



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2016 – 04:28 AM EDT

PDB ID : 4P3Q
Title : Room-temperature WT DHFR, time-averaged ensemble
Authors : Keedy, D.A.; van den Bedem, H.; Fraser, J.S.
Deposited on : 2014-03-10
Resolution : 1.35 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : **FAILED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

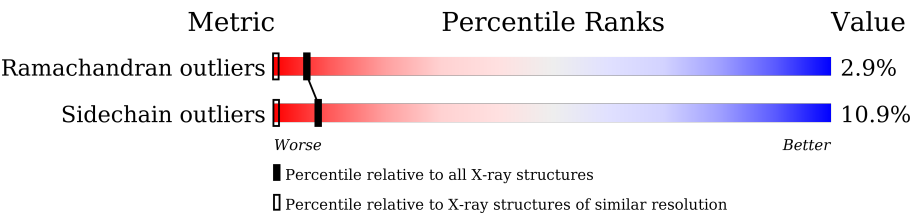
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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)) |
|-----------------------|-----------------------------|---|
| Ramachandran outliers | 100387 | 2280 (1.40-1.32) |
| Sidechain outliers | 100360 | 2279 (1.40-1.32) |














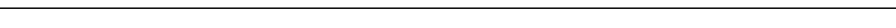











The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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.

Note EDS failed to run properly.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | 1-A | 159 | <div><div>87%</div><div>11%</div><div>.</div></div> |
| 1 | 10-A | 159 | <div><div>89%</div><div>8%</div><div>..</div></div> |
| 1 | 100-A | 159 | <div><div>87%</div><div>11%</div><div>.</div></div> |
| 1 | 101-A | 159 | <div><div>92%</div><div>6%</div><div>.</div></div> |
| 1 | 102-A | 159 | <div><div>90%</div><div>9%</div><div>..</div></div> |
| 1 | 103-A | 159 | <div><div>87%</div><div>10%</div><div>.</div></div> |
| 1 | 104-A | 159 | <div><div>89%</div><div>9%</div><div>.</div></div> |
| 1 | 105-A | 159 | <div><div>87%</div><div>9%</div><div>..</div></div> |
| 1 | 106-A | 159 | <div><div>82%</div><div>16%</div><div>.</div></div> |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 107-A | 159 |  83% 13% . |
| 1 | 108-A | 159 |  84% 14% .. |
| 1 | 109-A | 159 |  84% 14% .. |
| 1 | 11-A | 159 |  87% 9% .. |
| 1 | 110-A | 159 |  85% 12% . |
| 1 | 111-A | 159 |  85% 13% .. |
| 1 | 112-A | 159 |  85% 13% .. |
| 1 | 113-A | 159 |  81% 14% . . |
| 1 | 114-A | 159 |  82% 12% 5% . |
| 1 | 115-A | 159 |  80% 15% . . |
| 1 | 116-A | 159 |  83% 13% . . |
| 1 | 117-A | 159 |  83% 13% . . |
| 1 | 118-A | 159 |  84% 13% . . |
| 1 | 119-A | 159 |  87% 12% . |
| 1 | 12-A | 159 |  86% 11% . |
| 1 | 120-A | 159 |  91% 8% . |
| 1 | 121-A | 159 |  86% 13% . |
| 1 | 122-A | 159 |  86% 11% . |
| 1 | 123-A | 159 |  87% 11% . |
| 1 | 124-A | 159 |  87% 13% . |
| 1 | 125-A | 159 |  87% 12% . |
| 1 | 126-A | 159 |  90% 9% . |
| 1 | 127-A | 159 |  90% 9% . |
| 1 | 128-A | 159 |  88% 11% . |
| 1 | 129-A | 159 |  92% 7% . |














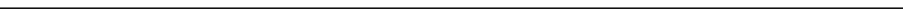











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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 13-A | 159 |  91% 8% . |
| 1 | 130-A | 159 |  92% 6% . |
| 1 | 131-A | 159 |  86% 13% . |
| 1 | 132-A | 159 |  89% 8% .. |
| 1 | 133-A | 159 |  90% 8% .. |
| 1 | 134-A | 159 |  89% 9% . |
| 1 | 135-A | 159 |  92% 7% .. |
| 1 | 136-A | 159 |  86% 11% .. |
| 1 | 137-A | 159 |  87% 8% .. |
| 1 | 138-A | 159 |  85% 11% .. |
| 1 | 139-A | 159 |  87% 11% .. |
| 1 | 14-A | 159 |  87% 11% .. |
| 1 | 140-A | 159 |  88% 9% .. |
| 1 | 141-A | 159 |  86% 11% .. |
| 1 | 142-A | 159 |  84% 13% .. |
| 1 | 143-A | 159 |  87% 9% .. |
| 1 | 144-A | 159 |  80% 15% . . |
| 1 | 145-A | 159 |  84% 13% .. |
| 1 | 146-A | 159 |  84% 13% .. |
| 1 | 147-A | 159 |  87% 11% .. |
| 1 | 148-A | 159 |  86% 11% .. |
| 1 | 149-A | 159 |  87% 11% . |
| 1 | 15-A | 159 |  87% 11% . |
| 1 | 150-A | 159 |  84% 14% . |
| 1 | 151-A | 159 |  85% 13% . |











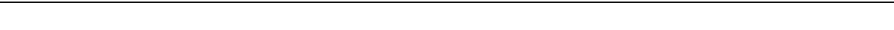

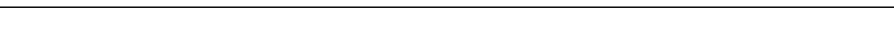
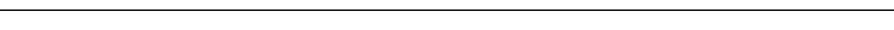











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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 152-A | 159 |  90% 9% . |
| 1 | 153-A | 159 |  87% 9% . . |
| 1 | 154-A | 159 |  88% 8% . |
| 1 | 155-A | 159 |  86% 11% . |
| 1 | 156-A | 159 |  81% 17% . |
| 1 | 157-A | 159 |  77% 20% . |
| 1 | 158-A | 159 |  86% 10% . . |
| 1 | 159-A | 159 |  84% 9% 6% . |
| 1 | 16-A | 159 |  86% 12% . . |
| 1 | 160-A | 159 |  86% 12% . . |
| 1 | 161-A | 159 |  86% 10% . . |
| 1 | 162-A | 159 |  86% 10% . . |
| 1 | 163-A | 159 |  86% 12% . |
| 1 | 164-A | 159 |  86% 9% . . |
| 1 | 165-A | 159 |  87% 11% . . |
| 1 | 166-A | 159 |  88% 10% . . |
| 1 | 167-A | 159 |  82% 13% . . |
| 1 | 17-A | 159 |  87% 11% . . |
| 1 | 18-A | 159 |  90% 9% . |
| 1 | 19-A | 159 |  89% 10% . . |
| 1 | 2-A | 159 |  89% 9% . |
| 1 | 20-A | 159 |  86% 13% . |
| 1 | 21-A | 159 |  88% 11% . |
| 1 | 22-A | 159 |  89% 9% . |
| 1 | 23-A | 159 |  88% 9% . |














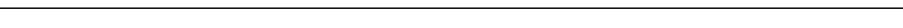











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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 24-A | 159 |  87% 11% . |
| 1 | 25-A | 159 |  84% 14% . |
| 1 | 26-A | 159 |  87% 12% .. |
| 1 | 27-A | 159 |  85% 13% . |
| 1 | 28-A | 159 |  84% 11% . . |
| 1 | 29-A | 159 |  81% 16% . . |
| 1 | 3-A | 159 |  88% 10% .. |
| 1 | 30-A | 159 |  81% 14% 5% |
| 1 | 31-A | 159 |  83% 11% 6% |
| 1 | 32-A | 159 |  79% 16% . . |
| 1 | 33-A | 159 |  83% 9% 6% . |
| 1 | 34-A | 159 |  79% 17% . |
| 1 | 35-A | 159 |  84% 12% . . |
| 1 | 36-A | 159 |  83% 13% . . |
| 1 | 37-A | 159 |  82% 15% . |
| 1 | 38-A | 159 |  82% 15% . |
| 1 | 39-A | 159 |  81% 16% . |
| 1 | 4-A | 159 |  84% 14% .. |
| 1 | 40-A | 159 |  84% 12% . . |
| 1 | 41-A | 159 |  84% 13% . . |
| 1 | 42-A | 159 |  86% 11% .. |
| 1 | 43-A | 159 |  87% 11% .. |
| 1 | 44-A | 159 |  87% 11% . |
| 1 | 45-A | 159 |  84% 13% . |
| 1 | 46-A | 159 |  86% 13% . |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | 47-A | 159 |  86% 11% .. |
| 1 | 48-A | 159 |  90% 7% .. |
| 1 | 49-A | 159 |  87% 10% .. |
| 1 | 5-A | 159 |  91% 6% .. |
| 1 | 50-A | 159 |  84% 12% .. |
| 1 | 51-A | 159 |  86% 11% .. |
| 1 | 52-A | 159 |  85% 12% .. |
| 1 | 53-A | 159 |  86% 9% .. |
| 1 | 54-A | 159 |  87% 12% . |
| 1 | 55-A | 159 |  87% 12% . |
| 1 | 56-A | 159 |  87% 9% . |
| 1 | 57-A | 159 |  87% 10% .. |
| 1 | 58-A | 159 |  89% 10% . |
| 1 | 59-A | 159 |  92% 6% . |
| 1 | 6-A | 159 |  84% 13% . |
| 1 | 60-A | 159 |  85% 12% . |
| 1 | 61-A | 159 |  86% 11% .. |
| 1 | 62-A | 159 |  85% 14% . |
| 1 | 63-A | 159 |  89% 11% |
| 1 | 64-A | 159 |  91% 8% . |
| 1 | 65-A | 159 |  87% 12% . |
| 1 | 66-A | 159 |  87% 9% .. |
| 1 | 67-A | 159 |  89% 8% . |
| 1 | 68-A | 159 |  89% 8% .. |
| 1 | 69-A | 159 |  87% 9% .. |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | 7-A | 159 |  82% 15% .. |
| 1 | 70-A | 159 |  87% 10% .. |
| 1 | 71-A | 159 |  87% 9% . |
| 1 | 72-A | 159 |  84% 13% .. |
| 1 | 73-A | 159 |  87% 9% .. |
| 1 | 74-A | 159 |  86% 11% .. |
| 1 | 75-A | 159 |  88% 10% . |
| 1 | 76-A | 159 |  85% 14% . |
| 1 | 77-A | 159 |  90% 9% . |
| 1 | 78-A | 159 |  84% 14% . |
| 1 | 79-A | 159 |  87% 10% .. |
| 1 | 8-A | 159 |  84% 12% .. |
| 1 | 80-A | 159 |  84% 12% .. |
| 1 | 81-A | 159 |  88% 8% .. |
| 1 | 82-A | 159 |  87% 10% .. |
| 1 | 83-A | 159 |  87% 11% .. |
| 1 | 84-A | 159 |  91% 8% . |
| 1 | 85-A | 159 |  86% 12% . |
| 1 | 86-A | 159 |  89% 9% .. |
| 1 | 87-A | 159 |  91% 6% . |
| 1 | 88-A | 159 |  87% 12% . |
| 1 | 89-A | 159 |  87% 11% . |
| 1 | 9-A | 159 |  87% 9% .. |
| 1 | 90-A | 159 |  87% 10% . |
| 1 | 91-A | 159 |  89% 9% . |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | 92-A | 159 |  88% 10% . |
| 1 | 93-A | 159 |  89% 9% . |
| 1 | 94-A | 159 |  84% 15% . |
| 1 | 95-A | 159 |  84% 14% .. |
| 1 | 96-A | 159 |  87% 10% . |
| 1 | 97-A | 159 |  86% 11% . |
| 1 | 98-A | 159 |  86% 13% . |
| 1 | 99-A | 159 |  86% 14% . |

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 451154 atoms, of which 211088 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 | 1223 | 217 | 239 | 7 | | | | |
| 1 | 2-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | | |
| 1 | 3-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | | |
| 1 | 4-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | | |
| 1 | 5-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | | |
| 1 | 6-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | | |
| 1 | 7-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | | |
| 1 | 8-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | | |
| 1 | 9-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | | |
| 1 | 10-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | | |
| 1 | 11-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | | |
| 1 | 12-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | | |
| 1 | 13-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | | |
| 1 | 14-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | | |
| 1 | 15-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | | |
| 1 | 16-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 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 | 1223 | 217 | 239 | 7 | | | |
| 1 | 18-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 19-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 20-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 21-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 22-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 23-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 24-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 25-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 26-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 27-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 28-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 29-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 30-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 31-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 32-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 33-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 34-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 35-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 36-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 37-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 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 | 1223 | 217 | 239 | 7 | | | |
| 1 | 39-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 40-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 41-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 42-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 43-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 44-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 45-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 46-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 47-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 48-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 49-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 50-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 51-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 52-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 53-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 54-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 55-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 56-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 57-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 58-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 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 | 1223 | 217 | 239 | 7 | | | |
| 1 | 60-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 61-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 62-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 63-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 64-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 65-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 66-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 67-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 68-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 69-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 70-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 71-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 72-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 73-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 74-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 75-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 76-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 77-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 78-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 79-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 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 | 1223 | 217 | 239 | 7 | | | |
| 1 | 81-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 82-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 83-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 84-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 85-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 86-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 87-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 88-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 89-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 90-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 91-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 92-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 93-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 94-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 95-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 96-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 97-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 98-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 99-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 100-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 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 | 1223 | 217 | 239 | 7 | | | |
| 1 | 102-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 103-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 104-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 105-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 106-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 107-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 108-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 109-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 110-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 111-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 112-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 113-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 114-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 115-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 116-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 117-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 118-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 119-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 120-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 121-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 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 | 1223 | 217 | 239 | 7 | | | |
| 1 | 123-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 124-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 125-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 126-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 127-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 128-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 129-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 130-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 131-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 132-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 133-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 134-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 135-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 136-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 137-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 138-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 139-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 140-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 141-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 142-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |

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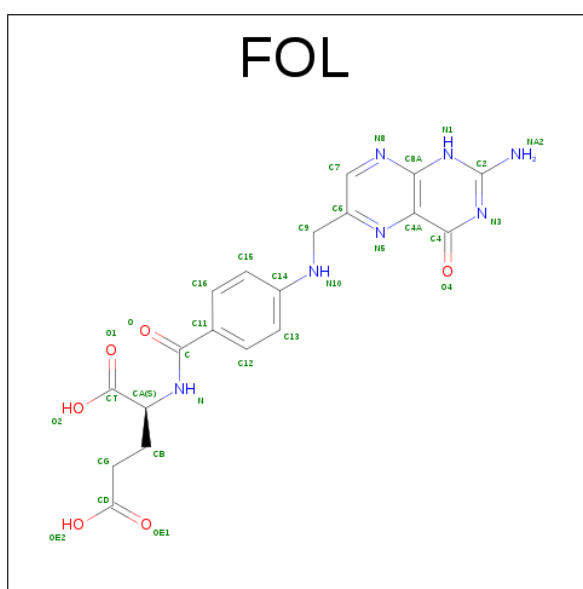
| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 1 | 143-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 144-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 145-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 146-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 147-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 148-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 149-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 150-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 151-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 152-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 153-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 154-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 155-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 156-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 157-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 158-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 159-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 160-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 161-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 162-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 163-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 1 | 164-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 165-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 166-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |
| 1 | 167-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1223 | 217 | 239 | 7 | | | |

- Molecule 2 is FOLIC ACID (three-letter code: FOL) (formula: C₁₉H₁₉N₇O₆).



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

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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 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 114-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 115-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 116-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 117-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 118-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 119-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 120-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 121-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 122-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 123-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 124-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 125-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 126-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 127-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 128-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 129-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 130-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 131-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 132-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 133-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 | 134-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 135-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 136-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 137-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 138-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 139-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 140-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 141-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 142-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 143-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 144-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 145-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 146-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 147-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 148-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 149-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 150-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 151-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 152-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 153-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 154-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 | 155-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 156-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 157-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 158-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 159-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 160-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 161-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 162-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 163-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 164-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 165-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 166-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 167-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3 | 122-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 110-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 37-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 80-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 94-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 167-A | 2 | Total 2 | Ca 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3 | 162-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 60-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 148-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 123-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 44-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 150-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 128-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 135-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 50-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 138-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 104-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 12-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 114-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 19-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 165-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 73-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 1-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 53-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 143-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 25-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 131-A | 2 | Total 2 | Ca 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3 | 32-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 93-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 77-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 161-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 58-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 130-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 57-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 29-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 101-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 3-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 11-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 84-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 98-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 144-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 127-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 154-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 108-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 16-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 65-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 117-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 41-A | 2 | Total 2 | Ca 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3 | 5-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 8-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 21-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 109-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 102-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 113-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 36-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 81-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 160-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 97-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 61-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 149-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 48-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 124-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 45-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 153-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 129-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 134-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 35-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 105-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 7-A | 2 | Total 2 | Ca 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3 | 15-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 88-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 18-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 72-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 159-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 52-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 140-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 26-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 120-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 118-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 89-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 31-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 82-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 92-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 76-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 46-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 137-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 56-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 106-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 10-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 85-A | 2 | Total 2 | Ca 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3 | 145-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 157-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 39-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 133-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 91-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 66-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 79-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 55-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 22-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 103-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 112-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 86-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 96-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 62-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 146-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 49-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 125-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 42-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 152-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 119-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 34-A | 2 | Total 2 | Ca 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3 | 14-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 63-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 68-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 71-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 158-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 141-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 27-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 163-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 121-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 111-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 30-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 83-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 95-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 2-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 9-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 75-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 47-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 151-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 136-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 51-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 139-A | 2 | Total 2 | Ca 2 | 0 | 0 |

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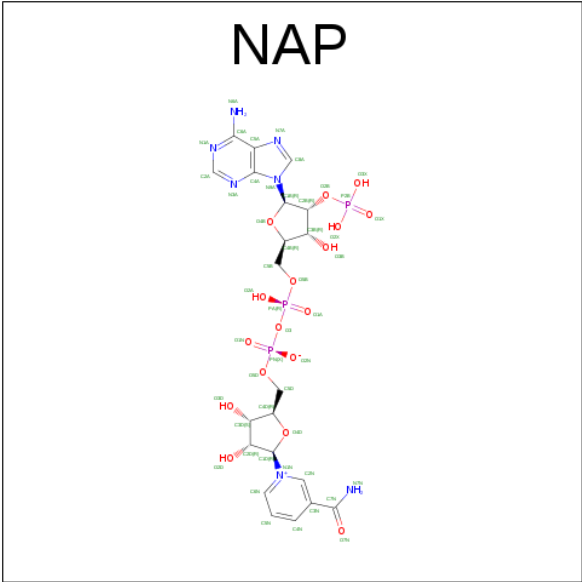
| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3 | 107-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 13-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 115-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 74-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 142-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 24-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 156-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 4-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 38-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 132-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 33-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 116-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 164-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 90-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 67-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 166-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 78-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 59-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 54-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 23-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 28-A | 2 | Total 2 | Ca 2 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 3 | 100-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 87-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 99-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 6-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 147-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 126-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 43-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 155-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 17-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 64-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 69-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 70-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 40-A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 3 | 20-A | 2 | Total 2 | Ca 2 | 0 | 0 |

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 4 | 1-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 2-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 3-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 4-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 5-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 6-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 7-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 8-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 9-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 10-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 11-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 12-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 13-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 14-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 4 | 15-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 16-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 17-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 18-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 19-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 20-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 21-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 22-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 23-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 24-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 25-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 26-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 27-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 28-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 29-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 30-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 31-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 32-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 33-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 34-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 35-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 4 | 36-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 37-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 38-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 39-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 40-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 41-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 42-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 43-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 44-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 45-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 46-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 47-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 48-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 49-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 50-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 51-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 52-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 53-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 54-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 55-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 56-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 4 | 57-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 58-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 59-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 60-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 61-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 62-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 63-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 64-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 65-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 66-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 67-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 68-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 69-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 70-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 71-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 72-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 73-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 74-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 75-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 76-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 77-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 4 | 78-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 79-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 80-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 81-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 82-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 83-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 84-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 85-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 86-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 87-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 88-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 89-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 90-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 91-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 92-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 93-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 94-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 95-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 96-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 97-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 98-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 4 | 99-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 100-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 101-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 102-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 103-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 104-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 105-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 106-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 107-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 108-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 109-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 110-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 111-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 112-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 113-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 114-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 115-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 116-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 117-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 118-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 119-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 4 | 120-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 121-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 122-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 123-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 124-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 125-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 126-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 127-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 128-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 129-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 130-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 131-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 132-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 133-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 134-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 135-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 136-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 137-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 138-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 139-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 140-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 4 | 141-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 142-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 143-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 144-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 145-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 146-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 147-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 148-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 149-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 150-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 151-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 152-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 153-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 154-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 155-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 156-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 157-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 158-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 159-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 160-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 161-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 4 | 162-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 163-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 164-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 165-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 166-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |
| 4 | 167-A | 1 | Total 72 | C 21 | H 24 | N 7 | O 17 | P 3 | 0 | 0 |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|---------|---------|
| 5 | 1-A | 83 | Total | O | 0 | 0 |
| | | | 83 | 83 | | |
| 5 | 2-A | 83 | Total | O | 0 | 0 |
| | | | 83 | 83 | | |
| 5 | 3-A | 79 | Total | O | 0 | 0 |
| | | | 79 | 79 | | |
| 5 | 4-A | 68 | Total | O | 0 | 0 |
| | | | 68 | 68 | | |
| 5 | 5-A | 75 | Total | O | 0 | 0 |
| | | | 75 | 75 | | |
| 5 | 6-A | 80 | Total | O | 0 | 0 |
| | | | 80 | 80 | | |
| 5 | 7-A | 99 | Total | O | 0 | 0 |
| | | | 99 | 99 | | |
| 5 | 8-A | 89 | Total | O | 0 | 0 |
| | | | 89 | 89 | | |
| 5 | 9-A | 79 | Total | O | 0 | 0 |
| | | | 79 | 79 | | |
| 5 | 10-A | 79 | Total | O | 0 | 0 |
| | | | 79 | 79 | | |
| 5 | 11-A | 82 | Total | O | 0 | 0 |
| | | | 82 | 82 | | |
| 5 | 12-A | 88 | Total | O | 0 | 0 |
| | | | 88 | 88 | | |
| 5 | 13-A | 89 | Total | O | 0 | 0 |
| | | | 89 | 89 | | |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 5 | 14-A | 96 | Total O 96 96 | 0 | 0 |
| 5 | 15-A | 96 | Total O 96 96 | 0 | 0 |
| 5 | 16-A | 94 | Total O 94 94 | 0 | 0 |
| 5 | 17-A | 84 | Total O 84 84 | 0 | 0 |
| 5 | 18-A | 89 | Total O 89 89 | 0 | 0 |
| 5 | 19-A | 80 | Total O 80 80 | 0 | 0 |
| 5 | 20-A | 73 | Total O 73 73 | 0 | 0 |
| 5 | 21-A | 92 | Total O 92 92 | 0 | 0 |
| 5 | 22-A | 91 | Total O 91 91 | 0 | 0 |
| 5 | 23-A | 94 | Total O 94 94 | 0 | 0 |
| 5 | 24-A | 95 | Total O 95 95 | 0 | 0 |
| 5 | 25-A | 76 | Total O 76 76 | 0 | 0 |
| 5 | 26-A | 83 | Total O 83 83 | 0 | 0 |
| 5 | 27-A | 81 | Total O 81 81 | 0 | 0 |
| 5 | 28-A | 81 | Total O 81 81 | 0 | 0 |
| 5 | 29-A | 83 | Total O 83 83 | 0 | 0 |
| 5 | 30-A | 84 | Total O 84 84 | 0 | 0 |
| 5 | 31-A | 86 | Total O 86 86 | 0 | 0 |
| 5 | 32-A | 85 | Total O 85 85 | 0 | 0 |
| 5 | 33-A | 86 | Total O 86 86 | 0 | 0 |
| 5 | 34-A | 93 | Total O 93 93 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5 | 35-A | 93 | Total 93 | O 93 | 0 | 0 |
| 5 | 36-A | 77 | Total 77 | O 77 | 0 | 0 |
| 5 | 37-A | 82 | Total 82 | O 82 | 0 | 0 |
| 5 | 38-A | 87 | Total 87 | O 87 | 0 | 0 |
| 5 | 39-A | 93 | Total 93 | O 93 | 0 | 0 |
| 5 | 40-A | 84 | Total 84 | O 84 | 0 | 0 |
| 5 | 41-A | 82 | Total 82 | O 82 | 0 | 0 |
| 5 | 42-A | 83 | Total 83 | O 83 | 0 | 0 |
| 5 | 43-A | 95 | Total 95 | O 95 | 0 | 0 |
| 5 | 44-A | 100 | Total 100 | O 100 | 0 | 0 |
| 5 | 45-A | 93 | Total 93 | O 93 | 0 | 0 |
| 5 | 46-A | 92 | Total 92 | O 92 | 0 | 0 |
| 5 | 47-A | 98 | Total 98 | O 98 | 0 | 0 |
| 5 | 48-A | 92 | Total 92 | O 92 | 0 | 0 |
| 5 | 49-A | 89 | Total 89 | O 89 | 0 | 0 |
| 5 | 50-A | 78 | Total 78 | O 78 | 0 | 0 |
| 5 | 51-A | 68 | Total 68 | O 68 | 0 | 0 |
| 5 | 52-A | 77 | Total 77 | O 77 | 0 | 0 |
| 5 | 53-A | 87 | Total 87 | O 87 | 0 | 0 |
| 5 | 54-A | 92 | Total 92 | O 92 | 0 | 0 |
| 5 | 55-A | 92 | Total 92 | O 92 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5 | 56-A | 82 | Total 82 | O 82 | 0 | 0 |
| 5 | 57-A | 86 | Total 86 | O 86 | 0 | 0 |
| 5 | 58-A | 89 | Total 89 | O 89 | 0 | 0 |
| 5 | 59-A | 96 | Total 96 | O 96 | 0 | 0 |
| 5 | 60-A | 96 | Total 96 | O 96 | 0 | 0 |
| 5 | 61-A | 98 | Total 98 | O 98 | 0 | 0 |
| 5 | 62-A | 100 | Total 100 | O 100 | 0 | 0 |
| 5 | 63-A | 97 | Total 97 | O 97 | 0 | 0 |
| 5 | 64-A | 87 | Total 87 | O 87 | 0 | 0 |
| 5 | 65-A | 83 | Total 83 | O 83 | 0 | 0 |
| 5 | 66-A | 77 | Total 77 | O 77 | 0 | 0 |
| 5 | 67-A | 78 | Total 78 | O 78 | 0 | 0 |
| 5 | 68-A | 79 | Total 79 | O 79 | 0 | 0 |
| 5 | 69-A | 79 | Total 79 | O 79 | 0 | 0 |
| 5 | 70-A | 85 | Total 85 | O 85 | 0 | 0 |
| 5 | 71-A | 91 | Total 91 | O 91 | 0 | 0 |
| 5 | 72-A | 101 | Total 101 | O 101 | 0 | 0 |
| 5 | 73-A | 94 | Total 94 | O 94 | 0 | 0 |
| 5 | 74-A | 85 | Total 85 | O 85 | 0 | 0 |
| 5 | 75-A | 92 | Total 92 | O 92 | 0 | 0 |
| 5 | 76-A | 82 | Total 82 | O 82 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5 | 77-A | 85 | Total 85 | O 85 | 0 | 0 |
| 5 | 78-A | 84 | Total 84 | O 84 | 0 | 0 |
| 5 | 79-A | 86 | Total 86 | O 86 | 0 | 0 |
| 5 | 80-A | 85 | Total 85 | O 85 | 0 | 0 |
| 5 | 81-A | 92 | Total 92 | O 92 | 0 | 0 |
| 5 | 82-A | 91 | Total 91 | O 91 | 0 | 0 |
| 5 | 83-A | 98 | Total 98 | O 98 | 0 | 0 |
| 5 | 84-A | 94 | Total 94 | O 94 | 0 | 0 |
| 5 | 85-A | 94 | Total 94 | O 94 | 0 | 0 |
| 5 | 86-A | 88 | Total 88 | O 88 | 0 | 0 |
| 5 | 87-A | 84 | Total 84 | O 84 | 0 | 0 |
| 5 | 88-A | 82 | Total 82 | O 82 | 0 | 0 |
| 5 | 89-A | 92 | Total 92 | O 92 | 0 | 0 |
| 5 | 90-A | 98 | Total 98 | O 98 | 0 | 0 |
| 5 | 91-A | 75 | Total 75 | O 75 | 0 | 0 |
| 5 | 92-A | 77 | Total 77 | O 77 | 0 | 0 |
| 5 | 93-A | 78 | Total 78 | O 78 | 0 | 0 |
| 5 | 94-A | 92 | Total 92 | O 92 | 0 | 0 |
| 5 | 95-A | 101 | Total 101 | O 101 | 0 | 0 |
| 5 | 96-A | 106 | Total 106 | O 106 | 0 | 0 |
| 5 | 97-A | 94 | Total 94 | O 94 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 5 | 98-A | 86 | Total 86 | O 86 | 0 | 0 |
| 5 | 99-A | 87 | Total 87 | O 87 | 0 | 0 |
| 5 | 100-A | 80 | Total 80 | O 80 | 0 | 0 |
| 5 | 101-A | 76 | Total 76 | O 76 | 0 | 0 |
| 5 | 102-A | 80 | Total 80 | O 80 | 0 | 0 |
| 5 | 103-A | 89 | Total 89 | O 89 | 0 | 0 |
| 5 | 104-A | 88 | Total 88 | O 88 | 0 | 0 |
| 5 | 105-A | 97 | Total 97 | O 97 | 0 | 0 |
| 5 | 106-A | 85 | Total 85 | O 85 | 0 | 0 |
| 5 | 107-A | 87 | Total 87 | O 87 | 0 | 0 |
| 5 | 108-A | 93 | Total 93 | O 93 | 0 | 0 |
| 5 | 109-A | 82 | Total 82 | O 82 | 0 | 0 |
| 5 | 110-A | 82 | Total 82 | O 82 | 0 | 0 |
| 5 | 111-A | 75 | Total 75 | O 75 | 0 | 0 |
| 5 | 112-A | 85 | Total 85 | O 85 | 0 | 0 |
| 5 | 113-A | 97 | Total 97 | O 97 | 0 | 0 |
| 5 | 114-A | 98 | Total 98 | O 98 | 0 | 0 |
| 5 | 115-A | 86 | Total 86 | O 86 | 0 | 0 |
| 5 | 116-A | 89 | Total 89 | O 89 | 0 | 0 |
| 5 | 117-A | 85 | Total 85 | O 85 | 0 | 0 |
| 5 | 118-A | 89 | Total 89 | O 89 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 5 | 119-A | 88 | Total | O | 0 | 0 |
| | | | 88 | 88 | | |
| 5 | 120-A | 95 | Total | O | 0 | 0 |
| | | | 95 | 95 | | |
| 5 | 121-A | 93 | Total | O | 0 | 0 |
| | | | 93 | 93 | | |
| 5 | 122-A | 90 | Total | O | 0 | 0 |
| | | | 90 | 90 | | |
| 5 | 123-A | 82 | Total | O | 0 | 0 |
| | | | 82 | 82 | | |
| 5 | 124-A | 81 | Total | O | 0 | 0 |
| | | | 81 | 81 | | |
| 5 | 125-A | 84 | Total | O | 0 | 0 |
| | | | 84 | 84 | | |
| 5 | 126-A | 101 | Total | O | 0 | 0 |
| | | | 101 | 101 | | |
| 5 | 127-A | 96 | Total | O | 0 | 0 |
| | | | 96 | 96 | | |
| 5 | 128-A | 90 | Total | O | 0 | 0 |
| | | | 90 | 90 | | |
| 5 | 129-A | 89 | Total | O | 0 | 0 |
| | | | 89 | 89 | | |
| 5 | 130-A | 81 | Total | O | 0 | 0 |
| | | | 81 | 81 | | |
| 5 | 131-A | 75 | Total | O | 0 | 0 |
| | | | 75 | 75 | | |
| 5 | 132-A | 87 | Total | O | 0 | 0 |
| | | | 87 | 87 | | |
| 5 | 133-A | 96 | Total | O | 0 | 0 |
| | | | 96 | 96 | | |
| 5 | 134-A | 89 | Total | O | 0 | 0 |
| | | | 89 | 89 | | |
| 5 | 135-A | 89 | Total | O | 0 | 0 |
| | | | 89 | 89 | | |
| 5 | 136-A | 87 | Total | O | 0 | 0 |
| | | | 87 | 87 | | |
| 5 | 137-A | 88 | Total | O | 0 | 0 |
| | | | 88 | 88 | | |
| 5 | 138-A | 88 | Total | O | 0 | 0 |
| | | | 88 | 88 | | |
| 5 | 139-A | 96 | Total | O | 0 | 0 |
| | | | 96 | 96 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5 | 140-A | 88 | Total 88 | O 88 | 0 | 0 |
| 5 | 141-A | 80 | Total 80 | O 80 | 0 | 0 |
| 5 | 142-A | 80 | Total 80 | O 80 | 0 | 0 |
| 5 | 143-A | 83 | Total 83 | O 83 | 0 | 0 |
| 5 | 144-A | 84 | Total 84 | O 84 | 0 | 0 |
| 5 | 145-A | 99 | Total 99 | O 99 | 0 | 0 |
| 5 | 146-A | 101 | Total 101 | O 101 | 0 | 0 |
| 5 | 147-A | 105 | Total 105 | O 105 | 0 | 0 |
| 5 | 148-A | 103 | Total 103 | O 103 | 0 | 0 |
| 5 | 149-A | 86 | Total 86 | O 86 | 0 | 0 |
| 5 | 150-A | 94 | Total 94 | O 94 | 0 | 0 |
| 5 | 151-A | 92 | Total 92 | O 92 | 0 | 0 |
| 5 | 152-A | 89 | Total 89 | O 89 | 0 | 0 |
| 5 | 153-A | 99 | Total 99 | O 99 | 0 | 0 |
| 5 | 154-A | 98 | Total 98 | O 98 | 0 | 0 |
| 5 | 155-A | 78 | Total 78 | O 78 | 0 | 0 |
| 5 | 156-A | 79 | Total 79 | O 79 | 0 | 0 |
| 5 | 157-A | 80 | Total 80 | O 80 | 0 | 0 |
| 5 | 158-A | 78 | Total 78 | O 78 | 0 | 0 |
| 5 | 159-A | 82 | Total 82 | O 82 | 0 | 0 |
| 5 | 160-A | 82 | Total 82 | O 82 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|---------|
| 5 | 161-A | 86 | Total 86 | O 86 | 0 | 0 |
| 5 | 162-A | 84 | Total 84 | O 84 | 0 | 0 |
| 5 | 163-A | 91 | Total 91 | O 91 | 0 | 0 |
| 5 | 164-A | 92 | Total 92 | O 92 | 0 | 0 |
| 5 | 165-A | 90 | Total 90 | O 90 | 0 | 0 |
| 5 | 166-A | 81 | Total 81 | O 81 | 0 | 0 |
| 5 | 167-A | 89 | Total 89 | O 89 | 0 | 0 |

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

Note EDS failed to run properly.

- Molecule 1: Dihydrofolate reductase

Chain 1-A:  87% 11% .




- Molecule 1: Dihydrofolate reductase

Chain 2-A:  89% 9% .




- Molecule 1: Dihydrofolate reductase

Chain 3-A:  88% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 4-A:  84% 14% ..




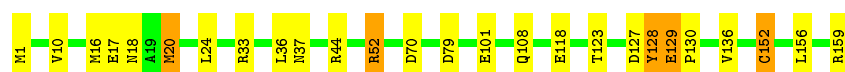
- Molecule 1: Dihydrofolate reductase

Chain 5-A:  91% 6% ..




- Molecule 1: Dihydrofolate reductase

Chain 6-A:  84% 13% .




- Molecule 1: Dihydrofolate reductase

Chain 7-A:  82% 15% . .




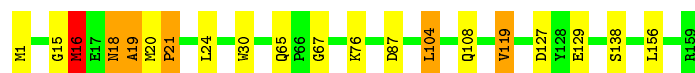
- Molecule 1: Dihydrofolate reductase

Chain 8-A:  84% 12% . .



- Molecule 1: Dihydrofolate reductase

Chain 9-A:  87% 9% . .



- Molecule 1: Dihydrofolate reductase

Chain 10-A:  89% 8% . .




- Molecule 1: Dihydrofolate reductase

Chain 11-A:  87% 9% . .



- Molecule 1: Dihydrofolate reductase

Chain 12-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 13-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 14-A: 87% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 15-A: 87% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 16-A: 86% 12% ..



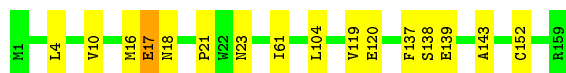
- Molecule 1: Dihydrofolate reductase

Chain 17-A: 87% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 18-A: 90% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 19-A: 89% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 20-A: 86% 13% .



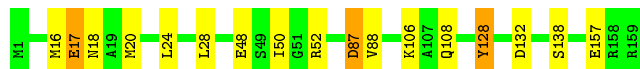
- Molecule 1: Dihydrofolate reductase

Chain 21-A:  88% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 22-A:  89% 9% .



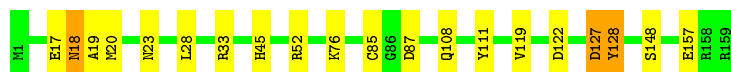
- Molecule 1: Dihydrofolate reductase

Chain 23-A:  88% 9% .



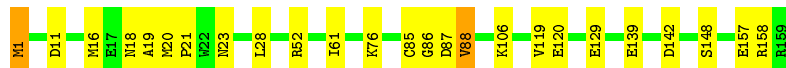
- Molecule 1: Dihydrofolate reductase

Chain 24-A:  87% 11% .




- Molecule 1: Dihydrofolate reductase

Chain 25-A:  84% 14% .




- Molecule 1: Dihydrofolate reductase

Chain 26-A:  87% 12% ..




- Molecule 1: Dihydrofolate reductase

Chain 27-A:  85% 13% .




- Molecule 1: Dihydrofolate reductase

Chain 28-A:  84% 11% . .




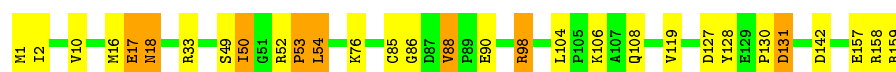
- Molecule 1: Dihydrofolate reductase

Chain 29-A:  81% 16% . .



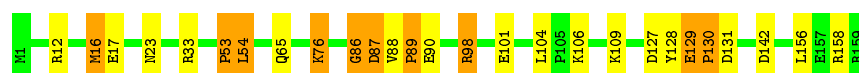
- Molecule 1: Dihydrofolate reductase

Chain 30-A:  81% 14% 5%




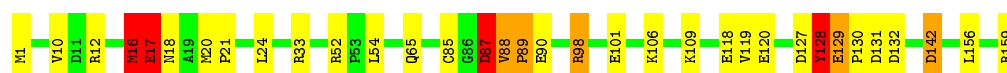
- Molecule 1: Dihydrofolate reductase

Chain 31-A:  83% 11% 6%



- Molecule 1: Dihydrofolate reductase

Chain 32-A:  79% 16% . .




- Molecule 1: Dihydrofolate reductase

Chain 33-A:  83% 9% 6% .




- Molecule 1: Dihydrofolate reductase

Chain 34-A:  79% 17% .



- Molecule 1: Dihydrofolate reductase

Chain 35-A:  84% 12% . .



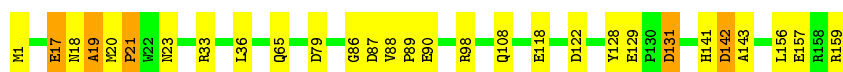
- Molecule 1: Dihydrofolate reductase

Chain 36-A: 83% 13% ..



- Molecule 1: Dihydrofolate reductase

Chain 37-A: 82% 15% .



- Molecule 1: Dihydrofolate reductase

Chain 38-A: 82% 15% .



- Molecule 1: Dihydrofolate reductase

Chain 39-A: 81% 16% .



- Molecule 1: Dihydrofolate reductase

Chain 40-A: 84% 12% ..



- Molecule 1: Dihydrofolate reductase

Chain 41-A: 84% 13% ..




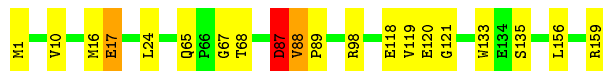
- Molecule 1: Dihydrofolate reductase

Chain 42-A: 86% 11% ..




- Molecule 1: Dihydrofolate reductase

Chain 43-A:  87% 11% ..




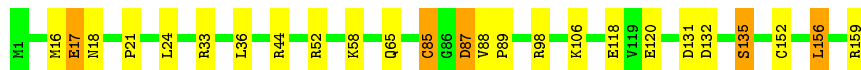
- Molecule 1: Dihydrofolate reductase

Chain 44-A:  87% 11% .




- Molecule 1: Dihydrofolate reductase

Chain 45-A:  84% 13% .




- Molecule 1: Dihydrofolate reductase

Chain 46-A:  86% 13% .



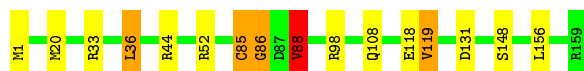
- Molecule 1: Dihydrofolate reductase

Chain 47-A:  86% 11% ..




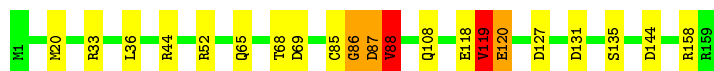
- Molecule 1: Dihydrofolate reductase

Chain 48-A:  90% 7% ..




- Molecule 1: Dihydrofolate reductase

Chain 49-A:  87% 10% ..




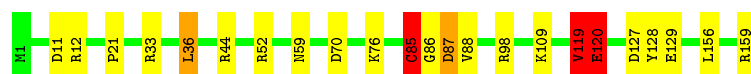
- Molecule 1: Dihydrofolate reductase

Chain 50-A:  84% 12% ..




- Molecule 1: Dihydrofolate reductase

Chain 51-A:  86% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 52-A:  85% 12% ..



- Molecule 1: Dihydrofolate reductase

Chain 53-A:  86% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 54-A:  87% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 55-A:  87% 12% .



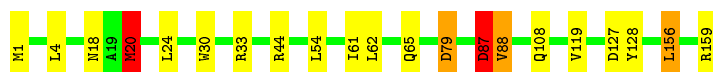
- Molecule 1: Dihydrofolate reductase

Chain 56-A:  87% 9% .



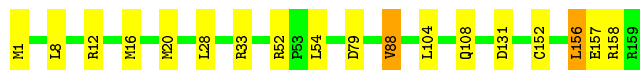
- Molecule 1: Dihydrofolate reductase

Chain 57-A:  87% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 58-A: 89% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 59-A: 92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 60-A: 85% 12% .



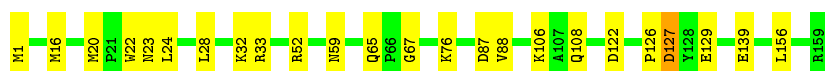
- Molecule 1: Dihydrofolate reductase

Chain 61-A: 86% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 62-A: 85% 14% .



- Molecule 1: Dihydrofolate reductase

Chain 63-A: 89% 11%



- Molecule 1: Dihydrofolate reductase

Chain 64-A: 91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 65-A:  87% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 66-A:  87% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 67-A:  89% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 68-A:  89% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 69-A:  87% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 70-A:  87% 10% ..




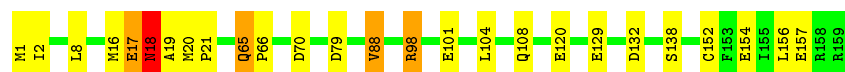
- Molecule 1: Dihydrofolate reductase

Chain 71-A:  87% 9% .




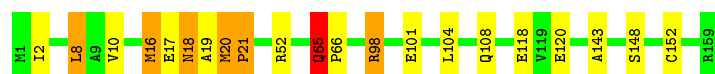
- Molecule 1: Dihydrofolate reductase

Chain 72-A:  84% 13% . .




- Molecule 1: Dihydrofolate reductase

Chain 73-A:  87% 9% . .



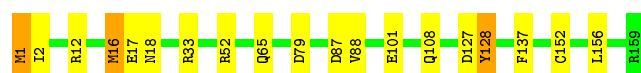
- Molecule 1: Dihydrofolate reductase

Chain 74-A:  86% 11% . .




- Molecule 1: Dihydrofolate reductase

Chain 75-A:  88% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 76-A:  85% 14% .




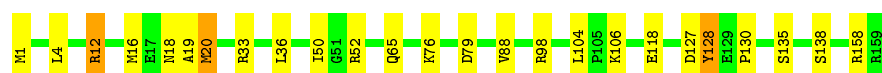
- Molecule 1: Dihydrofolate reductase

Chain 77-A:  90% 9% .




- Molecule 1: Dihydrofolate reductase

Chain 78-A:  84% 14% .



- Molecule 1: Dihydrofolate reductase

Chain 79-A:  87% 10% . .



- Molecule 1: Dihydrofolate reductase

Chain 80-A: 84% 12% ..



- Molecule 1: Dihydrofolate reductase

Chain 81-A: 88% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 82-A: 87% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 83-A: 87% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 84-A: 91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 85-A: 86% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 86-A: 89% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 87-A:  91% 6%



- Molecule 1: Dihydrofolate reductase

Chain 88-A:  87% 12%



- Molecule 1: Dihydrofolate reductase

Chain 89-A:  87% 11%



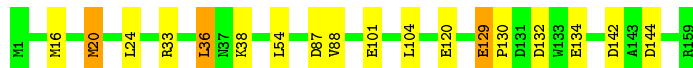
- Molecule 1: Dihydrofolate reductase

Chain 90-A:  87% 10%



- Molecule 1: Dihydrofolate reductase

Chain 91-A:  89% 9%



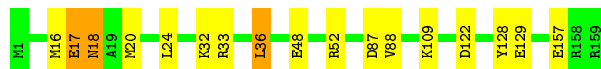
- Molecule 1: Dihydrofolate reductase

Chain 92-A:  88% 10%




- Molecule 1: Dihydrofolate reductase

Chain 93-A:  89% 9%



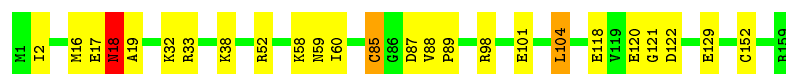
- Molecule 1: Dihydrofolate reductase

Chain 94-A:  84% 15% .



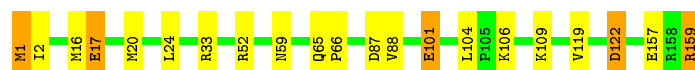
- Molecule 1: Dihydrofolate reductase

Chain 95-A:  84% 14% ..




- Molecule 1: Dihydrofolate reductase

Chain 96-A:  87% 10% .




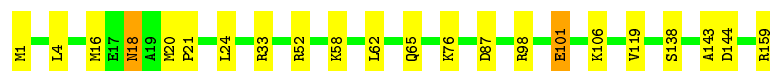
- Molecule 1: Dihydrofolate reductase

Chain 97-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 98-A:  86% 13% .



- Molecule 1: Dihydrofolate reductase

Chain 99-A:  86% 14% .



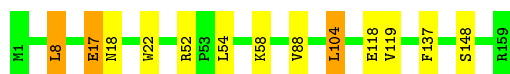
- Molecule 1: Dihydrofolate reductase

Chain 100-A:  87% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 101-A:  92% 6% .



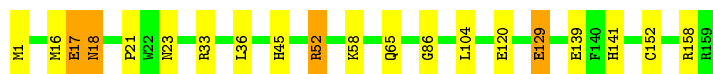
- Molecule 1: Dihydrofolate reductase

Chain 102-A: 90% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 103-A: 87% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 104-A: 89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 105-A: 87% 9% ..



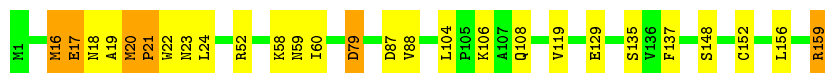
- Molecule 1: Dihydrofolate reductase

Chain 106-A: 82% 16% .



- Molecule 1: Dihydrofolate reductase

Chain 107-A: 83% 13% .




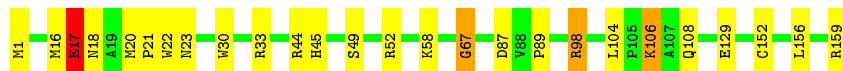
- Molecule 1: Dihydrofolate reductase

Chain 108-A: 84% 14% ..



- Molecule 1: Dihydrofolate reductase

Chain 109-A:  84% 14% ..



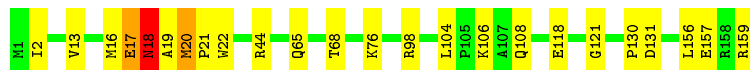
- Molecule 1: Dihydrofolate reductase

Chain 110-A:  85% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 111-A:  85% 13% ..




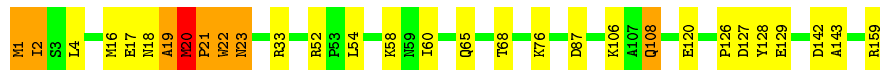
- Molecule 1: Dihydrofolate reductase

Chain 112-A:  85% 13% ..




- Molecule 1: Dihydrofolate reductase

Chain 113-A:  81% 14% . .




- Molecule 1: Dihydrofolate reductase

Chain 114-A:  82% 12% 5% .




- Molecule 1: Dihydrofolate reductase

Chain 115-A:  80% 15% . .




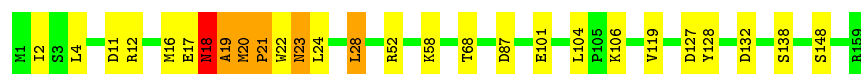
- Molecule 1: Dihydrofolate reductase

Chain 116-A:  83% 13% ..



- Molecule 1: Dihydrofolate reductase

Chain 117-A:  83% 13% ..



- Molecule 1: Dihydrofolate reductase

Chain 118-A:  84% 13% ..



- Molecule 1: Dihydrofolate reductase

Chain 119-A:  87% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 120-A:  91% 8% .




- Molecule 1: Dihydrofolate reductase

Chain 121-A:  86% 13% .



- Molecule 1: Dihydrofolate reductase

Chain 122-A:  86% 11% .



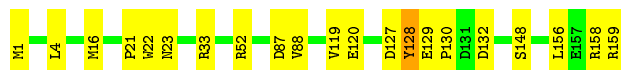
- Molecule 1: Dihydrofolate reductase

Chain 123-A:  87% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 124-A: 87% 13%



- Molecule 1: Dihydrofolate reductase

Chain 125-A: 87% 12%



- Molecule 1: Dihydrofolate reductase

Chain 126-A: 90% 9%



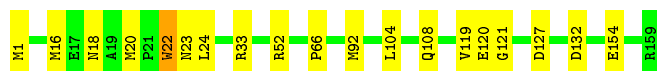
- Molecule 1: Dihydrofolate reductase

Chain 127-A: 90% 9%



- Molecule 1: Dihydrofolate reductase

Chain 128-A: 88% 11%



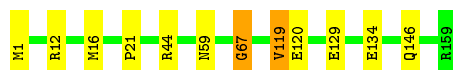
- Molecule 1: Dihydrofolate reductase

Chain 129-A: 92% 7%



- Molecule 1: Dihydrofolate reductase

Chain 130-A: 92% 6%



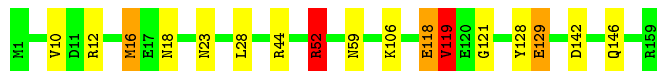
- Molecule 1: Dihydrofolate reductase

Chain 131-A:  86% 13% .



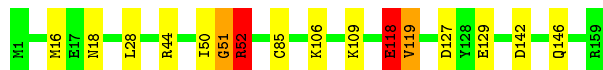
- Molecule 1: Dihydrofolate reductase

Chain 132-A:  89% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 133-A:  90% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 134-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 135-A:  92% 7% ..



- Molecule 1: Dihydrofolate reductase

Chain 136-A:  86% 11% ..




- Molecule 1: Dihydrofolate reductase

Chain 137-A:  87% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 138-A:  85% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 139-A:  87% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 140-A:  88% 9% ..




- Molecule 1: Dihydrofolate reductase

Chain 141-A:  86% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 142-A:  84% 13% ..




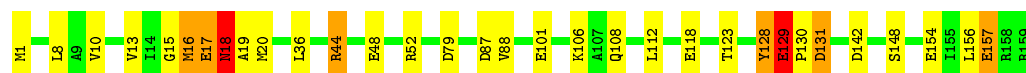
- Molecule 1: Dihydrofolate reductase

Chain 143-A:  87% 9% ..




- Molecule 1: Dihydrofolate reductase

Chain 144-A:  80% 15% ..



- Molecule 1: Dihydrofolate reductase

Chain 145-A:  84% 13% ..



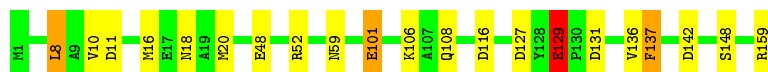
- Molecule 1: Dihydrofolate reductase

Chain 146-A: 84% 13% ..



- Molecule 1: Dihydrofolate reductase

Chain 147-A: 87% 11% ..



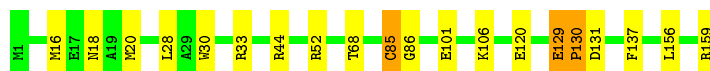
- Molecule 1: Dihydrofolate reductase

Chain 148-A: 86% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 149-A: 87% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 150-A: 84% 14% .



- Molecule 1: Dihydrofolate reductase

Chain 151-A: 85% 13% .



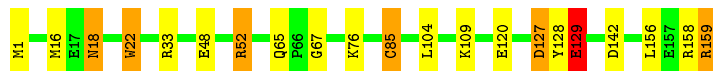
- Molecule 1: Dihydrofolate reductase

Chain 152-A: 90% 9% .



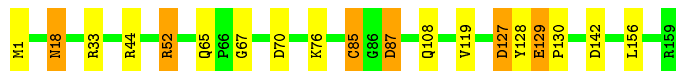
- Molecule 1: Dihydrofolate reductase

Chain 153-A:  87% 9% . .



- Molecule 1: Dihydrofolate reductase

Chain 154-A:  88% 8% .




- Molecule 1: Dihydrofolate reductase

Chain 155-A:  86% 11% .




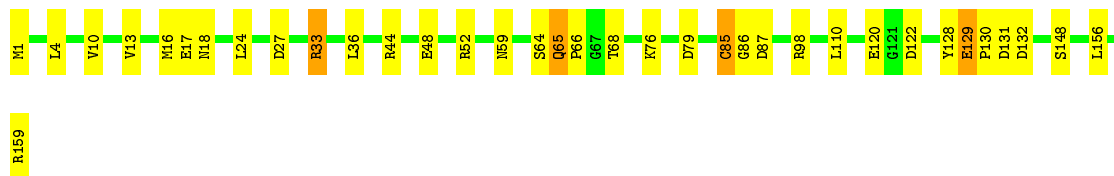
- Molecule 1: Dihydrofolate reductase

Chain 156-A:  81% 17% .




- Molecule 1: Dihydrofolate reductase

Chain 157-A:  77% 20% .




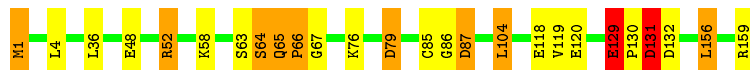
- Molecule 1: Dihydrofolate reductase

Chain 158-A:  86% 10% . .

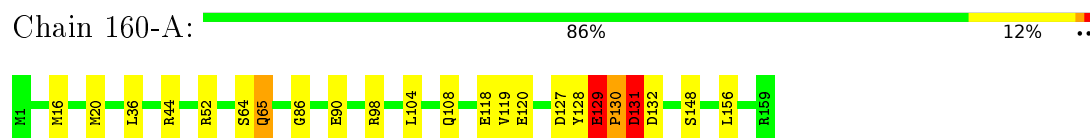


- Molecule 1: Dihydrofolate reductase

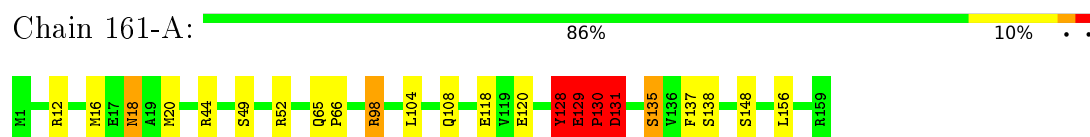
Chain 159-A:  84% 9% 6% .



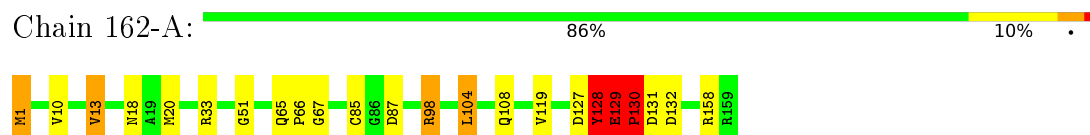
- Molecule 1: Dihydrofolate reductase



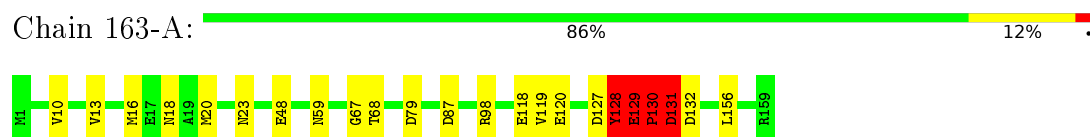
- Molecule 1: Dihydrofolate reductase



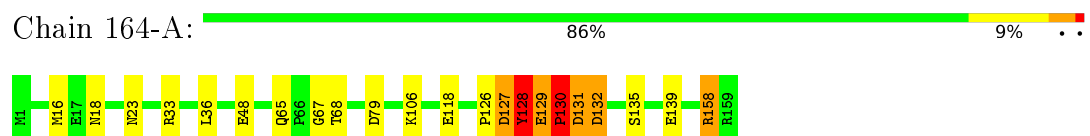
- Molecule 1: Dihydrofolate reductase



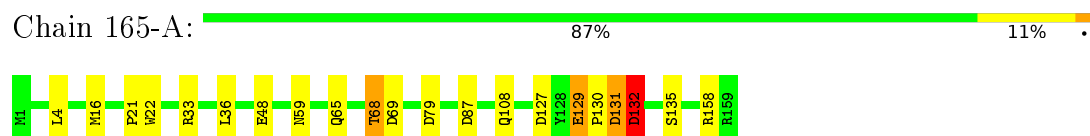
- Molecule 1: Dihydrofolate reductase



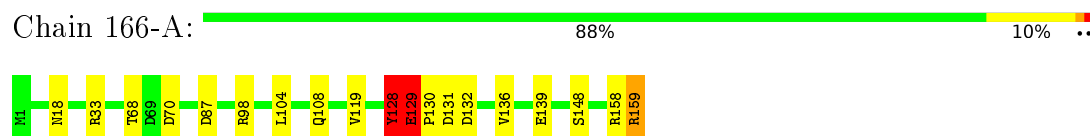
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



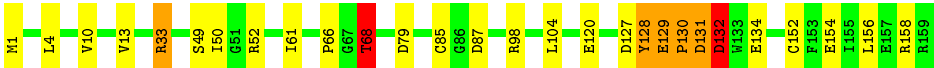
- Molecule 1: Dihydrofolate reductase

Chain 167-A:

82%

13%

..



4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 34.32Å 45.51Å 98.91Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 41.34 – 1.35 | Depositor |
| % Data completeness (in resolution range) | 91.6 (41.34-1.35) | Depositor |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.50 (at 1.35Å) | Xtriage |
| Refinement program | PHENIX (phenix.ensemble_refinement: 1.8.4_1496) | Depositor |
| R, R_{free} | 0.118 , 0.153 | Depositor |
| Wilson B-factor (Å ²) | 11.3 | Xtriage |
| Anisotropy | 0.174 | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 451154 | wwPDB-VP |
| Average B, all atoms (Å ²) | 9.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.87% 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, CA, NAP

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 | 0.70 | 0/1302 | 0.91 | 3/1770 (0.2%) |
| 1 | 2-A | 0.71 | 0/1302 | 0.91 | 2/1770 (0.1%) |
| 1 | 3-A | 0.70 | 0/1302 | 1.01 | 4/1770 (0.2%) |
| 1 | 4-A | 0.76 | 2/1302 (0.2%) | 0.97 | 5/1770 (0.3%) |
| 1 | 5-A | 0.73 | 0/1302 | 1.03 | 3/1770 (0.2%) |
| 1 | 6-A | 0.91 | 4/1302 (0.3%) | 1.03 | 6/1770 (0.3%) |
| 1 | 7-A | 0.94 | 6/1302 (0.5%) | 1.09 | 8/1770 (0.5%) |
| 1 | 8-A | 0.86 | 5/1302 (0.4%) | 1.14 | 11/1770 (0.6%) |
| 1 | 9-A | 0.82 | 0/1302 | 1.00 | 6/1770 (0.3%) |
| 1 | 10-A | 0.66 | 0/1302 | 0.87 | 2/1770 (0.1%) |
| 1 | 11-A | 0.73 | 1/1302 (0.1%) | 0.94 | 4/1770 (0.2%) |
| 1 | 12-A | 0.73 | 1/1302 (0.1%) | 0.98 | 3/1770 (0.2%) |
| 1 | 13-A | 0.67 | 1/1302 (0.1%) | 0.91 | 2/1770 (0.1%) |
| 1 | 14-A | 0.78 | 1/1302 (0.1%) | 0.92 | 2/1770 (0.1%) |
| 1 | 15-A | 0.76 | 0/1302 | 0.94 | 1/1770 (0.1%) |
| 1 | 16-A | 0.72 | 0/1302 | 0.99 | 5/1770 (0.3%) |
| 1 | 17-A | 0.75 | 3/1302 (0.2%) | 0.94 | 2/1770 (0.1%) |
| 1 | 18-A | 0.74 | 1/1302 (0.1%) | 0.91 | 1/1770 (0.1%) |
| 1 | 19-A | 0.73 | 2/1302 (0.2%) | 0.90 | 1/1770 (0.1%) |
| 1 | 20-A | 0.76 | 2/1302 (0.2%) | 0.93 | 7/1770 (0.4%) |
| 1 | 21-A | 0.76 | 2/1302 (0.2%) | 0.97 | 5/1770 (0.3%) |
| 1 | 22-A | 0.71 | 0/1302 | 0.99 | 4/1770 (0.2%) |
| 1 | 23-A | 0.75 | 0/1302 | 0.95 | 4/1770 (0.2%) |
| 1 | 24-A | 0.71 | 0/1302 | 0.95 | 3/1770 (0.2%) |
| 1 | 25-A | 0.72 | 0/1302 | 0.93 | 2/1770 (0.1%) |
| 1 | 26-A | 0.78 | 0/1302 | 0.95 | 4/1770 (0.2%) |
| 1 | 27-A | 0.78 | 0/1302 | 0.98 | 5/1770 (0.3%) |
| 1 | 28-A | 0.80 | 1/1302 (0.1%) | 1.04 | 5/1770 (0.3%) |
| 1 | 29-A | 0.86 | 4/1302 (0.3%) | 1.01 | 4/1770 (0.2%) |
| 1 | 30-A | 0.85 | 1/1302 (0.1%) | 1.18 | 8/1770 (0.5%) |
| 1 | 31-A | 0.91 | 3/1302 (0.2%) | 1.17 | 9/1770 (0.5%) |
| 1 | 32-A | 0.99 | 4/1302 (0.3%) | 1.15 | 13/1770 (0.7%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 33-A | 0.91 | 2/1302 (0.2%) | 1.15 | 10/1770 (0.6%) |
| 1 | 34-A | 0.95 | 5/1302 (0.4%) | 1.09 | 10/1770 (0.6%) |
| 1 | 35-A | 0.88 | 3/1302 (0.2%) | 1.08 | 7/1770 (0.4%) |
| 1 | 36-A | 0.86 | 3/1302 (0.2%) | 1.08 | 8/1770 (0.5%) |
| 1 | 37-A | 0.82 | 2/1302 (0.2%) | 1.06 | 6/1770 (0.3%) |
| 1 | 38-A | 0.81 | 1/1302 (0.1%) | 1.02 | 9/1770 (0.5%) |
| 1 | 39-A | 0.79 | 3/1302 (0.2%) | 1.09 | 10/1770 (0.6%) |
| 1 | 40-A | 0.81 | 1/1302 (0.1%) | 1.07 | 10/1770 (0.6%) |
| 1 | 41-A | 0.71 | 0/1302 | 1.09 | 7/1770 (0.4%) |
| 1 | 42-A | 0.73 | 0/1302 | 1.04 | 10/1770 (0.6%) |
| 1 | 43-A | 0.74 | 1/1302 (0.1%) | 1.03 | 8/1770 (0.5%) |
| 1 | 44-A | 0.74 | 1/1302 (0.1%) | 0.94 | 3/1770 (0.2%) |
| 1 | 45-A | 0.71 | 1/1302 (0.1%) | 0.94 | 4/1770 (0.2%) |
| 1 | 46-A | 0.76 | 2/1302 (0.2%) | 1.00 | 4/1770 (0.2%) |
| 1 | 47-A | 0.76 | 1/1302 (0.1%) | 1.03 | 7/1770 (0.4%) |
| 1 | 48-A | 0.71 | 0/1302 | 0.96 | 4/1770 (0.2%) |
| 1 | 49-A | 0.77 | 3/1302 (0.2%) | 0.96 | 6/1770 (0.3%) |
| 1 | 50-A | 0.76 | 1/1302 (0.1%) | 1.06 | 5/1770 (0.3%) |
| 1 | 51-A | 0.79 | 3/1302 (0.2%) | 1.01 | 4/1770 (0.2%) |
| 1 | 52-A | 0.79 | 3/1302 (0.2%) | 1.10 | 8/1770 (0.5%) |
| 1 | 53-A | 0.74 | 1/1302 (0.1%) | 1.04 | 8/1770 (0.5%) |
| 1 | 54-A | 0.71 | 1/1302 (0.1%) | 0.92 | 2/1770 (0.1%) |
| 1 | 55-A | 0.74 | 1/1302 (0.1%) | 0.96 | 3/1770 (0.2%) |
| 1 | 56-A | 0.90 | 5/1302 (0.4%) | 1.09 | 7/1770 (0.4%) |
| 1 | 57-A | 0.80 | 2/1302 (0.2%) | 1.11 | 12/1770 (0.7%) |
| 1 | 58-A | 0.93 | 1/1302 (0.1%) | 1.09 | 10/1770 (0.6%) |
| 1 | 59-A | 0.86 | 2/1302 (0.2%) | 0.99 | 5/1770 (0.3%) |
| 1 | 60-A | 0.73 | 1/1302 (0.1%) | 0.94 | 6/1770 (0.3%) |
| 1 | 61-A | 0.70 | 1/1302 (0.1%) | 0.94 | 5/1770 (0.3%) |
| 1 | 62-A | 0.71 | 0/1302 | 0.93 | 3/1770 (0.2%) |
| 1 | 63-A | 0.73 | 0/1302 | 1.00 | 4/1770 (0.2%) |
| 1 | 64-A | 0.67 | 0/1302 | 0.88 | 1/1770 (0.1%) |
| 1 | 65-A | 0.68 | 0/1302 | 1.05 | 10/1770 (0.6%) |
| 1 | 66-A | 0.74 | 1/1302 (0.1%) | 1.01 | 6/1770 (0.3%) |
| 1 | 67-A | 0.78 | 1/1302 (0.1%) | 0.95 | 3/1770 (0.2%) |
| 1 | 68-A | 0.77 | 1/1302 (0.1%) | 1.10 | 12/1770 (0.7%) |
| 1 | 69-A | 0.81 | 1/1302 (0.1%) | 1.04 | 10/1770 (0.6%) |
| 1 | 70-A | 1.04 | 4/1302 (0.3%) | 1.00 | 5/1770 (0.3%) |
| 1 | 71-A | 0.95 | 4/1302 (0.3%) | 1.01 | 7/1770 (0.4%) |
| 1 | 72-A | 0.74 | 1/1302 (0.1%) | 1.00 | 4/1770 (0.2%) |
| 1 | 73-A | 0.73 | 2/1302 (0.2%) | 0.98 | 7/1770 (0.4%) |
| 1 | 74-A | 0.79 | 2/1302 (0.2%) | 1.00 | 5/1770 (0.3%) |
| 1 | 75-A | 0.79 | 3/1302 (0.2%) | 0.96 | 3/1770 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 76-A | 0.73 | 0/1302 | 0.96 | 5/1770 (0.3%) |
| 1 | 77-A | 0.72 | 0/1302 | 0.88 | 4/1770 (0.2%) |
| 1 | 78-A | 0.72 | 1/1302 (0.1%) | 0.97 | 4/1770 (0.2%) |
| 1 | 79-A | 0.72 | 0/1302 | 1.05 | 9/1770 (0.5%) |
| 1 | 80-A | 0.79 | 3/1302 (0.2%) | 1.05 | 7/1770 (0.4%) |
| 1 | 81-A | 0.86 | 4/1302 (0.3%) | 1.09 | 9/1770 (0.5%) |
| 1 | 82-A | 0.84 | 3/1302 (0.2%) | 1.07 | 6/1770 (0.3%) |
| 1 | 83-A | 0.91 | 4/1302 (0.3%) | 1.10 | 10/1770 (0.6%) |
| 1 | 84-A | 0.83 | 1/1302 (0.1%) | 1.09 | 6/1770 (0.3%) |
| 1 | 85-A | 0.71 | 1/1302 (0.1%) | 0.96 | 5/1770 (0.3%) |
| 1 | 86-A | 0.78 | 1/1302 (0.1%) | 1.00 | 3/1770 (0.2%) |
| 1 | 87-A | 0.74 | 1/1302 (0.1%) | 0.95 | 5/1770 (0.3%) |
| 1 | 88-A | 0.74 | 2/1302 (0.2%) | 0.98 | 3/1770 (0.2%) |
| 1 | 89-A | 0.74 | 2/1302 (0.2%) | 0.97 | 3/1770 (0.2%) |
| 1 | 90-A | 0.71 | 1/1302 (0.1%) | 0.99 | 4/1770 (0.2%) |
| 1 | 91-A | 0.76 | 0/1302 | 1.04 | 4/1770 (0.2%) |
| 1 | 92-A | 0.77 | 2/1302 (0.2%) | 1.03 | 4/1770 (0.2%) |
| 1 | 93-A | 0.74 | 0/1302 | 1.00 | 4/1770 (0.2%) |
| 1 | 94-A | 0.73 | 2/1302 (0.2%) | 0.94 | 3/1770 (0.2%) |
| 1 | 95-A | 0.84 | 6/1302 (0.5%) | 0.95 | 2/1770 (0.1%) |
| 1 | 96-A | 0.76 | 1/1302 (0.1%) | 0.99 | 4/1770 (0.2%) |
| 1 | 97-A | 0.72 | 2/1302 (0.2%) | 0.98 | 6/1770 (0.3%) |
| 1 | 98-A | 0.71 | 1/1302 (0.1%) | 1.00 | 7/1770 (0.4%) |
| 1 | 99-A | 0.69 | 2/1302 (0.2%) | 0.99 | 8/1770 (0.5%) |
| 1 | 100-A | 0.66 | 0/1302 | 0.95 | 5/1770 (0.3%) |
| 1 | 101-A | 0.76 | 1/1302 (0.1%) | 0.90 | 3/1770 (0.2%) |
| 1 | 102-A | 0.73 | 1/1302 (0.1%) | 0.90 | 2/1770 (0.1%) |
| 1 | 103-A | 0.71 | 0/1302 | 0.96 | 5/1770 (0.3%) |
| 1 | 104-A | 0.83 | 4/1302 (0.3%) | 1.05 | 4/1770 (0.2%) |
| 1 | 105-A | 0.88 | 4/1302 (0.3%) | 1.04 | 5/1770 (0.3%) |
| 1 | 106-A | 0.85 | 3/1302 (0.2%) | 1.10 | 7/1770 (0.4%) |
| 1 | 107-A | 0.86 | 2/1302 (0.2%) | 1.07 | 7/1770 (0.4%) |
| 1 | 108-A | 1.05 | 1/1302 (0.1%) | 1.14 | 4/1770 (0.2%) |
| 1 | 109-A | 0.84 | 3/1302 (0.2%) | 1.21 | 12/1770 (0.7%) |
| 1 | 110-A | 0.77 | 2/1302 (0.2%) | 1.11 | 4/1770 (0.2%) |
| 1 | 111-A | 0.74 | 1/1302 (0.1%) | 1.12 | 7/1770 (0.4%) |
| 1 | 112-A | 0.78 | 0/1302 | 1.02 | 4/1770 (0.2%) |
| 1 | 113-A | 0.80 | 2/1302 (0.2%) | 1.08 | 6/1770 (0.3%) |
| 1 | 114-A | 0.78 | 1/1302 (0.1%) | 1.08 | 10/1770 (0.6%) |
| 1 | 115-A | 0.81 | 3/1302 (0.2%) | 1.08 | 11/1770 (0.6%) |
| 1 | 116-A | 0.87 | 5/1302 (0.4%) | 1.02 | 5/1770 (0.3%) |
| 1 | 117-A | 0.82 | 2/1302 (0.2%) | 1.05 | 8/1770 (0.5%) |
| 1 | 118-A | 0.80 | 2/1302 (0.2%) | 0.98 | 3/1770 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|----------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 119-A | 0.74 | 0/1302 | 0.90 | 3/1770 (0.2%) |
| 1 | 120-A | 0.74 | 1/1302 (0.1%) | 0.99 | 7/1770 (0.4%) |
| 1 | 121-A | 0.79 | 1/1302 (0.1%) | 1.01 | 5/1770 (0.3%) |
| 1 | 122-A | 0.76 | 2/1302 (0.2%) | 1.04 | 6/1770 (0.3%) |
| 1 | 123-A | 0.72 | 0/1302 | 0.93 | 2/1770 (0.1%) |
| 1 | 124-A | 0.71 | 0/1302 | 0.93 | 0/1770 |
| 1 | 125-A | 0.74 | 1/1302 (0.1%) | 0.93 | 2/1770 (0.1%) |
| 1 | 126-A | 0.67 | 0/1302 | 0.91 | 4/1770 (0.2%) |
| 1 | 127-A | 0.71 | 2/1302 (0.2%) | 0.97 | 4/1770 (0.2%) |
| 1 | 128-A | 0.74 | 1/1302 (0.1%) | 0.89 | 1/1770 (0.1%) |
| 1 | 129-A | 0.78 | 2/1302 (0.2%) | 0.87 | 3/1770 (0.2%) |
| 1 | 130-A | 0.68 | 0/1302 | 0.96 | 5/1770 (0.3%) |
| 1 | 131-A | 0.85 | 2/1302 (0.2%) | 1.09 | 9/1770 (0.5%) |
| 1 | 132-A | 0.77 | 2/1302 (0.2%) | 1.02 | 7/1770 (0.4%) |
| 1 | 133-A | 0.85 | 3/1302 (0.2%) | 1.02 | 3/1770 (0.2%) |
| 1 | 134-A | 0.84 | 2/1302 (0.2%) | 1.01 | 3/1770 (0.2%) |
| 1 | 135-A | 0.71 | 0/1302 | 0.91 | 3/1770 (0.2%) |
| 1 | 136-A | 0.71 | 1/1302 (0.1%) | 0.99 | 7/1770 (0.4%) |
| 1 | 137-A | 0.71 | 1/1302 (0.1%) | 0.99 | 7/1770 (0.4%) |
| 1 | 138-A | 0.75 | 3/1302 (0.2%) | 1.01 | 5/1770 (0.3%) |
| 1 | 139-A | 0.75 | 0/1302 | 0.99 | 5/1770 (0.3%) |
| 1 | 140-A | 0.78 | 1/1302 (0.1%) | 0.97 | 5/1770 (0.3%) |
| 1 | 141-A | 0.85 | 3/1302 (0.2%) | 0.97 | 4/1770 (0.2%) |
| 1 | 142-A | 0.77 | 3/1302 (0.2%) | 1.00 | 6/1770 (0.3%) |
| 1 | 143-A | 0.82 | 1/1302 (0.1%) | 1.00 | 6/1770 (0.3%) |
| 1 | 144-A | 0.93 | 7/1302 (0.5%) | 1.10 | 11/1770 (0.6%) |
| 1 | 145-A | 0.74 | 1/1302 (0.1%) | 1.02 | 6/1770 (0.3%) |
| 1 | 146-A | 0.84 | 3/1302 (0.2%) | 1.04 | 7/1770 (0.4%) |
| 1 | 147-A | 0.80 | 1/1302 (0.1%) | 1.00 | 5/1770 (0.3%) |
| 1 | 148-A | 0.74 | 1/1302 (0.1%) | 1.06 | 6/1770 (0.3%) |
| 1 | 149-A | 0.83 | 3/1302 (0.2%) | 1.03 | 5/1770 (0.3%) |
| 1 | 150-A | 0.69 | 1/1302 (0.1%) | 0.94 | 2/1770 (0.1%) |
| 1 | 151-A | 0.76 | 1/1302 (0.1%) | 1.06 | 9/1770 (0.5%) |
| 1 | 152-A | 0.79 | 3/1302 (0.2%) | 0.99 | 5/1770 (0.3%) |
| 1 | 153-A | 0.75 | 2/1302 (0.2%) | 0.95 | 4/1770 (0.2%) |
| 1 | 154-A | 0.76 | 1/1302 (0.1%) | 1.03 | 8/1770 (0.5%) |
| 1 | 155-A | 0.79 | 1/1302 (0.1%) | 1.12 | 11/1770 (0.6%) |
| 1 | 156-A | 0.86 | 5/1302 (0.4%) | 1.02 | 4/1770 (0.2%) |
| 1 | 157-A | 0.99 | 7/1302 (0.5%) | 1.20 | 11/1770 (0.6%) |
| 1 | 158-A | 0.91 | 1/1302 (0.1%) | 1.14 | 10/1770 (0.6%) |
| 1 | 159-A | 1.03 | 11/1302 (0.8%) | 1.15 | 11/1770 (0.6%) |
| 1 | 160-A | 0.78 | 0/1302 | 1.02 | 6/1770 (0.3%) |
| 1 | 161-A | 0.80 | 1/1302 (0.1%) | 1.04 | 6/1770 (0.3%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 162-A | 0.86 | 6/1302 (0.5%) | 1.00 | 6/1770 (0.3%) |
| 1 | 163-A | 0.78 | 2/1302 (0.2%) | 0.96 | 4/1770 (0.2%) |
| 1 | 164-A | 0.76 | 1/1302 (0.1%) | 0.96 | 4/1770 (0.2%) |
| 1 | 165-A | 0.74 | 1/1302 (0.1%) | 0.97 | 5/1770 (0.3%) |
| 1 | 166-A | 0.77 | 1/1302 (0.1%) | 1.00 | 8/1770 (0.5%) |
| 1 | 167-A | 0.76 | 2/1302 (0.2%) | 1.01 | 7/1770 (0.4%) |
| All | All | 0.79 | 287/217434 (0.1%) | 1.01 | 932/295590 (0.3%) |

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 | 1 |
| 1 | 3-A | 0 | 1 |
| 1 | 4-A | 0 | 3 |
| 1 | 5-A | 0 | 3 |
| 1 | 6-A | 0 | 2 |
| 1 | 7-A | 0 | 5 |
| 1 | 8-A | 0 | 4 |
| 1 | 9-A | 0 | 5 |
| 1 | 10-A | 0 | 5 |
| 1 | 11-A | 0 | 2 |
| 1 | 12-A | 0 | 3 |
| 1 | 13-A | 0 | 3 |
| 1 | 14-A | 0 | 3 |
| 1 | 15-A | 0 | 1 |
| 1 | 16-A | 0 | 3 |
| 1 | 17-A | 0 | 4 |
| 1 | 18-A | 0 | 2 |
| 1 | 19-A | 0 | 2 |
| 1 | 20-A | 0 | 2 |
| 1 | 21-A | 0 | 2 |
| 1 | 22-A | 0 | 1 |
| 1 | 23-A | 0 | 3 |
| 1 | 24-A | 0 | 2 |
| 1 | 25-A | 0 | 3 |
| 1 | 26-A | 0 | 3 |
| 1 | 27-A | 0 | 1 |
| 1 | 28-A | 0 | 3 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 29-A | 0 | 1 |
| 1 | 30-A | 0 | 1 |
| 1 | 31-A | 0 | 2 |
| 1 | 32-A | 0 | 4 |
| 1 | 33-A | 0 | 6 |
| 1 | 34-A | 0 | 3 |
| 1 | 35-A | 0 | 2 |
| 1 | 36-A | 0 | 4 |
| 1 | 37-A | 0 | 2 |
| 1 | 38-A | 0 | 2 |
| 1 | 39-A | 0 | 1 |
| 1 | 40-A | 0 | 2 |
| 1 | 41-A | 0 | 4 |
| 1 | 42-A | 0 | 2 |
| 1 | 43-A | 0 | 1 |
| 1 | 44-A | 0 | 2 |
| 1 | 45-A | 0 | 2 |
| 1 | 46-A | 0 | 3 |
| 1 | 47-A | 0 | 1 |
| 1 | 48-A | 0 | 2 |
| 1 | 49-A | 0 | 4 |
| 1 | 50-A | 0 | 4 |
| 1 | 51-A | 0 | 3 |
| 1 | 52-A | 0 | 4 |
| 1 | 53-A | 0 | 4 |
| 1 | 57-A | 0 | 1 |
| 1 | 61-A | 0 | 1 |
| 1 | 62-A | 0 | 1 |
| 1 | 63-A | 0 | 1 |
| 1 | 66-A | 0 | 3 |
| 1 | 67-A | 0 | 1 |
| 1 | 68-A | 0 | 2 |
| 1 | 69-A | 0 | 1 |
| 1 | 70-A | 0 | 1 |
| 1 | 71-A | 0 | 2 |
| 1 | 72-A | 0 | 4 |
| 1 | 73-A | 0 | 2 |
| 1 | 74-A | 0 | 1 |
| 1 | 75-A | 0 | 1 |
| 1 | 78-A | 0 | 1 |
| 1 | 79-A | 0 | 2 |
| 1 | 80-A | 0 | 2 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 81-A | 0 | 2 |
| 1 | 82-A | 0 | 1 |
| 1 | 83-A | 0 | 1 |
| 1 | 84-A | 0 | 1 |
| 1 | 85-A | 0 | 1 |
| 1 | 86-A | 0 | 2 |
| 1 | 88-A | 0 | 1 |
| 1 | 89-A | 0 | 2 |
| 1 | 90-A | 0 | 2 |
| 1 | 91-A | 0 | 1 |
| 1 | 94-A | 0 | 1 |
| 1 | 95-A | 0 | 1 |
| 1 | 97-A | 0 | 1 |
| 1 | 98-A | 0 | 1 |
| 1 | 99-A | 0 | 1 |
| 1 | 100-A | 0 | 1 |
| 1 | 102-A | 0 | 1 |
| 1 | 104-A | 0 | 2 |
| 1 | 105-A | 0 | 4 |
| 1 | 107-A | 0 | 3 |
| 1 | 108-A | 0 | 2 |
| 1 | 109-A | 0 | 2 |
| 1 | 110-A | 0 | 2 |
| 1 | 111-A | 0 | 2 |
| 1 | 112-A | 0 | 2 |
| 1 | 113-A | 0 | 5 |
| 1 | 114-A | 0 | 4 |
| 1 | 115-A | 0 | 3 |
| 1 | 116-A | 0 | 3 |
| 1 | 117-A | 0 | 4 |
| 1 | 122-A | 0 | 3 |
| 1 | 124-A | 0 | 1 |
| 1 | 126-A | 0 | 1 |
| 1 | 127-A | 0 | 1 |
| 1 | 130-A | 0 | 1 |
| 1 | 131-A | 0 | 2 |
| 1 | 132-A | 0 | 3 |
| 1 | 133-A | 0 | 3 |
| 1 | 134-A | 0 | 1 |
| 1 | 136-A | 0 | 2 |
| 1 | 137-A | 0 | 2 |
| 1 | 138-A | 0 | 3 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 139-A | 0 | 1 |
| 1 | 140-A | 0 | 2 |
| 1 | 141-A | 0 | 1 |
| 1 | 143-A | 0 | 2 |
| 1 | 144-A | 0 | 2 |
| 1 | 145-A | 0 | 4 |
| 1 | 146-A | 0 | 4 |
| 1 | 147-A | 0 | 1 |
| 1 | 149-A | 0 | 2 |
| 1 | 150-A | 0 | 2 |
| 1 | 151-A | 0 | 2 |
| 1 | 152-A | 0 | 2 |
| 1 | 154-A | 0 | 1 |
| 1 | 155-A | 0 | 2 |
| 1 | 156-A | 0 | 1 |
| 1 | 157-A | 0 | 3 |
| 1 | 158-A | 0 | 2 |
| 1 | 159-A | 0 | 5 |
| 1 | 160-A | 0 | 3 |
| 1 | 161-A | 0 | 3 |
| 1 | 162-A | 0 | 5 |
| 1 | 163-A | 0 | 5 |
| 1 | 164-A | 0 | 5 |
| 1 | 165-A | 0 | 1 |
| 1 | 166-A | 0 | 2 |
| 1 | 167-A | 0 | 1 |
| All | All | 0 | 312 |

All (287) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1 | 70-A | 152 | CYS | CB-SG | 24.25 | 2.23 | 1.82 |
| 1 | 108-A | 152 | CYS | CB-SG | 21.03 | 2.18 | 1.82 |
| 1 | 71-A | 152 | CYS | CB-SG | 18.24 | 2.13 | 1.82 |
| 1 | 58-A | 152 | CYS | CB-SG | 16.08 | 2.09 | 1.82 |
| 1 | 129-A | 152 | CYS | CB-SG | 13.95 | 2.06 | 1.82 |
| 1 | 149-A | 85 | CYS | CB-SG | 12.27 | 2.03 | 1.82 |
| 1 | 107-A | 152 | CYS | CB-SG | 12.07 | 2.02 | 1.82 |
| 1 | 152-A | 152 | CYS | CB-SG | 11.46 | 2.01 | 1.82 |
| 1 | 95-A | 152 | CYS | CB-SG | 10.51 | 2.00 | 1.82 |
| 1 | 67-A | 152 | CYS | CB-SG | 10.29 | 1.99 | 1.82 |
| 1 | 106-A | 152 | CYS | CB-SG | 10.15 | 1.99 | 1.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 6-A | 152 | CYS | CB-SG | 10.09 | 1.99 | 1.82 |
| 1 | 32-A | 17 | GLU | CB-CG | 9.95 | 1.71 | 1.52 |
| 1 | 141-A | 152 | CYS | CB-SG | -9.49 | 1.66 | 1.82 |
| 1 | 34-A | 158 | ARG | CG-CD | 9.26 | 1.75 | 1.51 |
| 1 | 146-A | 17 | GLU | CB-CG | 9.14 | 1.69 | 1.52 |
| 1 | 104-A | 139 | GLU | CB-CG | 9.05 | 1.69 | 1.52 |
| 1 | 51-A | 85 | CYS | CB-SG | -8.80 | 1.67 | 1.82 |
| 1 | 159-A | 64 | SER | CA-CB | 8.52 | 1.65 | 1.52 |
| 1 | 66-A | 157 | GLU | CG-CD | 8.51 | 1.64 | 1.51 |
| 1 | 144-A | 10 | VAL | CA-CB | 8.40 | 1.72 | 1.54 |
| 1 | 69-A | 88 | VAL | CB-CG2 | -8.36 | 1.35 | 1.52 |
| 1 | 50-A | 85 | CYS | CB-SG | -8.35 | 1.68 | 1.82 |
| 1 | 97-A | 101 | GLU | CB-CG | 8.35 | 1.68 | 1.52 |
| 1 | 162-A | 13 | VAL | CB-CG1 | -8.34 | 1.35 | 1.52 |
| 1 | 96-A | 101 | GLU | CB-CG | 8.14 | 1.67 | 1.52 |
| 1 | 56-A | 98 | ARG | CG-CD | -8.12 | 1.31 | 1.51 |
| 1 | 156-A | 118 | GLU | CB-CG | 8.10 | 1.67 | 1.52 |
| 1 | 70-A | 22 | TRP | CB-CG | 8.09 | 1.64 | 1.50 |
| 1 | 159-A | 129 | GLU | CD-OE2 | 8.09 | 1.34 | 1.25 |
| 1 | 105-A | 17 | GLU | CB-CG | 8.04 | 1.67 | 1.52 |
| 1 | 89-A | 88 | VAL | CB-CG2 | -7.97 | 1.36 | 1.52 |
| 1 | 6-A | 10 | VAL | CB-CG2 | -7.95 | 1.36 | 1.52 |
| 1 | 52-A | 85 | CYS | CB-SG | -7.94 | 1.68 | 1.82 |
| 1 | 14-A | 118 | GLU | CB-CG | 7.91 | 1.67 | 1.52 |
| 1 | 87-A | 88 | VAL | CB-CG2 | -7.88 | 1.36 | 1.52 |
| 1 | 75-A | 152 | CYS | CB-SG | -7.84 | 1.69 | 1.82 |
| 1 | 144-A | 16 | MET | N-CA | 7.80 | 1.61 | 1.46 |
| 1 | 78-A | 20 | MET | CG-SD | 7.70 | 2.01 | 1.81 |
| 1 | 159-A | 48 | GLU | CB-CG | 7.67 | 1.66 | 1.52 |
| 1 | 29-A | 120 | GLU | CB-CG | 7.65 | 1.66 | 1.52 |
| 1 | 95-A | 101 | GLU | CB-CG | 7.61 | 1.66 | 1.52 |
| 1 | 116-A | 152 | CYS | CB-SG | 7.55 | 1.95 | 1.82 |
| 1 | 74-A | 101 | GLU | CB-CG | 7.52 | 1.66 | 1.52 |
| 1 | 106-A | 18 | ASN | N-CA | -7.45 | 1.31 | 1.46 |
| 1 | 116-A | 85 | CYS | CB-SG | -7.43 | 1.69 | 1.82 |
| 1 | 164-A | 48 | GLU | CB-CG | 7.43 | 1.66 | 1.52 |
| 1 | 138-A | 157 | GLU | CB-CG | 7.39 | 1.66 | 1.52 |
| 1 | 144-A | 154 | GLU | CB-CG | 7.39 | 1.66 | 1.52 |
| 1 | 29-A | 120 | GLU | CG-CD | 7.30 | 1.62 | 1.51 |
| 1 | 33-A | 158 | ARG | CG-CD | 7.29 | 1.70 | 1.51 |
| 1 | 21-A | 21 | PRO | CA-C | 7.22 | 1.67 | 1.52 |
| 1 | 59-A | 58 | LYS | CE-NZ | -7.22 | 1.31 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | 32-A | 101 | GLU | CB-CG | -7.21 | 1.38 | 1.52 |
| 1 | 40-A | 152 | CYS | CB-SG | 7.19 | 1.94 | 1.82 |
| 1 | 8-A | 101 | GLU | CB-CG | -7.17 | 1.38 | 1.52 |
| 1 | 131-A | 120 | GLU | CB-CG | 7.06 | 1.65 | 1.52 |
| 1 | 35-A | 129 | GLU | CB-CG | 7.04 | 1.65 | 1.52 |
| 1 | 56-A | 88 | VAL | CB-CG1 | -6.98 | 1.38 | 1.52 |
| 1 | 116-A | 18 | ASN | CB-CG | -6.97 | 1.35 | 1.51 |
| 1 | 83-A | 88 | VAL | CB-CG2 | -6.90 | 1.38 | 1.52 |
| 1 | 105-A | 88 | VAL | CB-CG2 | -6.90 | 1.38 | 1.52 |
| 1 | 162-A | 129 | GLU | CB-CG | 6.84 | 1.65 | 1.52 |
| 1 | 104-A | 139 | GLU | CG-CD | 6.84 | 1.62 | 1.51 |
| 1 | 20-A | 17 | GLU | CG-CD | -6.83 | 1.41 | 1.51 |
| 1 | 115-A | 118 | GLU | CB-CG | 6.83 | 1.65 | 1.52 |
| 1 | 159-A | 64 | SER | CB-OG | -6.79 | 1.33 | 1.42 |
| 1 | 34-A | 158 | ARG | CD-NE | 6.78 | 1.57 | 1.46 |
| 1 | 18-A | 139 | GLU | CB-CG | 6.75 | 1.65 | 1.52 |
| 1 | 161-A | 118 | GLU | CB-CG | 6.70 | 1.64 | 1.52 |
| 1 | 158-A | 85 | CYS | CB-SG | 6.70 | 1.93 | 1.82 |
| 1 | 46-A | 152 | CYS | CB-SG | 6.63 | 1.93 | 1.82 |
| 1 | 104-A | 88 | VAL | CB-CG2 | -6.63 | 1.39 | 1.52 |
| 1 | 113-A | 16 | MET | CB-CG | 6.63 | 1.72 | 1.51 |
| 1 | 138-A | 129 | GLU | CD-OE1 | -6.61 | 1.18 | 1.25 |
| 1 | 159-A | 48 | GLU | CG-CD | 6.59 | 1.61 | 1.51 |
| 1 | 133-A | 85 | CYS | CB-SG | -6.58 | 1.71 | 1.82 |
| 1 | 29-A | 38 | LYS | CE-NZ | -6.57 | 1.32 | 1.49 |
| 1 | 159-A | 129 | GLU | CG-CD | 6.55 | 1.61 | 1.51 |
| 1 | 82-A | 119 | VAL | CB-CG1 | -6.54 | 1.39 | 1.52 |
| 1 | 131-A | 120 | GLU | CG-CD | 6.54 | 1.61 | 1.51 |
| 1 | 98-A | 101 | GLU | CG-CD | 6.53 | 1.61 | 1.51 |
| 1 | 153-A | 85 | CYS | CB-SG | -6.53 | 1.71 | 1.82 |
| 1 | 105-A | 17 | GLU | CG-CD | 6.51 | 1.61 | 1.51 |
| 1 | 80-A | 128 | TYR | CD1-CE1 | 6.50 | 1.49 | 1.39 |
| 1 | 36-A | 129 | GLU | CB-CG | 6.50 | 1.64 | 1.52 |
| 1 | 116-A | 9 | ALA | CA-CB | -6.48 | 1.38 | 1.52 |
| 1 | 39-A | 157 | GLU | CB-CG | 6.47 | 1.64 | 1.52 |
| 1 | 30-A | 85 | CYS | CB-SG | -6.46 | 1.71 | 1.82 |
| 1 | 159-A | 58 | LYS | CE-NZ | 6.45 | 1.65 | 1.49 |
| 1 | 17-A | 101 | GLU | CB-CG | 6.44 | 1.64 | 1.52 |
| 1 | 136-A | 108 | GLN | CB-CG | 6.43 | 1.70 | 1.52 |
| 1 | 142-A | 152 | CYS | CB-SG | 6.38 | 1.93 | 1.82 |
| 1 | 71-A | 22 | TRP | CB-CG | 6.35 | 1.61 | 1.50 |
| 1 | 155-A | 142 | ASP | CB-CG | -6.32 | 1.38 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 142-A | 120 | GLU | CB-CG | 6.31 | 1.64 | 1.52 |
| 1 | 162-A | 119 | VAL | CB-CG2 | -6.29 | 1.39 | 1.52 |
| 1 | 92-A | 10 | VAL | CB-CG1 | -6.28 | 1.39 | 1.52 |
| 1 | 36-A | 20 | MET | N-CA | 6.28 | 1.58 | 1.46 |
| 1 | 144-A | 15 | GLY | CA-C | 6.27 | 1.61 | 1.51 |
| 1 | 159-A | 129 | GLU | CD-OE1 | 6.25 | 1.32 | 1.25 |
| 1 | 4-A | 154 | GLU | CB-CG | 6.24 | 1.64 | 1.52 |
| 1 | 81-A | 85 | CYS | CB-SG | -6.22 | 1.71 | 1.82 |
| 1 | 95-A | 88 | VAL | CB-CG1 | -6.21 | 1.39 | 1.52 |
| 1 | 88-A | 152 | CYS | CB-SG | 6.21 | 1.92 | 1.82 |
| 1 | 149-A | 101 | GLU | CB-CG | 6.20 | 1.64 | 1.52 |
| 1 | 31-A | 101 | GLU | CB-CG | 6.16 | 1.63 | 1.52 |
| 1 | 110-A | 19 | ALA | CA-CB | 6.16 | 1.65 | 1.52 |
| 1 | 157-A | 48 | GLU | CB-CG | 6.16 | 1.63 | 1.52 |
| 1 | 31-A | 76 | LYS | CE-NZ | 6.15 | 1.64 | 1.49 |
| 1 | 159-A | 131 | ASP | CB-CG | 6.13 | 1.64 | 1.51 |
| 1 | 145-A | 13 | VAL | CB-CG2 | -6.12 | 1.40 | 1.52 |
| 1 | 109-A | 17 | GLU | CG-CD | 6.12 | 1.61 | 1.51 |
| 1 | 115-A | 101 | GLU | CB-CG | 6.12 | 1.63 | 1.52 |
| 1 | 95-A | 38 | LYS | CE-NZ | 6.10 | 1.64 | 1.49 |
| 1 | 156-A | 159 | ARG | CG-CD | 6.09 | 1.67 | 1.51 |
| 1 | 162-A | 85 | CYS | CB-SG | -6.07 | 1.72 | 1.82 |
| 1 | 7-A | 128 | TYR | CB-CG | -6.05 | 1.42 | 1.51 |
| 1 | 149-A | 101 | GLU | CG-CD | 6.04 | 1.61 | 1.51 |
| 1 | 32-A | 142 | ASP | CB-CG | 6.04 | 1.64 | 1.51 |
| 1 | 156-A | 118 | GLU | CG-CD | 6.02 | 1.60 | 1.51 |
| 1 | 6-A | 101 | GLU | CB-CG | -6.02 | 1.40 | 1.52 |
| 1 | 57-A | 79 | ASP | CB-CG | 6.02 | 1.64 | 1.51 |
| 1 | 61-A | 88 | VAL | CB-CG2 | -6.01 | 1.40 | 1.52 |
| 1 | 33-A | 89 | PRO | CA-CB | -5.96 | 1.41 | 1.53 |
| 1 | 167-A | 85 | CYS | CB-SG | -5.96 | 1.72 | 1.81 |
| 1 | 109-A | 106 | LYS | CB-CG | 5.96 | 1.68 | 1.52 |
| 1 | 144-A | 157 | GLU | CB-CG | -5.95 | 1.40 | 1.52 |
| 1 | 92-A | 129 | GLU | CB-CG | 5.93 | 1.63 | 1.52 |
| 1 | 57-A | 159 | ARG | CG-CD | 5.92 | 1.66 | 1.51 |
| 1 | 32-A | 159 | ARG | CG-CD | 5.92 | 1.66 | 1.51 |
| 1 | 117-A | 101 | GLU | CB-CG | 5.91 | 1.63 | 1.52 |
| 1 | 6-A | 159 | ARG | CG-CD | 5.91 | 1.66 | 1.51 |
| 1 | 165-A | 108 | GLN | CG-CD | 5.90 | 1.64 | 1.51 |
| 1 | 95-A | 101 | GLU | CG-CD | 5.89 | 1.60 | 1.51 |
| 1 | 121-A | 98 | ARG | CG-CD | 5.89 | 1.66 | 1.51 |
| 1 | 157-A | 48 | GLU | CG-CD | 5.88 | 1.60 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 38-A | 108 | GLN | CB-CG | -5.87 | 1.36 | 1.52 |
| 1 | 118-A | 157 | GLU | CB-CG | 5.87 | 1.63 | 1.52 |
| 1 | 157-A | 44 | ARG | CG-CD | 5.86 | 1.66 | 1.51 |
| 1 | 37-A | 157 | GLU | CB-CG | 5.85 | 1.63 | 1.52 |
| 1 | 60-A | 98 | ARG | CG-CD | 5.84 | 1.66 | 1.51 |
| 1 | 144-A | 101 | GLU | CB-CG | 5.84 | 1.63 | 1.52 |
| 1 | 36-A | 108 | GLN | CB-CG | 5.83 | 1.68 | 1.52 |
| 1 | 56-A | 154 | GLU | CD-OE2 | 5.83 | 1.32 | 1.25 |
| 1 | 115-A | 18 | ASN | CB-CG | -5.83 | 1.37 | 1.51 |
| 1 | 73-A | 152 | CYS | CB-SG | -5.82 | 1.72 | 1.81 |
| 1 | 20-A | 120 | GLU | CB-CG | 5.82 | 1.63 | 1.52 |
| 1 | 43-A | 133 | TRP | CB-CG | -5.82 | 1.39 | 1.50 |
| 1 | 157-A | 129 | GLU | CG-CD | -5.80 | 1.43 | 1.51 |
| 1 | 109-A | 17 | GLU | CB-CG | 5.80 | 1.63 | 1.52 |
| 1 | 157-A | 85 | CYS | CB-SG | -5.80 | 1.72 | 1.81 |
| 1 | 97-A | 101 | GLU | CG-CD | 5.78 | 1.60 | 1.51 |
| 1 | 81-A | 101 | GLU | CB-CG | -5.77 | 1.41 | 1.52 |
| 1 | 86-A | 85 | CYS | CB-SG | -5.76 | 1.72 | 1.81 |
| 1 | 166-A | 132 | ASP | CA-C | 5.76 | 1.68 | 1.52 |
| 1 | 80-A | 126 | PRO | CA-C | 5.75 | 1.64 | 1.52 |
| 1 | 162-A | 10 | VAL | CB-CG2 | -5.75 | 1.40 | 1.52 |
| 1 | 39-A | 19 | ALA | CA-CB | -5.74 | 1.40 | 1.52 |
| 1 | 54-A | 118 | GLU | CB-CG | 5.73 | 1.63 | 1.52 |
| 1 | 19-A | 152 | CYS | CB-SG | -5.72 | 1.72 | 1.81 |
| 1 | 55-A | 129 | GLU | CG-CD | 5.72 | 1.60 | 1.51 |
| 1 | 163-A | 129 | GLU | CG-CD | 5.72 | 1.60 | 1.51 |
| 1 | 157-A | 48 | GLU | CD-OE2 | 5.71 | 1.31 | 1.25 |
| 1 | 11-A | 17 | GLU | CB-CG | 5.70 | 1.62 | 1.52 |
| 1 | 52-A | 129 | GLU | CB-CG | 5.69 | 1.62 | 1.52 |
| 1 | 99-A | 120 | GLU | CB-CG | 5.69 | 1.62 | 1.52 |
| 1 | 59-A | 20 | MET | CB-CG | 5.68 | 1.69 | 1.51 |
| 1 | 28-A | 18 | ASN | C-O | -5.66 | 1.12 | 1.23 |
| 1 | 7-A | 10 | VAL | CB-CG2 | -5.65 | 1.41 | 1.52 |
| 1 | 71-A | 154 | GLU | CG-CD | 5.65 | 1.60 | 1.51 |
| 1 | 101-A | 88 | VAL | CB-CG2 | -5.64 | 1.41 | 1.52 |
| 1 | 49-A | 119 | VAL | CB-CG2 | -5.64 | 1.41 | 1.52 |
| 1 | 138-A | 157 | GLU | CG-CD | 5.62 | 1.60 | 1.51 |
| 1 | 74-A | 79 | ASP | CB-CG | 5.60 | 1.63 | 1.51 |
| 1 | 122-A | 98 | ARG | CG-CD | 5.60 | 1.66 | 1.51 |
| 1 | 47-A | 16 | MET | CB-CG | 5.59 | 1.69 | 1.51 |
| 1 | 71-A | 154 | GLU | CB-CG | 5.58 | 1.62 | 1.52 |
| 1 | 125-A | 118 | GLU | CB-CG | 5.58 | 1.62 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | 35-A | 106 | LYS | CD-CE | 5.57 | 1.65 | 1.51 |
| 1 | 94-A | 101 | GLU | CB-CG | 5.57 | 1.62 | 1.52 |
| 1 | 114-A | 20 | MET | CB-CG | 5.56 | 1.69 | 1.51 |
| 1 | 7-A | 79 | ASP | CB-CG | 5.55 | 1.63 | 1.51 |
| 1 | 99-A | 120 | GLU | CG-CD | 5.54 | 1.60 | 1.51 |
| 1 | 81-A | 101 | GLU | CG-CD | -5.54 | 1.43 | 1.51 |
| 1 | 4-A | 157 | GLU | CB-CG | -5.53 | 1.41 | 1.52 |
| 1 | 107-A | 159 | ARG | CG-CD | -5.51 | 1.38 | 1.51 |
| 1 | 90-A | 134 | GLU | CB-CG | 5.51 | 1.62 | 1.52 |
| 1 | 12-A | 120 | GLU | CG-CD | 5.51 | 1.60 | 1.51 |
| 1 | 133-A | 119 | VAL | N-CA | 5.51 | 1.57 | 1.46 |
| 1 | 133-A | 118 | GLU | CB-CG | -5.51 | 1.41 | 1.52 |
| 1 | 148-A | 128 | TYR | CD2-CE2 | -5.50 | 1.31 | 1.39 |
| 1 | 105-A | 129 | GLU | CB-CG | -5.49 | 1.41 | 1.52 |
| 1 | 83-A | 85 | CYS | CB-SG | -5.47 | 1.72 | 1.81 |
| 1 | 51-A | 119 | VAL | CA-CB | 5.46 | 1.66 | 1.54 |
| 1 | 83-A | 152 | CYS | CB-SG | -5.46 | 1.73 | 1.81 |
| 1 | 111-A | 18 | ASN | CB-CG | 5.46 | 1.63 | 1.51 |
| 1 | 44-A | 152 | CYS | CB-SG | 5.46 | 1.91 | 1.82 |
| 1 | 34-A | 18 | ASN | CA-C | 5.46 | 1.67 | 1.52 |
| 1 | 73-A | 101 | GLU | CG-CD | 5.46 | 1.60 | 1.51 |
| 1 | 132-A | 119 | VAL | CB-CG1 | 5.45 | 1.64 | 1.52 |
| 1 | 134-A | 120 | GLU | CG-CD | -5.45 | 1.43 | 1.51 |
| 1 | 147-A | 101 | GLU | CB-CG | 5.44 | 1.62 | 1.52 |
| 1 | 159-A | 85 | CYS | CB-SG | -5.44 | 1.73 | 1.81 |
| 1 | 152-A | 128 | TYR | CD1-CE1 | -5.42 | 1.31 | 1.39 |
| 1 | 81-A | 129 | GLU | CG-CD | 5.42 | 1.60 | 1.51 |
| 1 | 132-A | 129 | GLU | CB-CG | 5.42 | 1.62 | 1.52 |
| 1 | 17-A | 139 | GLU | CG-CD | 5.40 | 1.60 | 1.51 |
| 1 | 52-A | 44 | ARG | CG-CD | 5.40 | 1.65 | 1.51 |
| 1 | 152-A | 129 | GLU | CD-OE1 | -5.39 | 1.19 | 1.25 |
| 1 | 146-A | 17 | GLU | CG-CD | 5.38 | 1.60 | 1.51 |
| 1 | 7-A | 120 | GLU | CG-CD | 5.37 | 1.60 | 1.51 |
| 1 | 34-A | 22 | TRP | CA-CB | 5.36 | 1.65 | 1.53 |
| 1 | 122-A | 18 | ASN | CB-CG | 5.35 | 1.63 | 1.51 |
| 1 | 7-A | 101 | GLU | CB-CG | -5.35 | 1.42 | 1.52 |
| 1 | 31-A | 89 | PRO | CA-C | -5.34 | 1.42 | 1.52 |
| 1 | 116-A | 118 | GLU | CB-CG | 5.33 | 1.62 | 1.52 |
| 1 | 72-A | 157 | GLU | CB-CG | -5.33 | 1.42 | 1.52 |
| 1 | 84-A | 98 | ARG | CG-CD | 5.32 | 1.65 | 1.51 |
| 1 | 53-A | 101 | GLU | CB-CG | -5.32 | 1.42 | 1.52 |
| 1 | 70-A | 21 | PRO | CA-C | 5.32 | 1.63 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 19-A | 17 | GLU | CG-CD | -5.31 | 1.44 | 1.51 |
| 1 | 141-A | 129 | GLU | CG-CD | 5.27 | 1.59 | 1.51 |
| 1 | 8-A | 68 | THR | CB-CG2 | -5.26 | 1.34 | 1.52 |
| 1 | 106-A | 20 | MET | CB-CG | 5.24 | 1.68 | 1.51 |
| 1 | 102-A | 139 | GLU | CG-CD | -5.24 | 1.44 | 1.51 |
| 1 | 49-A | 108 | GLN | CG-CD | 5.24 | 1.63 | 1.51 |
| 1 | 8-A | 17 | GLU | N-CA | 5.23 | 1.56 | 1.46 |
| 1 | 82-A | 88 | VAL | CB-CG2 | -5.23 | 1.41 | 1.52 |
| 1 | 94-A | 101 | GLU | CG-CD | 5.23 | 1.59 | 1.51 |
| 1 | 13-A | 120 | GLU | CB-CG | 5.23 | 1.62 | 1.52 |
| 1 | 156-A | 85 | CYS | CA-CB | -5.22 | 1.42 | 1.53 |
| 1 | 17-A | 152 | CYS | CB-SG | 5.21 | 1.91 | 1.82 |
| 1 | 8-A | 16 | MET | CG-SD | -5.21 | 1.67 | 1.81 |
| 1 | 157-A | 52 | ARG | CZ-NH2 | 5.21 | 1.39 | 1.33 |
| 1 | 75-A | 101 | GLU | CG-CD | -5.20 | 1.44 | 1.51 |
| 1 | 153-A | 129 | GLU | CD-OE2 | -5.20 | 1.20 | 1.25 |
| 1 | 39-A | 157 | GLU | CG-CD | 5.19 | 1.59 | 1.51 |
| 1 | 85-A | 98 | ARG | CG-CD | 5.19 | 1.65 | 1.51 |
| 1 | 95-A | 98 | ARG | CB-CG | -5.18 | 1.38 | 1.52 |
| 1 | 29-A | 20 | MET | CG-SD | 5.18 | 1.94 | 1.81 |
| 1 | 146-A | 154 | GLU | CB-CG | -5.18 | 1.42 | 1.52 |
| 1 | 34-A | 89 | PRO | C-O | 5.18 | 1.33 | 1.23 |
| 1 | 163-A | 48 | GLU | CG-CD | 5.18 | 1.59 | 1.51 |
| 1 | 143-A | 157 | GLU | CB-CG | -5.17 | 1.42 | 1.52 |
| 1 | 151-A | 129 | GLU | CG-CD | 5.17 | 1.59 | 1.51 |
| 1 | 49-A | 88 | VAL | CA-CB | 5.17 | 1.65 | 1.54 |
| 1 | 80-A | 118 | GLU | CB-CG | 5.17 | 1.61 | 1.52 |
| 1 | 118-A | 118 | GLU | CB-CG | 5.17 | 1.61 | 1.52 |
| 1 | 140-A | 146 | GLN | CB-CG | 5.17 | 1.66 | 1.52 |
| 1 | 75-A | 16 | MET | CB-CG | 5.17 | 1.67 | 1.51 |
| 1 | 159-A | 131 | ASP | CA-C | 5.16 | 1.66 | 1.52 |
| 1 | 142-A | 129 | GLU | CG-CD | 5.16 | 1.59 | 1.51 |
| 1 | 88-A | 10 | VAL | CB-CG2 | -5.15 | 1.42 | 1.52 |
| 1 | 127-A | 159 | ARG | CG-CD | -5.15 | 1.39 | 1.51 |
| 1 | 144-A | 131 | ASP | CB-CG | 5.15 | 1.62 | 1.51 |
| 1 | 45-A | 152 | CYS | CB-SG | -5.14 | 1.73 | 1.81 |
| 1 | 127-A | 158 | ARG | CG-CD | -5.14 | 1.39 | 1.51 |
| 1 | 167-A | 152 | CYS | CB-SG | 5.14 | 1.91 | 1.82 |
| 1 | 117-A | 119 | VAL | CB-CG1 | -5.14 | 1.42 | 1.52 |
| 1 | 137-A | 157 | GLU | CD-OE2 | 5.14 | 1.31 | 1.25 |
| 1 | 7-A | 159 | ARG | CG-CD | 5.13 | 1.64 | 1.51 |
| 1 | 156-A | 10 | VAL | CB-CG1 | -5.12 | 1.42 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 83-A | 130 | PRO | CA-C | 5.11 | 1.63 | 1.52 |
| 1 | 134-A | 146 | GLN | CB-CG | -5.11 | 1.38 | 1.52 |
| 1 | 110-A | 48 | GLU | CG-CD | 5.10 | 1.59 | 1.51 |
| 1 | 21-A | 118 | GLU | CG-CD | 5.10 | 1.59 | 1.51 |
| 1 | 129-A | 154 | GLU | CB-CG | -5.10 | 1.42 | 1.52 |
| 1 | 120-A | 16 | MET | CB-CG | 5.09 | 1.67 | 1.51 |
| 1 | 104-A | 108 | GLN | CB-CG | 5.08 | 1.66 | 1.52 |
| 1 | 154-A | 119 | VAL | CA-CB | 5.08 | 1.65 | 1.54 |
| 1 | 56-A | 154 | GLU | CG-CD | 5.08 | 1.59 | 1.51 |
| 1 | 8-A | 108 | GLN | CB-CG | 5.08 | 1.66 | 1.52 |
| 1 | 37-A | 129 | GLU | CG-CD | 5.07 | 1.59 | 1.51 |
| 1 | 46-A | 16 | MET | CB-CG | 5.07 | 1.67 | 1.51 |
| 1 | 141-A | 19 | ALA | CA-C | 5.07 | 1.66 | 1.52 |
| 1 | 35-A | 89 | PRO | CA-C | 5.06 | 1.62 | 1.52 |
| 1 | 150-A | 10 | VAL | CB-CG2 | -5.04 | 1.42 | 1.52 |
| 1 | 82-A | 128 | TYR | N-CA | 5.04 | 1.56 | 1.46 |
| 1 | 162-A | 129 | GLU | CD-OE2 | -5.04 | 1.20 | 1.25 |
| 1 | 70-A | 152 | CYS | CA-CB | 5.04 | 1.65 | 1.53 |
| 1 | 89-A | 142 | ASP | CB-CG | 5.02 | 1.62 | 1.51 |
| 1 | 113-A | 108 | GLN | CG-CD | 5.01 | 1.62 | 1.51 |
| 1 | 68-A | 20 | MET | N-CA | 5.01 | 1.56 | 1.46 |
| 1 | 56-A | 133 | TRP | CB-CG | -5.01 | 1.41 | 1.50 |
| 1 | 51-A | 159 | ARG | CG-CD | 5.00 | 1.64 | 1.51 |
| 1 | 128-A | 108 | GLN | CB-CG | 5.00 | 1.66 | 1.52 |

All (932) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | 110-A | 98 | ARG | NE-CZ-NH1 | 16.84 | 128.72 | 120.30 |
| 1 | 84-A | 36 | LEU | CA-CB-CG | 16.15 | 152.45 | 115.30 |
| 1 | 109-A | 98 | ARG | NE-CZ-NH2 | -15.74 | 112.43 | 120.30 |
| 1 | 109-A | 98 | ARG | NE-CZ-NH1 | 15.70 | 128.15 | 120.30 |
| 1 | 68-A | 20 | MET | C-N-CD | -14.29 | 89.16 | 120.60 |
| 1 | 113-A | 20 | MET | C-N-CD | -14.14 | 89.50 | 120.60 |
| 1 | 8-A | 20 | MET | C-N-CD | -13.50 | 90.90 | 120.60 |
| 1 | 108-A | 152 | CYS | CA-CB-SG | 13.44 | 138.19 | 114.00 |
| 1 | 111-A | 18 | ASN | N-CA-C | -13.42 | 74.76 | 111.00 |
| 1 | 30-A | 159 | ARG | NE-CZ-NH2 | -13.18 | 113.71 | 120.30 |
| 1 | 5-A | 129 | GLU | C-N-CD | -13.17 | 91.63 | 120.60 |
| 1 | 30-A | 159 | ARG | NE-CZ-NH1 | 12.99 | 126.80 | 120.30 |
| 1 | 66-A | 20 | MET | CG-SD-CE | 12.93 | 120.89 | 100.20 |
| 1 | 36-A | 88 | VAL | C-N-CD | -12.89 | 92.23 | 120.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | 104-A | 152 | CYS | CA-CB-SG | 12.23 | 136.01 | 114.00 |
| 1 | 158-A | 85 | CYS | CA-CB-SG | -12.21 | 92.03 | 114.00 |
| 1 | 47-A | 156 | LEU | CA-CB-CG | 12.16 | 143.26 | 115.30 |
| 1 | 106-A | 20 | MET | CG-SD-CE | 12.13 | 119.61 | 100.20 |
| 1 | 110-A | 98 | ARG | NE-CZ-NH2 | -12.11 | 114.25 | 120.30 |
| 1 | 107-A | 159 | ARG | NE-CZ-NH1 | 12.01 | 126.30 | 120.30 |
| 1 | 127-A | 158 | ARG | NE-CZ-NH1 | 11.72 | 126.16 | 120.30 |
| 1 | 41-A | 88 | VAL | C-N-CD | -11.70 | 94.87 | 120.60 |
| 1 | 52-A | 85 | CYS | CA-CB-SG | -11.70 | 92.95 | 114.00 |
| 1 | 148-A | 129 | GLU | C-N-CD | -11.22 | 95.92 | 120.60 |
| 1 | 154-A | 85 | CYS | CA-CB-SG | 10.86 | 133.55 | 114.00 |
| 1 | 8-A | 16 | MET | CG-SD-CE | 10.75 | 117.40 | 100.20 |
| 1 | 81-A | 12 | ARG | NE-CZ-NH2 | -10.53 | 115.04 | 120.30 |
| 1 | 65-A | 98 | ARG | NE-CZ-NH2 | -10.40 | 115.10 | 120.30 |
| 1 | 155-A | 129 | GLU | C-N-CD | 10.29 | 150.01 | 128.40 |
| 1 | 50-A | 85 | CYS | CA-CB-SG | -10.27 | 95.51 | 114.00 |
| 1 | 4-A | 129 | GLU | C-N-CD | -10.24 | 98.06 | 120.60 |
| 1 | 95-A | 85 | CYS | CA-CB-SG | -10.24 | 95.56 | 114.00 |
| 1 | 59-A | 16 | MET | CA-CB-CG | 10.22 | 130.68 | 113.30 |
| 1 | 46-A | 152 | CYS | CA-CB-SG | 10.21 | 132.38 | 114.00 |
| 1 | 70-A | 20 | MET | C-N-CD | -10.15 | 98.27 | 120.60 |
| 1 | 41-A | 158 | ARG | NE-CZ-NH1 | 10.12 | 125.36 | 120.30 |
| 1 | 114-A | 20 | MET | C-N-CD | -10.10 | 98.39 | 120.60 |
| 1 | 32-A | 12 | ARG | NE-CZ-NH1 | 10.05 | 125.33 | 120.30 |
| 1 | 109-A | 20 | MET | C-N-CD | -10.05 | 98.49 | 120.60 |
| 1 | 65-A | 98 | ARG | NE-CZ-NH1 | 10.01 | 125.31 | 120.30 |
| 1 | 91-A | 36 | LEU | CA-CB-CG | 10.01 | 138.32 | 115.30 |
| 1 | 53-A | 86 | GLY | N-CA-C | -9.92 | 88.29 | 113.10 |
| 1 | 127-A | 158 | ARG | NE-CZ-NH2 | -9.81 | 115.39 | 120.30 |
| 1 | 149-A | 129 | GLU | C-N-CD | -9.75 | 99.16 | 120.60 |
| 1 | 58-A | 104 | LEU | CB-CG-CD1 | 9.69 | 127.47 | 111.00 |
| 1 | 52-A | 86 | GLY | N-CA-C | -9.64 | 88.99 | 113.10 |
| 1 | 16-A | 129 | GLU | C-N-CD | -9.63 | 99.41 | 120.60 |
| 1 | 153-A | 85 | CYS | CA-CB-SG | -9.59 | 96.73 | 114.00 |
| 1 | 3-A | 129 | GLU | C-N-CD | -9.53 | 99.64 | 120.60 |
| 1 | 63-A | 28 | LEU | CA-CB-CG | 9.41 | 136.93 | 115.30 |
| 1 | 50-A | 88 | VAL | N-CA-C | 9.36 | 136.28 | 111.00 |
| 1 | 90-A | 129 | GLU | C-N-CD | 9.36 | 148.06 | 128.40 |
| 1 | 152-A | 129 | GLU | C-N-CD | 9.37 | 148.07 | 128.40 |
| 1 | 144-A | 44 | ARG | NE-CZ-NH1 | 9.35 | 124.97 | 120.30 |
| 1 | 148-A | 12 | ARG | NE-CZ-NH2 | -9.35 | 115.63 | 120.30 |
| 1 | 46-A | 156 | LEU | CA-CB-CG | 9.33 | 136.75 | 115.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 66-A | 98 | ARG | NE-CZ-NH2 | -9.33 | 115.64 | 120.30 |
| 1 | 98-A | 20 | MET | CG-SD-CE | 9.32 | 115.12 | 100.20 |
| 1 | 39-A | 16 | MET | CG-SD-CE | -9.31 | 85.30 | 100.20 |
| 1 | 23-A | 20 | MET | N-CA-C | -9.31 | 85.87 | 111.00 |
| 1 | 53-A | 52 | ARG | NE-CZ-NH1 | 9.29 | 124.94 | 120.30 |
| 1 | 122-A | 20 | MET | CG-SD-CE | 9.29 | 115.06 | 100.20 |
| 1 | 69-A | 20 | MET | C-N-CD | -9.27 | 100.20 | 120.60 |
| 1 | 159-A | 79 | ASP | CB-CG-OD2 | 9.25 | 126.62 | 118.30 |
| 1 | 56-A | 98 | ARG | NE-CZ-NH1 | 9.23 | 124.92 | 120.30 |
| 1 | 83-A | 98 | ARG | NE-CZ-NH2 | 9.22 | 124.91 | 120.30 |
| 1 | 167-A | 132 | ASP | CB-CG-OD2 | 9.18 | 126.56 | 118.30 |
| 1 | 161-A | 20 | MET | CG-SD-CE | -9.14 | 85.58 | 100.20 |
| 1 | 120-A | 20 | MET | CG-SD-CE | -9.08 | 85.68 | 100.20 |
| 1 | 22-A | 20 | MET | CG-SD-CE | -9.07 | 85.68 | 100.20 |
| 1 | 54-A | 88 | VAL | CB-CA-C | 9.05 | 128.60 | 111.40 |
| 1 | 55-A | 52 | ARG | NE-CZ-NH1 | 9.00 | 124.80 | 120.30 |
| 1 | 86-A | 36 | LEU | CB-CG-CD1 | 8.99 | 126.28 | 111.00 |
| 1 | 103-A | 52 | ARG | NE-CZ-NH2 | -8.98 | 115.81 | 120.30 |
| 1 | 95-A | 104 | LEU | CB-CG-CD1 | 8.97 | 126.25 | 111.00 |
| 1 | 136-A | 131 | ASP | CB-CG-OD2 | -8.95 | 110.24 | 118.30 |
| 1 | 155-A | 85 | CYS | CA-CB-SG | 8.93 | 130.08 | 114.00 |
| 1 | 144-A | 131 | ASP | CB-CG-OD2 | 8.85 | 126.27 | 118.30 |
| 1 | 69-A | 98 | ARG | NE-CZ-NH1 | 8.85 | 124.72 | 120.30 |
| 1 | 87-A | 36 | LEU | CB-CG-CD1 | 8.82 | 126.00 | 111.00 |
| 1 | 42-A | 88 | VAL | C-N-CD | -8.81 | 101.21 | 120.60 |
| 1 | 107-A | 159 | ARG | NE-CZ-NH2 | -8.79 | 115.91 | 120.30 |
| 1 | 115-A | 20 | MET | C-N-CD | -8.75 | 101.35 | 120.60 |
| 1 | 117-A | 20 | MET | C-N-CD | -8.75 | 101.36 | 120.60 |
| 1 | 157-A | 79 | ASP | CB-CG-OD2 | -8.75 | 110.43 | 118.30 |
| 1 | 57-A | 159 | ARG | NE-CZ-NH1 | 8.72 | 124.66 | 120.30 |
| 1 | 99-A | 98 | ARG | NE-CZ-NH2 | -8.69 | 115.96 | 120.30 |
| 1 | 65-A | 12 | ARG | NE-CZ-NH1 | 8.67 | 124.64 | 120.30 |
| 1 | 78-A | 20 | MET | CG-SD-CE | 8.65 | 114.03 | 100.20 |
| 1 | 79-A | 20 | MET | CG-SD-CE | 8.64 | 114.02 | 100.20 |
| 1 | 159-A | 159 | ARG | NE-CZ-NH2 | -8.62 | 115.99 | 120.30 |
| 1 | 79-A | 104 | LEU | CB-CG-CD1 | 8.62 | 125.65 | 111.00 |
| 1 | 94-A | 20 | MET | CG-SD-CE | -8.59 | 86.46 | 100.20 |
| 1 | 112-A | 121 | GLY | N-CA-C | 8.56 | 134.50 | 113.10 |
| 1 | 109-A | 159 | ARG | NE-CZ-NH1 | 8.53 | 124.57 | 120.30 |
| 1 | 56-A | 79 | ASP | CB-CG-OD2 | 8.52 | 125.97 | 118.30 |
| 1 | 148-A | 130 | PRO | N-CA-C | -8.51 | 89.97 | 112.10 |
| 1 | 156-A | 85 | CYS | CA-CB-SG | -8.49 | 98.72 | 114.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 50-A | 159 | ARG | NE-CZ-NH1 | 8.45 | 124.53 | 120.30 |
| 1 | 99-A | 159 | ARG | NE-CZ-NH2 | -8.43 | 116.08 | 120.30 |
| 1 | 144-A | 129 | GLU | N-CA-C | 8.37 | 133.59 | 111.00 |
| 1 | 118-A | 20 | MET | CA-CB-CG | 8.35 | 127.49 | 113.30 |
| 1 | 120-A | 98 | ARG | NE-CZ-NH2 | 8.33 | 124.47 | 120.30 |
| 1 | 61-A | 156 | LEU | CA-CB-CG | 8.33 | 134.45 | 115.30 |
| 1 | 58-A | 20 | MET | CG-SD-CE | -8.30 | 86.92 | 100.20 |
| 1 | 114-A | 98 | ARG | NE-CZ-NH1 | 8.29 | 124.44 | 120.30 |
| 1 | 80-A | 127 | ASP | CB-CG-OD1 | 8.26 | 125.73 | 118.30 |
| 1 | 8-A | 20 | MET | C-N-CA | 8.24 | 156.59 | 122.00 |
| 1 | 21-A | 152 | CYS | CA-CB-SG | -8.24 | 99.17 | 114.00 |
| 1 | 41-A | 156 | LEU | CA-CB-CG | 8.20 | 134.16 | 115.30 |
| 1 | 15-A | 11 | ASP | CB-CG-OD1 | 8.20 | 125.68 | 118.30 |
| 1 | 131-A | 119 | VAL | N-CA-C | 8.19 | 133.11 | 111.00 |
| 1 | 155-A | 44 | ARG | NE-CZ-NH1 | 8.18 | 124.39 | 120.30 |
| 1 | 166-A | 129 | GLU | C-N-CD | -8.11 | 102.76 | 120.60 |
| 1 | 23-A | 20 | MET | CA-CB-CG | 8.05 | 126.99 | 113.30 |
| 1 | 121-A | 20 | MET | CA-CB-CG | 8.05 | 126.98 | 113.30 |
| 1 | 109-A | 159 | ARG | NE-CZ-NH2 | -8.04 | 116.28 | 120.30 |
| 1 | 146-A | 142 | ASP | CB-CG-OD2 | 8.01 | 125.50 | 118.30 |
| 1 | 151-A | 52 | ARG | NE-CZ-NH1 | 8.00 | 124.30 | 120.30 |
| 1 | 115-A | 22 | TRP | N-CA-C | 7.99 | 132.57 | 111.00 |
| 1 | 79-A | 127 | ASP | CB-CG-OD2 | 7.97 | 125.47 | 118.30 |
| 1 | 120-A | 158 | ARG | NE-CZ-NH1 | 7.94 | 124.27 | 120.30 |
| 1 | 157-A | 86 | GLY | N-CA-C | 7.93 | 132.94 | 113.10 |
| 1 | 66-A | 98 | ARG | NE-CZ-NH1 | 7.91 | 124.25 | 120.30 |
| 1 | 40-A | 17 | GLU | CB-CA-C | 7.90 | 126.19 | 110.40 |
| 1 | 30-A | 98 | ARG | NE-CZ-NH1 | 7.88 | 124.24 | 120.30 |
| 1 | 59-A | 20 | MET | CG-SD-CE | -7.87 | 87.61 | 100.20 |
| 1 | 5-A | 20 | MET | CG-SD-CE | 7.86 | 112.78 | 100.20 |
| 1 | 83-A | 98 | ARG | NE-CZ-NH1 | -7.85 | 116.37 | 120.30 |
| 1 | 131-A | 4 | LEU | CB-CG-CD2 | 7.84 | 124.33 | 111.00 |
| 1 | 51-A | 85 | CYS | CA-CB-SG | -7.84 | 99.89 | 114.00 |
| 1 | 107-A | 152 | CYS | CA-CB-SG | 7.84 | 128.11 | 114.00 |
| 1 | 47-A | 36 | LEU | CA-CB-CG | 7.83 | 133.31 | 115.30 |
| 1 | 73-A | 16 | MET | CB-CG-SD | 7.82 | 135.86 | 112.40 |
| 1 | 83-A | 36 | LEU | CA-CB-CG | 7.79 | 133.22 | 115.30 |
| 1 | 109-A | 1 | MET | CG-SD-CE | 7.79 | 112.66 | 100.20 |
| 1 | 31-A | 158 | ARG | CG-CD-NE | -7.77 | 95.48 | 111.80 |
| 1 | 132-A | 44 | ARG | NE-CZ-NH1 | 7.77 | 124.18 | 120.30 |
| 1 | 99-A | 159 | ARG | NE-CZ-NH1 | 7.74 | 124.17 | 120.30 |
| 1 | 165-A | 132 | ASP | CB-CG-OD1 | 7.74 | 125.26 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 37-A | 86 | GLY | N-CA-C | -7.73 | 93.77 | 113.10 |
| 1 | 58-A | 156 | LEU | CA-CB-CG | 7.73 | 133.08 | 115.30 |
| 1 | 33-A | 158 | ARG | NE-CZ-NH1 | 7.72 | 124.16 | 120.30 |
| 1 | 14-A | 104 | LEU | CB-CG-CD2 | 7.69 | 124.07 | 111.00 |
| 1 | 63-A | 1 | MET | CA-CB-CG | 7.68 | 126.36 | 113.30 |
| 1 | 50-A | 87 | ASP | CB-CG-OD2 | -7.65 | 111.42 | 118.30 |
| 1 | 111-A | 159 | ARG | NE-CZ-NH1 | 7.64 | 124.12 | 120.30 |
| 1 | 145-A | 112 | LEU | CB-CG-CD1 | -7.63 | 98.03 | 111.00 |
| 1 | 83-A | 128 | TYR | CA-CB-CG | 7.57 | 127.78 | 113.40 |
| 1 | 84-A | 36 | LEU | CB-CG-CD1 | -7.56 | 98.14 | 111.00 |
| 1 | 88-A | 129 | GLU | C-N-CD | 7.56 | 144.28 | 128.40 |
| 1 | 30-A | 98 | ARG | NE-CZ-NH2 | -7.55 | 116.52 | 120.30 |
| 1 | 157-A | 33 | ARG | NE-CZ-NH2 | -7.54 | 116.53 | 120.30 |
| 1 | 46-A | 17 | GLU | N-CA-C | -7.53 | 90.66 | 111.00 |
| 1 | 31-A | 127 | ASP | N-CA-CB | 7.53 | 124.16 | 110.60 |
| 1 | 166-A | 132 | ASP | N-CA-C | 7.53 | 131.33 | 111.00 |
| 1 | 114-A | 104 | LEU | CB-CG-CD2 | 7.52 | 123.78 | 111.00 |
| 1 | 71-A | 20 | MET | C-N-CD | -7.51 | 104.08 | 120.60 |
| 1 | 47-A | 79 | ASP | CB-CG-OD1 | -7.49 | 111.56 | 118.30 |
| 1 | 36-A | 122 | ASP | CB-CG-OD1 | -7.49 | 111.56 | 118.30 |
| 1 | 91-A | 20 | MET | CG-SD-CE | 7.49 | 112.17 | 100.20 |
| 1 | 122-A | 121 | GLY | N-CA-C | 7.48 | 131.80 | 113.10 |
| 1 | 90-A | 1 | MET | CB-CA-C | 7.47 | 125.33 | 110.40 |
| 1 | 85-A | 128 | TYR | CB-CA-C | 7.46 | 125.33 | 110.40 |
| 1 | 16-A | 159 | ARG | NE-CZ-NH1 | 7.44 | 124.02 | 120.30 |
| 1 | 122-A | 129 | GLU | C-N-CD | 7.42 | 143.98 | 128.40 |
| 1 | 32-A | 12 | ARG | NE-CZ-NH2 | -7.41 | 116.59 | 120.30 |
| 1 | 162-A | 104 | LEU | CB-CG-CD1 | 7.39 | 123.57 | 111.00 |
| 1 | 157-A | 85 | CYS | CA-CB-SG | -7.39 | 100.70 | 114.00 |
| 1 | 96-A | 20 | MET | CG-SD-CE | -7.38 | 88.40 | 100.20 |
| 1 | 31-A | 98 | ARG | NE-CZ-NH1 | 7.35 | 123.97 | 120.30 |
| 1 | 162-A | 1 | MET | CG-SD-CE | 7.35 | 111.95 | 100.20 |
| 1 | 98-A | 98 | ARG | NE-CZ-NH2 | -7.34 | 116.63 | 120.30 |
| 1 | 145-A | 129 | GLU | N-CA-C | 7.34 | 130.82 | 111.00 |
| 1 | 154-A | 156 | LEU | CA-CB-CG | 7.34 | 132.18 | 115.30 |
| 1 | 7-A | 44 | ARG | NE-CZ-NH2 | -7.34 | 116.63 | 120.30 |
| 1 | 50-A | 36 | LEU | CA-CB-CG | 7.33 | 132.16 | 115.30 |
| 1 | 146-A | 17 | GLU | CB-CA-C | 7.32 | 125.05 | 110.40 |
| 1 | 55-A | 52 | ARG | NE-CZ-NH2 | -7.32 | 116.64 | 120.30 |
| 1 | 128-A | 92 | MET | CB-CG-SD | -7.31 | 90.46 | 112.40 |
| 1 | 99-A | 98 | ARG | NE-CZ-NH1 | 7.31 | 123.96 | 120.30 |
| 1 | 7-A | 12 | ARG | NE-CZ-NH2 | -7.31 | 116.65 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 65-A | 12 | ARG | NE-CZ-NH2 | -7.30 | 116.65 | 120.30 |
| 1 | 121-A | 121 | GLY | N-CA-C | 7.29 | 131.32 | 113.10 |
| 1 | 40-A | 21 | PRO | N-CA-C | 7.28 | 131.04 | 112.10 |
| 1 | 77-A | 52 | ARG | NE-CZ-NH2 | -7.28 | 116.66 | 120.30 |
| 1 | 49-A | 36 | LEU | CA-CB-CG | 7.27 | 132.02 | 115.30 |
| 1 | 60-A | 158 | ARG | NE-CZ-NH2 | -7.27 | 116.67 | 120.30 |
| 1 | 75-A | 152 | CYS | CA-CB-SG | -7.26 | 100.93 | 114.00 |
| 1 | 33-A | 128 | TYR | CA-CB-CG | 7.26 | 127.19 | 113.40 |
| 1 | 97-A | 159 | ARG | NE-CZ-NH2 | -7.25 | 116.67 | 120.30 |
| 1 | 80-A | 128 | TYR | CB-CG-CD1 | 7.25 | 125.35 | 121.00 |
| 1 | 154-A | 129 | GLU | C-N-CD | 7.24 | 143.60 | 128.40 |
| 1 | 158-A | 156 | LEU | CA-CB-CG | 7.23 | 131.93 | 115.30 |
| 1 | 161-A | 131 | ASP | CB-CG-OD1 | 7.23 | 124.81 | 118.30 |
| 1 | 142-A | 18 | ASN | N-CA-C | 7.22 | 130.49 | 111.00 |
| 1 | 8-A | 12 | ARG | NE-CZ-NH2 | -7.21 | 116.69 | 120.30 |
| 1 | 9-A | 21 | PRO | N-CA-C | 7.21 | 130.85 | 112.10 |
| 1 | 53-A | 156 | LEU | CA-CB-CG | 7.21 | 131.88 | 115.30 |
| 1 | 93-A | 18 | ASN | CB-CA-C | 7.19 | 124.77 | 110.40 |
| 1 | 57-A | 87 | ASP | CB-CG-OD1 | -7.17 | 111.84 | 118.30 |
| 1 | 148-A | 1 | MET | CG-SD-CE | 7.17 | 111.67 | 100.20 |
| 1 | 39-A | 158 | ARG | NE-CZ-NH2 | 7.17 | 123.88 | 120.30 |
| 1 | 113-A | 159 | ARG | NE-CZ-NH1 | 7.16 | 123.88 | 120.30 |
| 1 | 4-A | 44 | ARG | NE-CZ-NH2 | -7.14 | 116.73 | 120.30 |
| 1 | 83-A | 142 | ASP | CB-CG-OD2 | 7.14 | 124.73 | 118.30 |
| 1 | 98-A | 98 | ARG | NE-CZ-NH1 | 7.09 | 123.85 | 120.30 |
| 1 | 12-A | 17 | GLU | N-CA-C | 7.09 | 130.15 | 111.00 |
| 1 | 82-A | 127 | ASP | CB-CG-OD1 | 7.08 | 124.67 | 118.30 |
| 1 | 147-A | 8 | LEU | CB-CG-CD1 | -7.08 | 98.97 | 111.00 |
| 1 | 65-A | 20 | MET | CG-SD-CE | 7.05 | 111.49 | 100.20 |
| 1 | 130-A | 119 | VAL | CA-CB-CG2 | 7.03 | 121.45 | 110.90 |
| 1 | 6-A | 156 | LEU | CA-CB-CG | 7.03 | 131.47 | 115.30 |
| 1 | 57-A | 4 | LEU | CB-CG-CD2 | 7.02 | 122.94 | 111.00 |
| 1 | 67-A | 20 | MET | N-CA-C | 7.00 | 129.89 | 111.00 |
| 1 | 63-A | 98 | ARG | NE-CZ-NH1 | -7.00 | 116.80 | 120.30 |
| 1 | 59-A | 20 | MET | CA-CB-CG | 6.99 | 125.19 | 113.30 |
| 1 | 68-A | 20 | MET | C-N-CA | 6.99 | 151.35 | 122.00 |
| 1 | 39-A | 98 | ARG | NE-CZ-NH1 | -6.98 | 116.81 | 120.30 |
| 1 | 36-A | 119 | VAL | N-CA-C | 6.97 | 129.82 | 111.00 |
| 1 | 136-A | 13 | VAL | CB-CA-C | -6.96 | 98.17 | 111.40 |
| 1 | 20-A | 108 | GLN | CA-CB-CG | 6.96 | 128.72 | 113.40 |
| 1 | 7-A | 12 | ARG | NE-CZ-NH1 | 6.95 | 123.77 | 120.30 |
| 1 | 43-A | 87 | ASP | N-CA-C | 6.94 | 129.74 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 80-A | 128 | TYR | CA-CB-CG | 6.94 | 126.58 | 113.40 |
| 1 | 90-A | 36 | LEU | CA-CB-CG | 6.93 | 131.23 | 115.30 |
| 1 | 52-A | 52 | ARG | NE-CZ-NH1 | 6.91 | 123.76 | 120.30 |
| 1 | 82-A | 158 | ARG | NE-CZ-NH1 | 6.90 | 123.75 | 120.30 |
| 1 | 74-A | 98 | ARG | NE-CZ-NH2 | -6.89 | 116.86 | 120.30 |
| 1 | 154-A | 44 | ARG | NE-CZ-NH2 | -6.86 | 116.87 | 120.30 |
| 1 | 114-A | 20 | MET | CB-CG-SD | 6.86 | 132.98 | 112.40 |
| 1 | 158-A | 36 | LEU | CB-CG-CD2 | 6.85 | 122.65 | 111.00 |
| 1 | 146-A | 142 | ASP | CB-CG-OD1 | -6.85 | 112.14 | 118.30 |
| 1 | 136-A | 131 | ASP | CB-CG-OD1 | 6.85 | 124.46 | 118.30 |
| 1 | 115-A | 18 | ASN | N-CA-C | 6.84 | 129.47 | 111.00 |
| 1 | 144-A | 156 | LEU | CA-CB-CG | 6.83 | 131.01 | 115.30 |
| 1 | 137-A | 16 | MET | CB-CG-SD | 6.83 | 132.89 | 112.40 |
| 1 | 68-A | 127 | ASP | CB-CG-OD2 | 6.81 | 124.43 | 118.30 |
| 1 | 51-A | 86 | GLY | N-CA-C | -6.81 | 96.07 | 113.10 |
| 1 | 45-A | 85 | CYS | CA-CB-SG | -6.80 | 101.76 | 114.00 |
| 1 | 32-A | 132 | ASP | CB-CG-OD1 | 6.79 | 124.42 | 118.30 |
| 1 | 81-A | 104 | LEU | CB-CG-CD1 | -6.79 | 99.46 | 111.00 |
| 1 | 100-A | 98 | ARG | NE-CZ-NH1 | 6.77 | 123.69 | 120.30 |
| 1 | 7-A | 44 | ARG | NE-CZ-NH1 | 6.77 | 123.69 | 120.30 |
| 1 | 12-A | 119 | VAL | CB-CA-C | -6.77 | 98.54 | 111.40 |
| 1 | 34-A | 79 | ASP | CB-CG-OD2 | 6.76 | 124.39 | 118.30 |
| 1 | 138-A | 12 | ARG | NE-CZ-NH2 | -6.76 | 116.92 | 120.30 |
| 1 | 52-A | 156 | LEU | CA-CB-CG | 6.76 | 130.86 | 115.30 |
| 1 | 47-A | 85 | CYS | CA-CB-SG | -6.76 | 101.84 | 114.00 |
| 1 | 70-A | 20 | MET | C-N-CA | 6.75 | 150.35 | 122.00 |
| 1 | 143-A | 129 | GLU | C-N-CD | 6.75 | 142.56 | 128.40 |
| 1 | 117-A | 12 | ARG | NE-CZ-NH2 | -6.74 | 116.93 | 120.30 |
| 1 | 159-A | 104 | LEU | CB-CG-CD1 | 6.74 | 122.47 | 111.00 |
| 1 | 126-A | 127 | ASP | CB-CG-OD1 | 6.74 | 124.37 | 118.30 |
| 1 | 97-A | 159 | ARG | NE-CZ-NH1 | 6.73 | 123.67 | 120.30 |
| 1 | 154-A | 52 | ARG | NE-CZ-NH2 | -6.73 | 116.93 | 120.30 |
| 1 | 154-A | 52 | ARG | NE-CZ-NH1 | 6.73 | 123.67 | 120.30 |
| 1 | 158-A | 52 | ARG | NE-CZ-NH1 | 6.72 | 123.66 | 120.30 |
| 1 | 143-A | 18 | ASN | N-CA-C | 6.71 | 129.12 | 111.00 |
| 1 | 70-A | 152 | CYS | CB-CA-C | 6.71 | 123.81 | 110.40 |
| 1 | 57-A | 156 | LEU | CA-CB-CG | 6.70 | 130.70 | 115.30 |
| 1 | 34-A | 44 | ARG | NE-CZ-NH1 | 6.69 | 123.64 | 120.30 |
| 1 | 97-A | 20 | MET | CB-CG-SD | 6.69 | 132.46 | 112.40 |
| 1 | 155-A | 44 | ARG | NE-CZ-NH2 | -6.68 | 116.96 | 120.30 |
| 1 | 159-A | 1 | MET | CG-SD-CE | -6.68 | 89.51 | 100.20 |
| 1 | 70-A | 20 | MET | N-CA-C | 6.67 | 129.01 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 33-A | 128 | TYR | N-CA-CB | -6.67 | 98.59 | 110.60 |
| 1 | 32-A | 16 | MET | CB-CG-SD | 6.66 | 132.37 | 112.40 |
| 1 | 131-A | 1 | MET | CG-SD-CE | 6.66 | 110.85 | 100.20 |
| 1 | 126-A | 20 | MET | CG-SD-CE | 6.66 | 110.85 | 100.20 |
| 1 | 122-A | 156 | LEU | CA-CB-CG | 6.65 | 130.59 | 115.30 |
| 1 | 74-A | 8 | LEU | CA-CB-CG | 6.64 | 130.58 | 115.30 |
| 1 | 33-A | 87 | ASP | N-CA-C | 6.64 | 128.93 | 111.00 |
| 1 | 33-A | 12 | ARG | NE-CZ-NH2 | -6.64 | 116.98 | 120.30 |
| 1 | 11-A | 21 | PRO | N-CA-C | 6.64 | 129.35 | 112.10 |
| 1 | 52-A | 36 | LEU | CB-CA-C | 6.63 | 122.80 | 110.20 |
| 1 | 151-A | 159 | ARG | NE-CZ-NH1 | 6.63 | 123.61 | 120.30 |
| 1 | 138-A | 16 | MET | CB-CG-SD | 6.62 | 132.26 | 112.40 |
| 1 | 34-A | 142 | ASP | CB-CG-OD2 | -6.62 | 112.34 | 118.30 |
| 1 | 37-A | 159 | ARG | NE-CZ-NH1 | 6.62 | 123.61 | 120.30 |
| 1 | 137-A | 1 | MET | CG-SD-CE | 6.61 | 110.78 | 100.20 |
| 1 | 80-A | 104 | LEU | CB-CG-CD1 | 6.61 | 122.23 | 111.00 |
| 1 | 16-A | 18 | ASN | N-CA-C | 6.58 | 128.78 | 111.00 |
| 1 | 37-A | 19 | ALA | N-CA-C | 6.58 | 128.76 | 111.00 |
| 1 | 39-A | 122 | ASP | CB-CG-OD1 | 6.58 | 124.22 | 118.30 |
| 1 | 129-A | 159 | ARG | NE-CZ-NH1 | 6.58 | 123.59 | 120.30 |
| 1 | 42-A | 87 | ASP | CB-CG-OD1 | 6.57 | 124.22 | 118.30 |
| 1 | 43-A | 98 | ARG | NE-CZ-NH1 | -6.57 | 117.02 | 120.30 |
| 1 | 93-A | 20 | MET | N-CA-C | -6.56 | 93.29 | 111.00 |
| 1 | 132-A | 119 | VAL | N-CA-C | 6.55 | 128.69 | 111.00 |
| 1 | 146-A | 16 | MET | CA-CB-CG | 6.55 | 124.44 | 113.30 |
| 1 | 32-A | 156 | LEU | CA-CB-CG | 6.55 | 130.36 | 115.30 |
| 1 | 32-A | 87 | ASP | CB-CG-OD2 | -6.54 | 112.41 | 118.30 |
| 1 | 121-A | 20 | MET | CB-CA-C | 6.54 | 123.49 | 110.40 |
| 1 | 42-A | 98 | ARG | NE-CZ-NH1 | -6.54 | 117.03 | 120.30 |
| 1 | 57-A | 20 | MET | CG-SD-CE | 6.54 | 110.67 | 100.20 |
| 1 | 16-A | 38 | LYS | CD-CE-NZ | -6.54 | 96.67 | 111.70 |
| 1 | 112-A | 33 | ARG | NE-CZ-NH1 | 6.53 | 123.56 | 120.30 |
| 1 | 110-A | 1 | MET | C-N-CA | -6.53 | 105.39 | 121.70 |
| 1 | 105-A | 18 | ASN | N-CA-C | -6.52 | 93.39 | 111.00 |
| 1 | 24-A | 111 | TYR | CA-CB-CG | -6.51 | 101.02 | 113.40 |
| 1 | 29-A | 17 | GLU | N-CA-C | -6.51 | 93.42 | 111.00 |
| 1 | 160-A | 64 | SER | N-CA-C | -6.50 | 93.46 | 111.00 |
| 1 | 106-A | 70 | ASP | CB-CG-OD1 | 6.49 | 124.14 | 118.30 |
| 1 | 74-A | 79 | ASP | CB-CG-OD1 | 6.48 | 124.13 | 118.30 |
| 1 | 160-A | 129 | GLU | C-N-CD | -6.47 | 106.38 | 120.60 |
| 1 | 32-A | 85 | CYS | CA-CB-SG | -6.46 | 102.37 | 114.00 |
| 1 | 144-A | 128 | TYR | CA-CB-CG | 6.46 | 125.67 | 113.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 143-A | 20 | MET | CA-CB-CG | 6.44 | 124.25 | 113.30 |
| 1 | 87-A | 1 | MET | CB-CG-SD | 6.43 | 131.68 | 112.40 |
| 1 | 116-A | 20 | MET | N-CA-C | -6.42 | 93.67 | 111.00 |
| 1 | 162-A | 130 | PRO | CA-N-CD | -6.42 | 102.52 | 111.50 |
| 1 | 106-A | 20 | MET | CA-CB-CG | 6.41 | 124.20 | 113.30 |
| 1 | 49-A | 87 | ASP | N-CA-C | 6.41 | 128.31 | 111.00 |
| 1 | 66-A | 157 | GLU | OE1-CD-OE2 | -6.40 | 115.62 | 123.30 |
| 1 | 155-A | 129 | GLU | C-N-CA | -6.40 | 95.12 | 122.00 |
| 1 | 80-A | 126 | PRO | N-CA-C | 6.39 | 128.72 | 112.10 |
| 1 | 57-A | 119 | VAL | CB-CA-C | -6.38 | 99.28 | 111.40 |
| 1 | 105-A | 20 | MET | C-N-CD | 6.38 | 141.80 | 128.40 |
| 1 | 109-A | 152 | CYS | CA-CB-SG | 6.38 | 125.48 | 114.00 |
| 1 | 9-A | 20 | MET | C-N-CD | -6.38 | 106.58 | 120.60 |
| 1 | 79-A | 119 | VAL | CB-CA-C | -6.37 | 99.30 | 111.40 |
| 1 | 113-A | 20 | MET | C-N-CA | 6.37 | 148.75 | 122.00 |
| 1 | 142-A | 152 | CYS | CA-CB-SG | 6.37 | 125.46 | 114.00 |
| 1 | 115-A | 11 | ASP | CB-CG-OD1 | 6.37 | 124.03 | 118.30 |
| 1 | 70-A | 152 | CYS | CA-CB-SG | 6.36 | 125.45 | 114.00 |
| 1 | 69-A | 16 | MET | CB-CG-SD | 6.34 | 131.43 | 112.40 |
| 1 | 38-A | 12 | ARG | NE-CZ-NH1 | 6.34 | 123.47 | 120.30 |
| 1 | 33-A | 129 | GLU | N-CA-C | 6.32 | 128.06 | 111.00 |
| 1 | 9-A | 104 | LEU | CB-CG-CD1 | 6.31 | 121.72 | 111.00 |
| 1 | 41-A | 19 | ALA | N-CA-C | 6.30 | 128.02 | 111.00 |
| 1 | 104-A | 18 | ASN | N-CA-C | -6.30 | 93.98 | 111.00 |
| 1 | 132-A | 118 | GLU | N-CA-C | 6.30 | 128.02 | 111.00 |
| 1 | 165-A | 16 | MET | CG-SD-CE | 6.30 | 110.28 | 100.20 |
| 1 | 98-A | 87 | ASP | CB-CG-OD1 | 6.30 | 123.97 | 118.30 |
| 1 | 141-A | 19 | ALA | N-CA-C | 6.30 | 128.00 | 111.00 |
| 1 | 30-A | 16 | MET | CG-SD-CE | 6.29 | 110.26 | 100.20 |
| 1 | 146-A | 131 | ASP | CB-CG-OD1 | -6.28 | 112.64 | 118.30 |
| 1 | 68-A | 79 | ASP | CB-CG-OD1 | 6.27 | 123.94 | 118.30 |
| 1 | 150-A | 136 | VAL | N-CA-C | -6.27 | 94.08 | 111.00 |
| 1 | 23-A | 20 | MET | CB-CG-SD | 6.27 | 131.20 | 112.40 |
| 1 | 9-A | 119 | VAL | CB-CA-C | -6.26 | 99.50 | 111.40 |
| 1 | 30-A | 127 | ASP | CB-CG-OD1 | -6.26 | 112.66 | 118.30 |
| 1 | 40-A | 22 | TRP | N-CA-C | -6.26 | 94.11 | 111.00 |
| 1 | 47-A | 87 | ASP | CB-CG-OD2 | 6.26 | 123.93 | 118.30 |
| 1 | 82-A | 142 | ASP | CB-CG-OD2 | 6.26 | 123.93 | 118.30 |
| 1 | 135-A | 120 | GLU | CB-CA-C | 6.26 | 122.91 | 110.40 |
| 1 | 35-A | 127 | ASP | N-CA-C | -6.25 | 94.12 | 111.00 |
| 1 | 157-A | 98 | ARG | NE-CZ-NH2 | 6.25 | 123.42 | 120.30 |
| 1 | 159-A | 4 | LEU | CB-CG-CD2 | 6.25 | 121.62 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 60-A | 127 | ASP | CB-CG-OD1 | 6.25 | 123.92 | 118.30 |
| 1 | 140-A | 1 | MET | CG-SD-CE | -6.24 | 90.21 | 100.20 |
| 1 | 31-A | 12 | ARG | NE-CZ-NH2 | -6.24 | 117.18 | 120.30 |
| 1 | 42-A | 87 | ASP | CB-CG-OD2 | -6.24 | 112.68 | 118.30 |
| 1 | 162-A | 104 | LEU | CB-CG-CD2 | -6.24 | 100.40 | 111.00 |
| 1 | 72-A | 88 | VAL | CG1-CB-CG2 | 6.22 | 120.86 | 110.90 |
| 1 | 134-A | 159 | ARG | NE-CZ-NH1 | -6.22 | 117.19 | 120.30 |
| 1 | 75-A | 1 | MET | CA-CB-CG | 6.22 | 123.87 | 113.30 |
| 1 | 39-A | 158 | ARG | CG-CD-NE | 6.21 | 124.85 | 111.80 |
| 1 | 138-A | 12 | ARG | NE-CZ-NH1 | 6.21 | 123.41 | 120.30 |
| 1 | 67-A | 87 | ASP | CB-CG-OD2 | 6.21 | 123.89 | 118.30 |
| 1 | 132-A | 44 | ARG | NE-CZ-NH2 | -6.21 | 117.19 | 120.30 |
| 1 | 115-A | 119 | VAL | CB-CA-C | -6.21 | 99.61 | 111.40 |
| 1 | 33-A | 131 | ASP | CB-CG-OD2 | -6.20 | 112.72 | 118.30 |
| 1 | 6-A | 44 | ARG | NE-CZ-NH1 | 6.20 | 123.40 | 120.30 |
| 1 | 21-A | 12 | ARG | NE-CZ-NH1 | 6.20 | 123.40 | 120.30 |
| 1 | 35-A | 18 | ASN | CB-CA-C | 6.19 | 122.78 | 110.40 |
| 1 | 145-A | 1 | MET | CG-SD-CE | -6.19 | 90.30 | 100.20 |
| 1 | 68-A | 52 | ARG | NE-CZ-NH1 | 6.19 | 123.39 | 120.30 |
| 1 | 31-A | 53 | PRO | N-CA-C | 6.19 | 128.19 | 112.10 |
| 1 | 107-A | 20 | MET | CB-CG-SD | 6.19 | 130.96 | 112.40 |
| 1 | 20-A | 159 | ARG | NE-CZ-NH1 | 6.18 | 123.39 | 120.30 |
| 1 | 71-A | 16 | MET | N-CA-C | -6.18 | 94.31 | 111.00 |
| 1 | 125-A | 16 | MET | CA-CB-CG | 6.18 | 123.81 | 113.30 |
| 1 | 8-A | 4 | LEU | CB-CG-CD1 | -6.18 | 100.50 | 111.00 |
| 1 | 158-A | 44 | ARG | NE-CZ-NH2 | 6.17 | 123.39 | 120.30 |
| 1 | 134-A | 159 | ARG | NE-CZ-NH2 | 6.17 | 123.39 | 120.30 |
| 1 | 138-A | 16 | MET | CG-SD-CE | 6.17 | 110.07 | 100.20 |
| 1 | 86-A | 104 | LEU | CB-CG-CD2 | -6.16 | 100.52 | 111.00 |
| 1 | 109-A | 17 | GLU | N-CA-CB | 6.16 | 121.69 | 110.60 |
| 1 | 153-A | 127 | ASP | N-CA-C | 6.16 | 127.64 | 111.00 |
| 1 | 68-A | 1 | MET | CB-CA-C | 6.16 | 122.72 | 110.40 |
| 1 | 136-A | 18 | ASN | CB-CA-C | -6.15 | 98.10 | 110.40 |
| 1 | 56-A | 87 | ASP | CB-CG-OD1 | 6.15 | 123.83 | 118.30 |
| 1 | 159-A | 156 | LEU | CA-CB-CG | 6.14 | 129.42 | 115.30 |
| 1 | 76-A | 16 | MET | CG-SD-CE | 6.13 | 110.01 | 100.20 |
| 1 | 56-A | 4 | LEU | CB-CG-CD2 | 6.13 | 121.42 | 111.00 |
| 1 | 53-A | 87 | ASP | CB-CG-OD1 | -6.13 | 112.78 | 118.30 |
| 1 | 151-A | 129 | GLU | C-N-CD | 6.13 | 141.27 | 128.40 |
| 1 | 117-A | 19 | ALA | N-CA-C | 6.13 | 127.54 | 111.00 |
| 1 | 21-A | 152 | CYS | CB-CA-C | -6.12 | 98.16 | 110.40 |
| 1 | 131-A | 1 | MET | CA-CB-CG | 6.11 | 123.69 | 113.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 156-A | 86 | GLY | N-CA-C | 6.11 | 128.38 | 113.10 |
| 1 | 38-A | 88 | VAL | C-N-CD | -6.11 | 107.17 | 120.60 |
| 1 | 93-A | 129 | GLU | CA-CB-CG | -6.11 | 99.96 | 113.40 |
| 1 | 135-A | 52 | ARG | NE-CZ-NH1 | 6.10 | 123.35 | 120.30 |
| 1 | 40-A | 159 | ARG | NE-CZ-NH2 | -6.10 | 117.25 | 120.30 |
| 1 | 166-A | 128 | TYR | CA-CB-CG | 6.10 | 124.98 | 113.40 |
| 1 | 17-A | 79 | ASP | CB-CG-OD1 | 6.10 | 123.79 | 118.30 |
| 1 | 65-A | 4 | LEU | CB-CG-CD2 | 6.09 | 121.36 | 111.00 |
| 1 | 136-A | 52 | ARG | CB-CG-CD | 6.09 | 127.44 | 111.60 |
| 1 | 147-A | 159 | ARG | NE-CZ-NH2 | -6.09 | 117.25 | 120.30 |
| 1 | 60-A | 158 | ARG | CG-CD-NE | -6.09 | 99.01 | 111.80 |
| 1 | 166-A | 159 | ARG | NE-CZ-NH2 | -6.09 | 117.26 | 120.30 |
| 1 | 58-A | 33 | ARG | NE-CZ-NH2 | 6.09 | 123.34 | 120.30 |
| 1 | 89-A | 142 | ASP | CB-CG-OD2 | 6.09 | 123.78 | 118.30 |
| 1 | 86-A | 159 | ARG | CG-CD-NE | -6.08 | 99.02 | 111.80 |
| 1 | 87-A | 104 | LEU | CB-CG-CD2 | -6.08 | 100.66 | 111.00 |
| 1 | 75-A | 101 | GLU | OE1-CD-OE2 | 6.08 | 130.60 | 123.30 |
| 1 | 158-A | 79 | ASP | CB-CG-OD2 | 6.08 | 123.77 | 118.30 |
| 1 | 56-A | 156 | LEU | CB-CG-CD1 | -6.08 | 100.67 | 111.00 |
| 1 | 12-A | 119 | VAL | N-CA-C | 6.07 | 127.40 | 111.00 |
| 1 | 155-A | 156 | LEU | CB-CG-CD2 | 6.07 | 121.32 | 111.00 |
| 1 | 99-A | 132 | ASP | CB-CG-OD2 | 6.07 | 123.76 | 118.30 |
| 1 | 127-A | 134 | GLU | CA-CB-CG | 6.07 | 126.75 | 113.40 |
| 1 | 108-A | 4 | LEU | CB-CG-CD2 | 6.07 | 121.31 | 111.00 |
| 1 | 16-A | 159 | ARG | NE-CZ-NH2 | -6.06 | 117.27 | 120.30 |
| 1 | 28-A | 20 | MET | N-CA-C | 6.06 | 127.37 | 111.00 |
| 1 | 126-A | 20 | MET | CB-CG-SD | -6.06 | 94.21 | 112.40 |
| 1 | 28-A | 32 | LYS | CD-CE-NZ | 6.05 | 125.62 | 111.70 |
| 1 | 48-A | 85 | CYS | N-CA-C | 6.05 | 127.34 | 111.00 |
| 1 | 82-A | 159 | ARG | NE-CZ-NH1 | 6.05 | 123.32 | 120.30 |
| 1 | 20-A | 36 | LEU | CB-CG-CD1 | 6.04 | 121.27 | 111.00 |
| 1 | 125-A | 20 | MET | N-CA-C | -6.03 | 94.72 | 111.00 |
| 1 | 103-A | 33 | ARG | NE-CZ-NH2 | -6.03 | 117.29 | 120.30 |
| 1 | 144-A | 15 | GLY | CA-C-O | -6.03 | 109.76 | 120.60 |
| 1 | 21-A | 12 | ARG | NE-CZ-NH2 | -6.02 | 117.29 | 120.30 |
| 1 | 39-A | 52 | ARG | NE-CZ-NH2 | -6.02 | 117.29 | 120.30 |
| 1 | 103-A | 52 | ARG | NE-CZ-NH1 | 6.02 | 123.31 | 120.30 |
| 1 | 68-A | 127 | ASP | CB-CA-C | 6.01 | 122.43 | 110.40 |
| 1 | 79-A | 127 | ASP | N-CA-C | 6.01 | 127.24 | 111.00 |
| 1 | 79-A | 127 | ASP | CB-CG-OD1 | -6.01 | 112.89 | 118.30 |
| 1 | 103-A | 129 | GLU | CA-CB-CG | 6.01 | 126.61 | 113.40 |
| 1 | 73-A | 98 | ARG | NE-CZ-NH1 | 6.00 | 123.30 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 40-A | 16 | MET | CG-SD-CE | 5.99 | 109.78 | 100.20 |
| 1 | 134-A | 16 | MET | CB-CG-SD | 5.99 | 130.37 | 112.40 |
| 1 | 165-A | 127 | ASP | N-CA-C | -5.99 | 94.84 | 111.00 |
| 1 | 32-A | 98 | ARG | CG-CD-NE | 5.98 | 124.36 | 111.80 |
| 1 | 76-A | 44 | ARG | NE-CZ-NH2 | -5.98 | 117.31 | 120.30 |
| 1 | 79-A | 129 | GLU | C-N-CA | -5.98 | 96.88 | 122.00 |
| 1 | 156-A | 16 | MET | CG-SD-CE | 5.98 | 109.77 | 100.20 |
| 1 | 96-A | 122 | ASP | N-CA-CB | -5.98 | 99.84 | 110.60 |
| 1 | 35-A | 104 | LEU | CB-CG-CD2 | 5.97 | 121.16 | 111.00 |
| 1 | 39-A | 104 | LEU | CB-CG-CD2 | 5.97 | 121.15 | 111.00 |
| 1 | 152-A | 159 | ARG | NE-CZ-NH1 | 5.97 | 123.29 | 120.30 |
| 1 | 10-A | 156 | LEU | CA-CB-CG | 5.97 | 129.03 | 115.30 |
| 1 | 119-A | 1 | MET | CG-SD-CE | -5.97 | 90.65 | 100.20 |
| 1 | 11-A | 156 | LEU | CA-CB-CG | 5.96 | 129.02 | 115.30 |
| 1 | 10-A | 119 | VAL | CB-CA-C | -5.96 | 100.08 | 111.40 |
| 1 | 131-A | 20 | MET | CB-CA-C | 5.96 | 122.31 | 110.40 |
| 1 | 47-A | 85 | CYS | N-CA-C | 5.96 | 127.08 | 111.00 |
| 1 | 45-A | 156 | LEU | CA-CB-CG | 5.95 | 128.99 | 115.30 |
| 1 | 122-A | 98 | ARG | CG-CD-NE | 5.95 | 124.30 | 111.80 |
| 1 | 27-A | 108 | GLN | CA-CB-CG | 5.95 | 126.49 | 113.40 |
| 1 | 32-A | 109 | LYS | CD-CE-NZ | 5.95 | 125.38 | 111.70 |
| 1 | 142-A | 4 | LEU | CB-CG-CD2 | 5.95 | 121.11 | 111.00 |
| 1 | 109-A | 156 | LEU | CA-CB-CG | 5.94 | 128.97 | 115.30 |
| 1 | 159-A | 132 | ASP | N-CA-C | 5.94 | 127.04 | 111.00 |
| 1 | 41-A | 159 | ARG | NE-CZ-NH2 | -5.94 | 117.33 | 120.30 |
| 1 | 29-A | 38 | LYS | CD-CE-NZ | -5.94 | 98.04 | 111.70 |
| 1 | 149-A | 44 | ARG | NE-CZ-NH1 | 5.94 | 123.27 | 120.30 |
| 1 | 85-A | 16 | MET | CG-SD-CE | -5.94 | 90.70 | 100.20 |
| 1 | 114-A | 52 | ARG | NE-CZ-NH1 | 5.93 | 123.27 | 120.30 |
| 1 | 25-A | 61 | ILE | CG1-CB-CG2 | -5.93 | 98.36 | 111.40 |
| 1 | 38-A | 142 | ASP | CB-CG-OD1 | 5.91 | 123.62 | 118.30 |
| 1 | 92-A | 4 | LEU | CB-CG-CD2 | 5.91 | 121.05 | 111.00 |
| 1 | 131-A | 20 | MET | CB-CG-SD | -5.91 | 94.69 | 112.40 |
| 1 | 2-A | 159 | ARG | NE-CZ-NH1 | 5.90 | 123.25 | 120.30 |
| 1 | 133-A | 44 | ARG | NE-CZ-NH2 | -5.90 | 117.35 | 120.30 |
| 1 | 130-A | 119 | VAL | N-CA-C | 5.89 | 126.92 | 111.00 |
| 1 | 131-A | 20 | MET | CA-CB-CG | 5.89 | 123.31 | 113.30 |
| 1 | 31-A | 16 | MET | CA-CB-CG | 5.89 | 123.31 | 113.30 |
| 1 | 108-A | 1 | MET | CG-SD-CE | 5.88 | 109.61 | 100.20 |
| 1 | 48-A | 88 | VAL | C-N-CD | 5.88 | 140.75 | 128.40 |
| 1 | 52-A | 36 | LEU | CB-CG-CD1 | -5.88 | 101.01 | 111.00 |
| 1 | 68-A | 16 | MET | CG-SD-CE | 5.88 | 109.61 | 100.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 84-A | 98 | ARG | CA-CB-CG | 5.88 | 126.33 | 113.40 |
| 1 | 109-A | 44 | ARG | NE-CZ-NH1 | 5.88 | 123.24 | 120.30 |
| 1 | 61-A | 159 | ARG | NE-CZ-NH2 | -5.88 | 117.36 | 120.30 |
| 1 | 136-A | 24 | LEU | CB-CG-CD1 | 5.88 | 120.99 | 111.00 |
| 1 | 106-A | 152 | CYS | CA-CB-SG | 5.88 | 124.58 | 114.00 |
| 1 | 147-A | 8 | LEU | CB-CG-CD2 | 5.87 | 120.99 | 111.00 |
| 1 | 159-A | 79 | ASP | CB-CG-OD1 | -5.87 | 113.02 | 118.30 |
| 1 | 82-A | 159 | ARG | NE-CZ-NH2 | -5.86 | 117.37 | 120.30 |
| 1 | 114-A | 129 | GLU | C-N-CA | -5.86 | 97.38 | 122.00 |
| 1 | 31-A | 130 | PRO | CA-C-O | -5.85 | 106.15 | 120.20 |
| 1 | 40-A | 4 | LEU | CB-CG-CD2 | 5.85 | 120.95 | 111.00 |
| 1 | 69-A | 17 | GLU | CB-CA-C | 5.85 | 122.09 | 110.40 |
| 1 | 119-A | 16 | MET | CA-CB-CG | 5.84 | 123.22 | 113.30 |
| 1 | 83-A | 4 | LEU | CB-CG-CD2 | 5.84 | 120.92 | 111.00 |
| 1 | 101-A | 104 | LEU | CB-CG-CD2 | 5.83 | 120.91 | 111.00 |
| 1 | 107-A | 79 | ASP | CB-CG-OD1 | 5.82 | 123.54 | 118.30 |
| 1 | 8-A | 159 | ARG | NE-CZ-NH1 | 5.82 | 123.21 | 120.30 |
| 1 | 130-A | 119 | VAL | CB-CA-C | -5.82 | 100.35 | 111.40 |
| 1 | 81-A | 4 | LEU | CB-CG-CD2 | 5.82 | 120.89 | 111.00 |
| 1 | 89-A | 36 | LEU | CA-CB-CG | 5.81 | 128.67 | 115.30 |
| 1 | 43-A | 159 | ARG | NE-CZ-NH2 | 5.81 | 123.20 | 120.30 |
| 1 | 160-A | 131 | ASP | CB-CG-OD1 | 5.81 | 123.53 | 118.30 |
| 1 | 6-A | 44 | ARG | NE-CZ-NH2 | -5.80 | 117.40 | 120.30 |
| 1 | 8-A | 12 | ARG | NE-CZ-NH1 | 5.80 | 123.20 | 120.30 |
| 1 | 117-A | 28 | LEU | CB-CG-CD1 | -5.80 | 101.15 | 111.00 |
| 1 | 119-A | 24 | LEU | CB-CG-CD1 | -5.80 | 101.15 | 111.00 |
| 1 | 164-A | 158 | ARG | NE-CZ-NH2 | -5.79 | 117.40 | 120.30 |
| 1 | 32-A | 129 | GLU | C-N-CD | -5.79 | 107.86 | 120.60 |
| 1 | 109-A | 44 | ARG | NE-CZ-NH2 | -5.79 | 117.41 | 120.30 |
| 1 | 65-A | 70 | ASP | CB-CG-OD1 | 5.79 | 123.51 | 118.30 |
| 1 | 166-A | 131 | ASP | C-N-CA | 5.79 | 136.17 | 121.70 |
| 1 | 139-A | 159 | ARG | NE-CZ-NH1 | 5.79 | 123.19 | 120.30 |
| 1 | 60-A | 156 | LEU | CA-CB-CG | 5.78 | 128.60 | 115.30 |
| 1 | 41-A | 159 | ARG | NE-CZ-NH1 | 5.77 | 123.19 | 120.30 |
| 1 | 92-A | 36 | LEU | CA-CB-CG | 5.77 | 128.58 | 115.30 |
| 1 | 3-A | 128 | TYR | CB-CG-CD2 | 5.77 | 124.46 | 121.00 |
| 1 | 26-A | 61 | ILE | CG1-CB-CG2 | -5.77 | 98.70 | 111.40 |
| 1 | 32-A | 159 | ARG | CB-CG-CD | 5.77 | 126.59 | 111.60 |
| 1 | 107-A | 20 | MET | CG-SD-CE | -5.77 | 90.97 | 100.20 |
| 1 | 45-A | 135 | SER | CB-CA-C | -5.77 | 99.15 | 110.10 |
| 1 | 118-A | 22 | TRP | N-CA-C | 5.77 | 126.57 | 111.00 |
| 1 | 120-A | 58 | LYS | CD-CE-NZ | 5.77 | 124.96 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 113-A | 129 | GLU | C-N-CD | 5.76 | 140.50 | 128.40 |
| 1 | 117-A | 22 | TRP | N-CA-C | 5.76 | 126.56 | 111.00 |
| 1 | 137-A | 127 | ASP | CB-CG-OD1 | 5.76 | 123.48 | 118.30 |
| 1 | 34-A | 158 | ARG | NE-CZ-NH1 | 5.76 | 123.18 | 120.30 |
| 1 | 116-A | 20 | MET | CB-CA-C | 5.76 | 121.91 | 110.40 |
| 1 | 106-A | 18 | ASN | N-CA-C | -5.75 | 95.47 | 111.00 |
| 1 | 148-A | 28 | LEU | CA-CB-CG | -5.75 | 102.08 | 115.30 |
| 1 | 9-A | 16 | MET | CA-CB-CG | 5.74 | 123.06 | 113.30 |
| 1 | 44-A | 85 | CYS | N-CA-C | 5.74 | 126.51 | 111.00 |
| 1 | 144-A | 44 | ARG | CG-CD-NE | 5.74 | 123.86 | 111.80 |
| 1 | 49-A | 131 | ASP | CB-CG-OD2 | -5.74 | 113.14 | 118.30 |
| 1 | 115-A | 104 | LEU | CB-CG-CD2 | 5.74 | 120.75 | 111.00 |
| 1 | 131-A | 159 | ARG | NE-CZ-NH2 | -5.74 | 117.43 | 120.30 |
| 1 | 51-A | 36 | LEU | CB-CG-CD1 | -5.74 | 101.25 | 111.00 |
| 1 | 55-A | 87 | ASP | N-CA-C | -5.74 | 95.51 | 111.00 |
| 1 | 115-A | 24 | LEU | CA-CB-CG | 5.74 | 128.49 | 115.30 |
| 1 | 160-A | 132 | ASP | CB-CG-OD1 | 5.73 | 123.46 | 118.30 |
| 1 | 69-A | 159 | ARG | NE-CZ-NH1 | 5.72 | 123.16 | 120.30 |
| 1 | 117-A | 12 | ARG | NE-CZ-NH1 | 5.72 | 123.16 | 120.30 |
| 1 | 41-A | 22 | TRP | N-CA-C | -5.72 | 95.55 | 111.00 |
| 1 | 157-A | 110 | LEU | CA-CB-CG | 5.72 | 128.45 | 115.30 |
| 1 | 157-A | 36 | LEU | CB-CG-CD2 | 5.72 | 120.72 | 111.00 |
| 1 | 152-A | 129 | GLU | C-N-CA | -5.71 | 98.01 | 122.00 |
| 1 | 42-A | 158 | ARG | NE-CZ-NH1 | 5.70 | 123.15 | 120.30 |
| 1 | 40-A | 158 | ARG | CG-CD-NE | 5.70 | 123.77 | 111.80 |
| 1 | 147-A | 16 | MET | CG-SD-CE | 5.70 | 109.32 | 100.20 |
| 1 | 105-A | 20 | MET | CG-SD-CE | -5.69 | 91.09 | 100.20 |
| 1 | 149-A | 86 | GLY | N-CA-C | 5.69 | 127.33 | 113.10 |
| 1 | 162-A | 98 | ARG | NE-CZ-NH1 | 5.69 | 123.15 | 120.30 |
| 1 | 39-A | 17 | GLU | CB-CA-C | 5.68 | 121.77 | 110.40 |
| 1 | 58-A | 131 | ASP | CB-CG-OD2 | -5.68 | 113.18 | 118.30 |
| 1 | 140-A | 131 | ASP | CB-CG-OD1 | 5.68 | 123.42 | 118.30 |
| 1 | 141-A | 44 | ARG | NE-CZ-NH1 | 5.68 | 123.14 | 120.30 |
| 1 | 144-A | 16 | MET | N-CA-CB | 5.68 | 120.82 | 110.60 |
| 1 | 165-A | 69 | ASP | N-CA-C | -5.68 | 95.66 | 111.00 |
| 1 | 87-A | 126 | PRO | N-CA-C | 5.68 | 126.86 | 112.10 |
| 1 | 136-A | 87 | ASP | CB-CA-C | 5.68 | 121.75 | 110.40 |
| 1 | 38-A | 12 | ARG | NE-CZ-NH2 | -5.67 | 117.46 | 120.30 |
| 1 | 46-A | 16 | MET | N-CA-CB | 5.67 | 120.81 | 110.60 |
| 1 | 132-A | 52 | ARG | N-CA-C | -5.67 | 95.68 | 111.00 |
| 1 | 71-A | 152 | CYS | CA-CB-SG | 5.67 | 124.21 | 114.00 |
| 1 | 157-A | 85 | CYS | N-CA-C | 5.67 | 126.31 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 18-A | 4 | LEU | CB-CG-CD2 | 5.67 | 120.64 | 111.00 |
| 1 | 114-A | 20 | MET | CA-CB-CG | 5.67 | 122.94 | 113.30 |
| 1 | 27-A | 61 | ILE | CG1-CB-CG2 | -5.66 | 98.94 | 111.40 |
| 1 | 13-A | 98 | ARG | NE-CZ-NH2 | -5.66 | 117.47 | 120.30 |
| 1 | 61-A | 20 | MET | CB-CG-SD | -5.66 | 95.43 | 112.40 |
| 1 | 83-A | 159 | ARG | NE-CZ-NH1 | 5.65 | 123.13 | 120.30 |
| 1 | 154-A | 87 | ASP | CB-CA-C | 5.65 | 121.70 | 110.40 |
| 1 | 161-A | 12 | ARG | NE-CZ-NH2 | -5.65 | 117.47 | 120.30 |
| 1 | 5-A | 129 | GLU | C-N-CA | 5.65 | 145.73 | 122.00 |
| 1 | 35-A | 19 | ALA | N-CA-C | 5.65 | 126.25 | 111.00 |
| 1 | 26-A | 4 | LEU | CB-CG-CD2 | 5.65 | 120.60 | 111.00 |
| 1 | 69-A | 22 | TRP | CA-CB-CG | 5.65 | 124.43 | 113.70 |
| 1 | 14-A | 131 | ASP | CB-CG-OD2 | -5.64 | 113.22 | 118.30 |
| 1 | 78-A | 16 | MET | CG-SD-CE | 5.64 | 109.23 | 100.20 |
| 1 | 29-A | 50 | ILE | N-CA-CB | 5.64 | 123.78 | 110.80 |
| 1 | 113-A | 16 | MET | CB-CG-SD | 5.64 | 129.32 | 112.40 |
| 1 | 167-A | 129 | GLU | C-N-CD | -5.64 | 108.19 | 120.60 |
| 1 | 143-A | 44 | ARG | NE-CZ-NH1 | 5.64 | 123.12 | 120.30 |
| 1 | 52-A | 33 | ARG | NE-CZ-NH1 | 5.64 | 123.12 | 120.30 |
| 1 | 65-A | 98 | ARG | CD-NE-CZ | 5.64 | 131.49 | 123.60 |
| 1 | 84-A | 129 | GLU | C-N-CD | 5.64 | 140.24 | 128.40 |
| 1 | 161-A | 98 | ARG | NE-CZ-NH1 | 5.63 | 123.12 | 120.30 |
| 1 | 77-A | 33 | ARG | NE-CZ-NH2 | -5.63 | 117.48 | 120.30 |
| 1 | 49-A | 88 | VAL | N-CA-CB | 5.63 | 123.89 | 111.50 |
| 1 | 146-A | 20 | MET | C-N-CD | -5.63 | 108.21 | 120.60 |
| 1 | 28-A | 159 | ARG | NE-CZ-NH2 | 5.63 | 123.11 | 120.30 |
| 1 | 84-A | 128 | TYR | CA-CB-CG | 5.62 | 124.09 | 113.40 |
| 1 | 149-A | 130 | PRO | N-CA-C | -5.62 | 97.47 | 112.10 |
| 1 | 152-A | 85 | CYS | N-CA-CB | 5.62 | 120.72 | 110.60 |
| 1 | 73-A | 20 | MET | C-N-CD | -5.62 | 108.23 | 120.60 |
| 1 | 71-A | 1 | MET | CG-SD-CE | 5.62 | 109.19 | 100.20 |
| 1 | 45-A | 131 | ASP | CB-CG-OD2 | -5.62 | 113.24 | 118.30 |
| 1 | 100-A | 159 | ARG | NE-CZ-NH2 | -5.62 | 117.49 | 120.30 |
| 1 | 167-A | 156 | LEU | CA-CB-CG | -5.62 | 102.38 | 115.30 |
| 1 | 108-A | 16 | MET | CA-CB-CG | 5.62 | 122.85 | 113.30 |
| 1 | 111-A | 104 | LEU | CB-CG-CD2 | 5.62 | 120.55 | 111.00 |
| 1 | 31-A | 130 | PRO | O-C-N | 5.61 | 131.68 | 122.70 |
| 1 | 53-A | 36 | LEU | CB-CG-CD2 | -5.61 | 101.46 | 111.00 |
| 1 | 111-A | 159 | ARG | NE-CZ-NH2 | -5.61 | 117.49 | 120.30 |
| 1 | 164-A | 131 | ASP | CB-CG-OD1 | -5.61 | 113.25 | 118.30 |
| 1 | 20-A | 4 | LEU | CB-CG-CD2 | -5.61 | 101.47 | 111.00 |
| 1 | 91-A | 38 | LYS | CD-CE-NZ | 5.61 | 124.60 | 111.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 166-A | 98 | ARG | CG-CD-NE | 5.61 | 123.58 | 111.80 |
| 1 | 61-A | 129 | GLU | C-N-CD | -5.61 | 108.27 | 120.60 |
| 1 | 59-A | 52 | ARG | NE-CZ-NH1 | 5.60 | 123.10 | 120.30 |
| 1 | 158-A | 129 | GLU | N-CA-CB | 5.60 | 120.68 | 110.60 |
| 1 | 73-A | 101 | GLU | OE1-CD-OE2 | -5.60 | 116.58 | 123.30 |
| 1 | 138-A | 11 | ASP | CB-CG-OD1 | -5.60 | 113.26 | 118.30 |
| 1 | 81-A | 33 | ARG | NE-CZ-NH1 | 5.60 | 123.10 | 120.30 |
| 1 | 33-A | 158 | ARG | NE-CZ-NH2 | -5.59 | 117.50 | 120.30 |
| 1 | 166-A | 158 | ARG | NE-CZ-NH1 | 5.59 | 123.10 | 120.30 |
| 1 | 115-A | 20 | MET | N-CA-C | -5.59 | 95.90 | 111.00 |
| 1 | 2-A | 159 | ARG | CG-CD-NE | 5.59 | 123.54 | 111.80 |
| 1 | 58-A | 156 | LEU | CB-CG-CD1 | 5.59 | 120.50 | 111.00 |
| 1 | 137-A | 18 | ASN | CB-CA-C | -5.59 | 99.22 | 110.40 |
| 1 | 62-A | 16 | MET | CB-CG-SD | -5.59 | 95.64 | 112.40 |
| 1 | 87-A | 4 | LEU | CB-CG-CD2 | -5.58 | 101.50 | 111.00 |
| 1 | 112-A | 33 | ARG | NE-CZ-NH2 | -5.58 | 117.51 | 120.30 |
| 1 | 57-A | 127 | ASP | CB-CG-OD1 | -5.58 | 113.28 | 118.30 |
| 1 | 157-A | 98 | ARG | NE-CZ-NH1 | -5.58 | 117.51 | 120.30 |
| 1 | 105-A | 1 | MET | CB-CG-SD | -5.57 | 95.68 | 112.40 |
| 1 | 40-A | 142 | ASP | CB-CG-OD1 | -5.57 | 113.29 | 118.30 |
| 1 | 73-A | 65 | GLN | C-N-CD | -5.57 | 108.35 | 120.60 |
| 1 | 114-A | 98 | ARG | NE-CZ-NH2 | -5.57 | 117.52 | 120.30 |
| 1 | 167-A | 4 | LEU | CB-CG-CD2 | 5.57 | 120.46 | 111.00 |
| 1 | 1-A | 132 | ASP | CB-CG-OD2 | 5.57 | 123.31 | 118.30 |
| 1 | 42-A | 98 | ARG | NE-CZ-NH2 | 5.57 | 123.08 | 120.30 |
| 1 | 3-A | 128 | TYR | CA-CB-CG | 5.56 | 123.96 | 113.40 |
| 1 | 57-A | 44 | ARG | NE-CZ-NH1 | 5.55 | 123.08 | 120.30 |
| 1 | 7-A | 121 | GLY | N-CA-C | 5.55 | 126.98 | 113.10 |
| 1 | 37-A | 131 | ASP | CB-CG-OD1 | 5.55 | 123.30 | 118.30 |
| 1 | 163-A | 129 | GLU | N-CA-C | -5.55 | 96.01 | 111.00 |
| 1 | 106-A | 98 | ARG | NE-CZ-NH1 | -5.55 | 117.53 | 120.30 |
| 1 | 159-A | 52 | ARG | NE-CZ-NH2 | -5.55 | 117.53 | 120.30 |
| 1 | 62-A | 106 | LYS | CB-CA-C | 5.55 | 121.49 | 110.40 |
| 1 | 159-A | 64 | SER | N-CA-C | 5.54 | 125.97 | 111.00 |
| 1 | 94-A | 104 | LEU | CB-CG-CD1 | 5.54 | 120.42 | 111.00 |
| 1 | 98-A | 159 | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 1 | 143-A | 16 | MET | N-CA-C | 5.54 | 125.95 | 111.00 |
| 1 | 48-A | 36 | LEU | CA-CB-CG | 5.53 | 128.03 | 115.30 |
| 1 | 33-A | 119 | VAL | N-CA-C | 5.53 | 125.93 | 111.00 |
| 1 | 160-A | 44 | ARG | NE-CZ-NH1 | 5.53 | 123.06 | 120.30 |
| 1 | 43-A | 88 | VAL | C-N-CD | -5.52 | 108.45 | 120.60 |
| 1 | 146-A | 16 | MET | CB-CA-C | 5.52 | 121.44 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 63-A | 16 | MET | CA-CB-CG | 5.52 | 122.69 | 113.30 |
| 1 | 166-A | 159 | ARG | NE-CZ-NH1 | 5.52 | 123.06 | 120.30 |
| 1 | 44-A | 152 | CYS | CA-CB-SG | 5.52 | 123.93 | 114.00 |
| 1 | 79-A | 12 | ARG | CA-CB-CG | 5.51 | 125.53 | 113.40 |
| 1 | 81-A | 158 | ARG | NE-CZ-NH1 | 5.51 | 123.06 | 120.30 |
| 1 | 139-A | 152 | CYS | CA-CB-SG | -5.51 | 104.08 | 114.00 |
| 1 | 155-A | 85 | CYS | N-CA-CB | 5.51 | 120.52 | 110.60 |
| 1 | 34-A | 44 | ARG | NE-CZ-NH2 | -5.51 | 117.55 | 120.30 |
| 1 | 133-A | 119 | VAL | CB-CA-C | -5.51 | 100.94 | 111.40 |
| 1 | 109-A | 16 | MET | C-N-CA | -5.50 | 107.94 | 121.70 |
| 1 | 158-A | 85 | CYS | N-CA-CB | -5.50 | 100.69 | 110.60 |
| 1 | 51-A | 12 | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 1 | 65-A | 33 | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 1 | 4-A | 44 | ARG | NE-CZ-NH1 | 5.50 | 123.05 | 120.30 |
| 1 | 29-A | 20 | MET | CB-CG-SD | 5.50 | 128.90 | 112.40 |
| 1 | 162-A | 130 | PRO | N-CA-C | 5.50 | 126.40 | 112.10 |
| 1 | 9-A | 21 | PRO | CA-N-CD | -5.50 | 103.80 | 111.50 |
| 1 | 151-A | 85 | CYS | CB-CA-C | 5.50 | 121.39 | 110.40 |
| 1 | 42-A | 4 | LEU | CB-CG-CD2 | 5.49 | 120.33 | 111.00 |
| 1 | 42-A | 33 | ARG | CB-CA-C | 5.49 | 121.38 | 110.40 |
| 1 | 60-A | 98 | ARG | CG-CD-NE | 5.49 | 123.33 | 111.80 |
| 1 | 139-A | 129 | GLU | N-CA-C | 5.49 | 125.83 | 111.00 |
| 1 | 165-A | 132 | ASP | CB-CG-OD2 | -5.49 | 113.36 | 118.30 |
| 1 | 137-A | 13 | VAL | CB-CA-C | -5.49 | 100.97 | 111.40 |
| 1 | 144-A | 20 | MET | CB-CG-SD | -5.49 | 95.94 | 112.40 |
| 1 | 8-A | 33 | ARG | CB-CG-CD | 5.49 | 125.86 | 111.60 |
| 1 | 77-A | 28 | LEU | CA-CB-CG | -5.49 | 102.69 | 115.30 |
| 1 | 59-A | 87 | ASP | CB-CG-OD1 | -5.48 | 113.36 | 118.30 |
| 1 | 137-A | 13 | VAL | N-CA-CB | 5.48 | 123.56 | 111.50 |
| 1 | 68-A | 52 | ARG | NE-CZ-NH2 | -5.48 | 117.56 | 120.30 |
| 1 | 57-A | 159 | ARG | CD-NE-CZ | 5.48 | 131.27 | 123.60 |
| 1 | 68-A | 33 | ARG | NE-CZ-NH1 | 5.48 | 123.04 | 120.30 |
| 1 | 140-A | 1 | MET | CB-CG-SD | 5.48 | 128.83 | 112.40 |
| 1 | 71-A | 22 | TRP | N-CA-CB | 5.48 | 120.46 | 110.60 |
| 1 | 27-A | 20 | MET | N-CA-C | 5.47 | 125.78 | 111.00 |
| 1 | 93-A | 36 | LEU | CB-CG-CD1 | 5.47 | 120.30 | 111.00 |
| 1 | 114-A | 16 | MET | CG-SD-CE | 5.47 | 108.96 | 100.20 |
| 1 | 111-A | 44 | ARG | NE-CZ-NH1 | 5.46 | 123.03 | 120.30 |
| 1 | 120-A | 16 | MET | CB-CG-SD | 5.46 | 128.78 | 112.40 |
| 1 | 85-A | 101 | GLU | CB-CA-C | -5.45 | 99.49 | 110.40 |
| 1 | 129-A | 152 | CYS | CA-CB-SG | 5.45 | 123.81 | 114.00 |
| 1 | 44-A | 20 | MET | CG-SD-CE | 5.44 | 108.91 | 100.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 164-A | 158 | ARG | NE-CZ-NH1 | 5.44 | 123.02 | 120.30 |
| 1 | 91-A | 33 | ARG | NE-CZ-NH2 | -5.44 | 117.58 | 120.30 |
| 1 | 97-A | 22 | TRP | N-CA-C | -5.44 | 96.32 | 111.00 |
| 1 | 71-A | 67 | GLY | N-CA-C | 5.43 | 126.69 | 113.10 |
| 1 | 151-A | 33 | ARG | NE-CZ-NH2 | -5.43 | 117.58 | 120.30 |
| 1 | 157-A | 159 | ARG | NE-CZ-NH1 | 5.43 | 123.02 | 120.30 |
| 1 | 123-A | 1 | MET | CG-SD-CE | -5.43 | 91.51 | 100.20 |
| 1 | 88-A | 129 | GLU | C-N-CA | -5.43 | 99.21 | 122.00 |
| 1 | 99-A | 12 | ARG | NE-CZ-NH2 | -5.43 | 117.59 | 120.30 |
| 1 | 30-A | 1 | MET | CA-CB-CG | 5.42 | 122.52 | 113.30 |
| 1 | 83-A | 127 | ASP | CB-CG-OD2 | 5.42 | 123.18 | 118.30 |
| 1 | 99-A | 1 | MET | CG-SD-CE | 5.42 | 108.87 | 100.20 |
| 1 | 161-A | 12 | ARG | NE-CZ-NH1 | 5.42 | 123.01 | 120.30 |
| 1 | 163-A | 128 | TYR | N-CA-C | -5.42 | 96.37 | 111.00 |
| 1 | 71-A | 154 | GLU | OE1-CD-OE2 | -5.42 | 116.80 | 123.30 |
| 1 | 17-A | 1 | MET | CG-SD-CE | -5.41 | 91.54 | 100.20 |
| 1 | 34-A | 12 | ARG | NE-CZ-NH2 | -5.41 | 117.59 | 120.30 |
| 1 | 36-A | 79 | ASP | CB-CG-OD2 | -5.41 | 113.43 | 118.30 |
| 1 | 105-A | 152 | CYS | N-CA-CB | -5.41 | 100.87 | 110.60 |
| 1 | 36-A | 79 | ASP | CB-CG-OD1 | 5.40 | 123.16 | 118.30 |
| 1 | 54-A | 1 | MET | CG-SD-CE | -5.40 | 91.56 | 100.20 |
| 1 | 3-A | 156 | LEU | CA-CB-CG | 5.40 | 127.71 | 115.30 |
| 1 | 34-A | 85 | CYS | N-CA-C | 5.39 | 125.56 | 111.00 |
| 1 | 161-A | 135 | SER | CB-CA-C | -5.39 | 99.86 | 110.10 |
| 1 | 142-A | 120 | GLU | CB-CA-C | 5.38 | 121.17 | 110.40 |
| 1 | 112-A | 44 | ARG | NE-CZ-NH1 | 5.38 | 122.99 | 120.30 |
| 1 | 155-A | 85 | CYS | CB-CA-C | -5.38 | 99.64 | 110.40 |
| 1 | 35-A | 132 | ASP | CB-CG-OD2 | -5.38 | 113.46 | 118.30 |
| 1 | 130-A | 44 | ARG | NE-CZ-NH2 | -5.38 | 117.61 | 120.30 |
| 1 | 114-A | 127 | ASP | N-CA-C | 5.38 | 125.52 | 111.00 |
| 1 | 11-A | 16 | MET | CA-CB-CG | 5.37 | 122.43 | 113.30 |
| 1 | 145-A | 132 | ASP | CB-CG-OD2 | 5.37 | 123.14 | 118.30 |
| 1 | 107-A | 16 | MET | C-N-CA | -5.37 | 108.28 | 121.70 |
| 1 | 69-A | 20 | MET | C-N-CA | 5.37 | 144.54 | 122.00 |
| 1 | 8-A | 128 | TYR | CA-CB-CG | 5.37 | 123.60 | 113.40 |
| 1 | 81-A | 127 | ASP | CB-CG-OD1 | 5.37 | 123.13 | 118.30 |
| 1 | 85-A | 44 | ARG | NE-CZ-NH2 | -5.37 | 117.62 | 120.30 |
| 1 | 38-A | 142 | ASP | CB-CG-OD2 | -5.37 | 113.47 | 118.30 |
| 1 | 65-A | 119 | VAL | N-CA-C | -5.37 | 96.51 | 111.00 |
| 1 | 40-A | 20 | MET | CG-SD-CE | 5.36 | 108.78 | 100.20 |
| 1 | 49-A | 88 | VAL | CA-CB-CG2 | 5.36 | 118.94 | 110.90 |
| 1 | 144-A | 128 | TYR | C-N-CA | 5.36 | 135.10 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 116-A | 12 | ARG | NE-CZ-NH2 | -5.35 | 117.62 | 120.30 |
| 1 | 147-A | 20 | MET | CG-SD-CE | -5.35 | 91.64 | 100.20 |
| 1 | 149-A | 159 | ARG | NE-CZ-NH1 | 5.35 | 122.97 | 120.30 |
| 1 | 48-A | 88 | VAL | N-CA-C | -5.34 | 96.58 | 111.00 |
| 1 | 32-A | 88 | VAL | C-N-CD | 5.34 | 139.61 | 128.40 |
| 1 | 8-A | 142 | ASP | CB-CG-OD1 | 5.34 | 123.10 | 118.30 |
| 1 | 106-A | 20 | MET | N-CA-C | 5.34 | 125.41 | 111.00 |
| 1 | 122-A | 12 | ARG | CG-CD-NE | -5.34 | 100.59 | 111.80 |
| 1 | 7-A | 79 | ASP | CB-CA-C | 5.33 | 121.06 | 110.40 |
| 1 | 72-A | 79 | ASP | CB-CG-OD1 | 5.33 | 123.10 | 118.30 |
| 1 | 163-A | 79 | ASP | CB-CG-OD1 | 5.33 | 123.10 | 118.30 |
| 1 | 56-A | 20 | MET | CG-SD-CE | 5.33 | 108.73 | 100.20 |
| 1 | 132-A | 12 | ARG | NE-CZ-NH2 | -5.33 | 117.63 | 120.30 |
| 1 | 81-A | 131 | ASP | N-CA-C | 5.33 | 125.39 | 111.00 |
| 1 | 1-A | 157 | GLU | OE1-CD-OE2 | -5.33 | 116.91 | 123.30 |
| 1 | 73-A | 98 | ARG | NE-CZ-NH2 | -5.33 | 117.64 | 120.30 |
| 1 | 120-A | 20 | MET | CA-CB-CG | 5.33 | 122.36 | 113.30 |
| 1 | 35-A | 106 | LYS | CD-CE-NZ | 5.33 | 123.95 | 111.70 |
| 1 | 13-A | 104 | LEU | CB-CG-CD2 | 5.32 | 120.05 | 111.00 |
| 1 | 34-A | 16 | MET | CB-CG-SD | 5.32 | 128.37 | 112.40 |
| 1 | 163-A | 129 | GLU | OE1-CD-OE2 | -5.32 | 116.92 | 123.30 |
| 1 | 164-A | 132 | ASP | N-CA-C | 5.32 | 125.36 | 111.00 |
| 1 | 155-A | 1 | MET | CG-SD-CE | -5.31 | 91.70 | 100.20 |
| 1 | 111-A | 2 | ILE | N-CA-C | -5.31 | 96.65 | 111.00 |
| 1 | 39-A | 52 | ARG | NE-CZ-NH1 | 5.31 | 122.95 | 120.30 |
| 1 | 129-A | 20 | MET | CA-CB-CG | 5.31 | 122.33 | 113.30 |
| 1 | 132-A | 16 | MET | CG-SD-CE | -5.31 | 91.70 | 100.20 |
| 1 | 77-A | 52 | ARG | NE-CZ-NH1 | 5.31 | 122.95 | 120.30 |
| 1 | 151-A | 52 | ARG | NE-CZ-NH2 | -5.30 | 117.65 | 120.30 |
| 1 | 26-A | 12 | ARG | NE-CZ-NH2 | -5.30 | 117.65 | 120.30 |
| 1 | 167-A | 68 | THR | N-CA-C | 5.30 | 125.31 | 111.00 |
| 1 | 154-A | 127 | ASP | N-CA-C | 5.29 | 125.30 | 111.00 |
| 1 | 22-A | 17 | GLU | CB-CA-C | 5.29 | 120.98 | 110.40 |
| 1 | 6-A | 52 | ARG | NE-CZ-NH2 | -5.29 | 117.65 | 120.30 |
| 1 | 155-A | 118 | GLU | CB-CA-C | -5.29 | 99.82 | 110.40 |
| 1 | 43-A | 87 | ASP | CB-CA-C | -5.28 | 99.83 | 110.40 |
| 1 | 78-A | 98 | ARG | CG-CD-NE | 5.28 | 122.90 | 111.80 |
| 1 | 42-A | 158 | ARG | NE-CZ-NH2 | -5.28 | 117.66 | 120.30 |
| 1 | 103-A | 16 | MET | N-CA-C | -5.28 | 96.74 | 111.00 |
| 1 | 158-A | 52 | ARG | NE-CZ-NH2 | -5.27 | 117.66 | 120.30 |
| 1 | 66-A | 118 | GLU | N-CA-C | -5.27 | 96.77 | 111.00 |
| 1 | 85-A | 159 | ARG | CG-CD-NE | -5.27 | 100.73 | 111.80 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 35-A | 142 | ASP | CB-CG-OD1 | 5.27 | 123.04 | 118.30 |
| 1 | 121-A | 20 | MET | CG-SD-CE | -5.27 | 91.77 | 100.20 |
| 1 | 84-A | 104 | LEU | CB-CG-CD1 | 5.27 | 119.95 | 111.00 |
| 1 | 57-A | 79 | ASP | CB-CG-OD2 | 5.26 | 123.04 | 118.30 |
| 1 | 117-A | 18 | ASN | N-CA-C | -5.26 | 96.79 | 111.00 |
| 1 | 144-A | 18 | ASN | CB-CA-C | -5.26 | 99.87 | 110.40 |
| 1 | 152-A | 136 | VAL | CB-CA-C | 5.26 | 121.40 | 111.40 |
| 1 | 116-A | 17 | GLU | N-CA-C | -5.26 | 96.79 | 111.00 |
| 1 | 43-A | 133 | TRP | CB-CA-C | -5.26 | 99.88 | 110.40 |
| 1 | 58-A | 79 | ASP | CB-CG-OD1 | -5.26 | 113.57 | 118.30 |
| 1 | 101-A | 54 | LEU | CA-CB-CG | 5.26 | 127.39 | 115.30 |
| 1 | 118-A | 16 | MET | CA-CB-CG | 5.26 | 122.24 | 113.30 |
| 1 | 38-A | 11 | ASP | CB-CG-OD1 | -5.25 | 113.57 | 118.30 |
| 1 | 27-A | 20 | MET | CB-CG-SD | 5.25 | 128.16 | 112.40 |
| 1 | 74-A | 19 | ALA | N-CA-C | -5.25 | 96.83 | 111.00 |
| 1 | 158-A | 63 | SER | CB-CA-C | -5.25 | 100.13 | 110.10 |
| 1 | 167-A | 33 | ARG | NE-CZ-NH1 | 5.25 | 122.92 | 120.30 |
| 1 | 38-A | 44 | ARG | NE-CZ-NH1 | 5.25 | 122.92 | 120.30 |
| 1 | 66-A | 98 | ARG | CG-CD-NE | 5.25 | 122.82 | 111.80 |
| 1 | 53-A | 159 | ARG | NE-CZ-NH2 | 5.24 | 122.92 | 120.30 |
| 1 | 97-A | 98 | ARG | NE-CZ-NH1 | 5.24 | 122.92 | 120.30 |
| 1 | 21-A | 131 | ASP | CB-CG-OD2 | -5.24 | 113.58 | 118.30 |
| 1 | 142-A | 131 | ASP | N-CA-C | 5.24 | 125.15 | 111.00 |
| 1 | 53-A | 98 | ARG | NE-CZ-NH1 | 5.23 | 122.92 | 120.30 |
| 1 | 57-A | 159 | ARG | NE-CZ-NH2 | -5.23 | 117.68 | 120.30 |
| 1 | 97-A | 1 | MET | N-CA-C | -5.23 | 96.87 | 111.00 |
| 1 | 25-A | 87 | ASP | N-CA-C | -5.23 | 96.88 | 111.00 |
| 1 | 92-A | 44 | ARG | NE-CZ-NH1 | 5.23 | 122.91 | 120.30 |
| 1 | 79-A | 131 | ASP | CB-CG-OD1 | 5.23 | 123.00 | 118.30 |
| 1 | 26-A | 12 | ARG | NE-CZ-NH1 | 5.22 | 122.91 | 120.30 |
| 1 | 64-A | 127 | ASP | CB-CG-OD2 | 5.22 | 123.00 | 118.30 |
| 1 | 43-A | 1 | MET | CG-SD-CE | 5.22 | 108.55 | 100.20 |
| 1 | 53-A | 128 | TYR | CA-CB-CG | 5.22 | 123.31 | 113.40 |
| 1 | 150-A | 137 | PHE | N-CA-C | 5.22 | 125.09 | 111.00 |
| 1 | 7-A | 129 | GLU | OE1-CD-OE2 | 5.21 | 129.56 | 123.30 |
| 1 | 90-A | 129 | GLU | N-CA-C | 5.21 | 125.08 | 111.00 |
| 1 | 89-A | 119 | VAL | N-CA-C | 5.21 | 125.08 | 111.00 |
| 1 | 62-A | 32 | LYS | CD-CE-NZ | 5.21 | 123.69 | 111.70 |
| 1 | 67-A | 152 | CYS | CA-CB-SG | 5.21 | 123.38 | 114.00 |
| 1 | 7-A | 79 | ASP | N-CA-CB | -5.21 | 101.23 | 110.60 |
| 1 | 43-A | 1 | MET | CA-CB-CG | 5.21 | 122.15 | 113.30 |
| 1 | 36-A | 20 | MET | N-CA-C | 5.21 | 125.05 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 24-A | 17 | GLU | CB-CA-C | 5.20 | 120.80 | 110.40 |
| 1 | 76-A | 16 | MET | CA-CB-CG | 5.20 | 122.14 | 113.30 |
| 1 | 4-A | 17 | GLU | N-CA-C | -5.20 | 96.96 | 111.00 |
| 1 | 61-A | 62 | LEU | CA-CB-CG | 5.20 | 127.26 | 115.30 |
| 1 | 126-A | 4 | LEU | CB-CG-CD2 | 5.20 | 119.84 | 111.00 |
| 1 | 60-A | 98 | ARG | NE-CZ-NH2 | 5.20 | 122.90 | 120.30 |
| 1 | 104-A | 52 | ARG | NE-CZ-NH2 | -5.20 | 117.70 | 120.30 |
| 1 | 36-A | 69 | ASP | N-CA-C | -5.19 | 96.98 | 111.00 |
| 1 | 127-A | 33 | ARG | CG-CD-NE | 5.19 | 122.70 | 111.80 |
| 1 | 88-A | 142 | ASP | CB-CA-C | -5.19 | 100.03 | 110.40 |
| 1 | 94-A | 1 | MET | CA-CB-CG | 5.18 | 122.11 | 113.30 |
| 1 | 143-A | 86 | GLY | N-CA-C | -5.18 | 100.15 | 113.10 |
| 1 | 80-A | 109 | LYS | CD-CE-NZ | 5.18 | 123.61 | 111.70 |
| 1 | 123-A | 128 | TYR | CA-CB-CG | 5.18 | 123.24 | 113.40 |
| 1 | 56-A | 133 | TRP | CB-CA-C | -5.17 | 100.06 | 110.40 |
| 1 | 28-A | 52 | ARG | CA-CB-CG | 5.17 | 124.77 | 113.40 |
| 1 | 34-A | 142 | ASP | CB-CG-OD1 | 5.17 | 122.95 | 118.30 |
| 1 | 47-A | 88 | VAL | C-N-CD | 5.17 | 139.25 | 128.40 |
| 1 | 38-A | 127 | ASP | CB-CG-OD2 | -5.17 | 113.65 | 118.30 |
| 1 | 101-A | 8 | LEU | CA-CB-CG | 5.16 | 127.17 | 115.30 |
| 1 | 153-A | 52 | ARG | CG-CD-NE | 5.16 | 122.62 | 111.80 |
| 1 | 6-A | 152 | CYS | CA-CB-SG | 5.15 | 123.28 | 114.00 |
| 1 | 160-A | 131 | ASP | CB-CG-OD2 | -5.15 | 113.66 | 118.30 |
| 1 | 20-A | 44 | ARG | NE-CZ-NH1 | 5.15 | 122.88 | 120.30 |
| 1 | 78-A | 12 | ARG | CA-CB-CG | 5.15 | 124.73 | 113.40 |
| 1 | 11-A | 156 | LEU | CB-CG-CD1 | 5.15 | 119.75 | 111.00 |
| 1 | 76-A | 127 | ASP | N-CA-CB | -5.15 | 101.34 | 110.60 |
| 1 | 142-A | 42 | MET | CG-SD-CE | 5.15 | 108.44 | 100.20 |
| 1 | 157-A | 33 | ARG | NE-CZ-NH1 | 5.15 | 122.87 | 120.30 |
| 1 | 81-A | 127 | ASP | N-CA-C | 5.15 | 124.89 | 111.00 |
| 1 | 68-A | 20 | MET | N-CA-C | 5.14 | 124.89 | 111.00 |
| 1 | 100-A | 44 | ARG | NE-CZ-NH1 | 5.14 | 122.87 | 120.30 |
| 1 | 30-A | 131 | ASP | CB-CG-OD1 | 5.14 | 122.93 | 118.30 |
| 1 | 81-A | 104 | LEU | CB-CG-CD2 | 5.14 | 119.74 | 111.00 |
| 1 | 49-A | 120 | GLU | CB-CA-C | -5.14 | 100.12 | 110.40 |
| 1 | 20-A | 20 | MET | CA-CB-CG | 5.14 | 122.03 | 113.30 |
| 1 | 22-A | 132 | ASP | CB-CG-OD2 | 5.14 | 122.92 | 118.30 |
| 1 | 69-A | 17 | GLU | CA-CB-CG | 5.14 | 124.70 | 113.40 |
| 1 | 151-A | 85 | CYS | CA-CB-SG | -5.14 | 104.75 | 114.00 |
| 1 | 156-A | 44 | ARG | NE-CZ-NH1 | 5.13 | 122.87 | 120.30 |
| 1 | 145-A | 112 | LEU | CB-CG-CD2 | 5.13 | 119.73 | 111.00 |
| 1 | 28-A | 19 | ALA | C-N-CA | 5.13 | 134.53 | 121.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 99-A | 12 | ARG | NE-CZ-NH1 | 5.13 | 122.86 | 120.30 |
| 1 | 133-A | 127 | ASP | N-CA-C | 5.13 | 124.85 | 111.00 |
| 1 | 58-A | 152 | CYS | CA-CB-SG | 5.13 | 123.23 | 114.00 |
| 1 | 159-A | 52 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 1 | 68-A | 21 | PRO | N-CA-C | 5.12 | 125.42 | 112.10 |
| 1 | 115-A | 129 | GLU | N-CA-CB | 5.12 | 119.82 | 110.60 |
| 1 | 69-A | 135 | SER | CB-CA-C | -5.12 | 100.37 | 110.10 |
| 1 | 104-A | 108 | GLN | CA-CB-CG | 5.12 | 124.66 | 113.40 |
| 1 | 145-A | 8 | LEU | CA-CB-CG | 5.12 | 127.08 | 115.30 |
| 1 | 153-A | 159 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 1 | 42-A | 1 | MET | CA-CB-CG | 5.12 | 122.00 | 113.30 |
| 1 | 83-A | 2 | ILE | CA-CB-CG1 | -5.12 | 101.28 | 111.00 |
| 1 | 72-A | 156 | LEU | CA-CB-CG | 5.11 | 127.06 | 115.30 |
| 1 | 20-A | 20 | MET | CG-SD-CE | 5.11 | 108.38 | 100.20 |
| 1 | 1-A | 131 | ASP | CB-CG-OD1 | 5.11 | 122.90 | 118.30 |
| 1 | 120-A | 98 | ARG | NE-CZ-NH1 | -5.11 | 117.75 | 120.30 |
| 1 | 141-A | 36 | LEU | CB-CG-CD2 | -5.11 | 102.31 | 111.00 |
| 1 | 141-A | 131 | ASP | N-CA-C | 5.11 | 124.79 | 111.00 |
| 1 | 73-A | 8 | LEU | CA-CB-CG | 5.11 | 127.05 | 115.30 |
| 1 | 80-A | 125 | PHE | C-N-CD | -5.11 | 109.37 | 120.60 |
| 1 | 58-A | 131 | ASP | CB-CG-OD1 | 5.10 | 122.89 | 118.30 |
| 1 | 37-A | 20 | MET | N-CA-C | 5.10 | 124.78 | 111.00 |
| 1 | 131-A | 44 | ARG | NE-CZ-NH1 | 5.10 | 122.85 | 120.30 |
| 1 | 151-A | 129 | GLU | C-N-CA | -5.10 | 100.57 | 122.00 |
| 1 | 39-A | 44 | ARG | NE-CZ-NH1 | 5.10 | 122.85 | 120.30 |
| 1 | 76-A | 20 | MET | CG-SD-CE | -5.10 | 92.04 | 100.20 |
| 1 | 4-A | 52 | ARG | NE-CZ-NH1 | 5.10 | 122.85 | 120.30 |
| 1 | 52-A | 159 | ARG | NE-CZ-NH2 | -5.09 | 117.75 | 120.30 |
| 1 | 102-A | 159 | ARG | NE-CZ-NH1 | 5.09 | 122.85 | 120.30 |
| 1 | 100-A | 159 | ARG | NE-CZ-NH1 | 5.09 | 122.84 | 120.30 |
| 1 | 155-A | 159 | ARG | NE-CZ-NH2 | -5.09 | 117.75 | 120.30 |
| 1 | 116-A | 16 | MET | N-CA-C | 5.09 | 124.74 | 111.00 |
| 1 | 83-A | 11 | ASP | CB-CG-OD1 | 5.09 | 122.88 | 118.30 |
| 1 | 117-A | 4 | LEU | CB-CG-CD2 | -5.08 | 102.36 | 111.00 |
| 1 | 69-A | 50 | ILE | CB-CA-C | -5.08 | 101.43 | 111.60 |
| 1 | 92-A | 128 | TYR | CB-CA-C | 5.08 | 120.57 | 110.40 |
| 1 | 151-A | 4 | LEU | CB-CG-CD2 | -5.08 | 102.36 | 111.00 |
| 1 | 111-A | 18 | ASN | CB-CA-C | 5.08 | 120.56 | 110.40 |
| 1 | 113-A | 21 | PRO | CA-N-CD | -5.08 | 104.39 | 111.50 |
| 1 | 137-A | 128 | TYR | CB-CA-C | 5.08 | 120.55 | 110.40 |
| 1 | 100-A | 104 | LEU | CB-CG-CD2 | 5.07 | 119.62 | 111.00 |
| 1 | 135-A | 131 | ASP | CB-CG-OD1 | 5.07 | 122.86 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 8-A | 1 | MET | CG-SD-CE | -5.06 | 92.10 | 100.20 |
| 1 | 24-A | 127 | ASP | N-CA-C | -5.06 | 97.34 | 111.00 |
| 1 | 27-A | 19 | ALA | C-N-CA | 5.06 | 134.35 | 121.70 |
| 1 | 37-A | 159 | ARG | NE-CZ-NH2 | -5.06 | 117.77 | 120.30 |
| 1 | 38-A | 44 | ARG | NE-CZ-NH2 | -5.06 | 117.77 | 120.30 |
| 1 | 82-A | 36 | LEU | CB-CG-CD2 | -5.06 | 102.40 | 111.00 |
| 1 | 96-A | 159 | ARG | CG-CD-NE | 5.05 | 122.41 | 111.80 |
| 1 | 23-A | 52 | ARG | NE-CZ-NH1 | 5.05 | 122.83 | 120.30 |
| 1 | 32-A | 128 | TYR | N-CA-C | 5.05 | 124.63 | 111.00 |
| 1 | 139-A | 159 | ARG | NE-CZ-NH2 | -5.05 | 117.78 | 120.30 |
| 1 | 139-A | 36 | LEU | CA-CB-CG | 5.05 | 126.91 | 115.30 |
| 1 | 148-A | 159 | ARG | NE-CZ-NH2 | 5.04 | 122.82 | 120.30 |
| 1 | 74-A | 127 | ASP | CB-CG-OD2 | 5.04 | 122.84 | 118.30 |
| 1 | 98-A | 4 | LEU | CB-CG-CD2 | 5.04 | 119.57 | 111.00 |
| 1 | 33-A | 44 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 1 | 140-A | 132 | ASP | CB-CG-OD2 | 5.04 | 122.83 | 118.30 |
| 1 | 167-A | 132 | ASP | N-CA-C | 5.04 | 124.59 | 111.00 |
| 1 | 98-A | 98 | ARG | CB-CA-C | -5.03 | 100.34 | 110.40 |
| 1 | 140-A | 44 | ARG | NE-CZ-NH1 | 5.03 | 122.81 | 120.30 |
| 1 | 34-A | 50 | ILE | CG1-CB-CG2 | -5.03 | 100.34 | 111.40 |
| 1 | 22-A | 128 | TYR | CA-CB-CG | 5.03 | 122.95 | 113.40 |
| 1 | 115-A | 1 | MET | CB-CG-SD | -5.03 | 97.33 | 112.40 |
| 1 | 31-A | 12 | ARG | NE-CZ-NH1 | 5.02 | 122.81 | 120.30 |
| 1 | 121-A | 20 | MET | N-CA-CB | -5.02 | 101.56 | 110.60 |
| 1 | 130-A | 12 | ARG | NE-CZ-NH2 | -5.02 | 117.79 | 120.30 |
| 1 | 6-A | 128 | TYR | CB-CA-C | -5.02 | 100.35 | 110.40 |
| 1 | 110-A | 98 | ARG | CD-NE-CZ | 5.02 | 130.63 | 123.60 |
| 1 | 96-A | 1 | MET | CA-CB-CG | 5.02 | 121.83 | 113.30 |
| 1 | 72-A | 98 | ARG | NE-CZ-NH1 | 5.02 | 122.81 | 120.30 |
| 1 | 19-A | 44 | ARG | NE-CZ-NH1 | 5.01 | 122.81 | 120.30 |
| 1 | 36-A | 88 | VAL | C-N-CA | 5.01 | 143.04 | 122.00 |
| 1 | 57-A | 44 | ARG | NE-CZ-NH2 | -5.01 | 117.80 | 120.30 |
| 1 | 115-A | 159 | ARG | CG-CD-NE | -5.01 | 101.28 | 111.80 |
| 1 | 102-A | 159 | ARG | NE-CZ-NH2 | -5.01 | 117.80 | 120.30 |
| 1 | 40-A | 44 | ARG | NE-CZ-NH1 | 5.01 | 122.80 | 120.30 |
| 1 | 58-A | 12 | ARG | NE-CZ-NH2 | -5.00 | 117.80 | 120.30 |

There are no chirality outliers.

All (312) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | 1-A | 128 | TYR | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | 10-A | 119 | VAL | Peptide |
| 1 | 10-A | 17 | GLU | Peptide |
| 1 | 10-A | 20 | MET | Peptide |
| 1 | 10-A | 21 | PRO | Peptide |
| 1 | 10-A | 67 | GLY | Peptide |
| 1 | 100-A | 18 | ASN | Peptide |
| 1 | 102-A | 17 | GLU | Peptide |
| 1 | 104-A | 128 | TYR | Peptide |
| 1 | 104-A | 16 | MET | Peptide |
| 1 | 105-A | 128 | TYR | Peptide |
| 1 | 105-A | 129 | GLU | Peptide |
| 1 | 105-A | 17 | GLU | Peptide |
| 1 | 105-A | 18 | ASN | Peptide |
| 1 | 107-A | 17 | GLU | Peptide |
| 1 | 107-A | 19 | ALA | Peptide |
| 1 | 107-A | 22 | TRP | Peptide |
| 1 | 108-A | 1 | MET | Peptide |
| 1 | 108-A | 18 | ASN | Peptide |
| 1 | 109-A | 17 | GLU | Peptide |
| 1 | 109-A | 67 | GLY | Peptide |
| 1 | 11-A | 119 | VAL | Peptide |
| 1 | 11-A | 16 | MET | Peptide |
| 1 | 110-A | 17 | GLU | Peptide |
| 1 | 110-A | 67 | GLY | Peptide |
| 1 | 111-A | 17 | GLU | Peptide |
| 1 | 111-A | 20 | MET | Peptide |
| 1 | 112-A | 1 | MET | Peptide |
| 1 | 112-A | 20 | MET | Peptide |
| 1 | 113-A | 1 | MET | Peptide |
| 1 | 113-A | 17 | GLU | Peptide |
| 1 | 113-A | 19 | ALA | Peptide |
| 1 | 113-A | 20 | MET | Peptide |
| 1 | 113-A | 22 | TRP | Peptide |
| 1 | 114-A | 128 | TYR | Peptide |
| 1 | 114-A | 17 | GLU | Peptide |
| 1 | 114-A | 19 | ALA | Peptide |
| 1 | 114-A | 20 | MET | Peptide |
| 1 | 115-A | 17 | GLU | Peptide |
| 1 | 115-A | 19 | ALA | Peptide |
| 1 | 115-A | 20 | MET | Peptide |
| 1 | 116-A | 121 | GLY | Peptide |
| 1 | 116-A | 19 | ALA | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|-------------------|
| 1 | 116-A | 22 | TRP | Peptide |
| 1 | 117-A | 17 | GLU | Peptide |
| 1 | 117-A | 18 | ASN | Mainchain,Peptide |
| 1 | 117-A | 21 | PRO | Peptide |
| 1 | 12-A | 119 | VAL | Peptide |
| 1 | 12-A | 16 | MET | Peptide |
| 1 | 12-A | 21 | PRO | Peptide |
| 1 | 122-A | 127 | ASP | Peptide |
| 1 | 122-A | 129 | GLU | Peptide |
| 1 | 122-A | 130 | PRO | Peptide |
| 1 | 124-A | 128 | TYR | Peptide |
| 1 | 126-A | 22 | TRP | Peptide |
| 1 | 127-A | 120 | GLU | Peptide |
| 1 | 13-A | 16 | MET | Peptide |
| 1 | 13-A | 17 | GLU | Peptide |
| 1 | 13-A | 21 | PRO | Peptide |
| 1 | 130-A | 67 | GLY | Peptide |
| 1 | 131-A | 118 | GLU | Peptide |
| 1 | 131-A | 128 | TYR | Peptide |
| 1 | 132-A | 118 | GLU | Peptide |
| 1 | 132-A | 119 | VAL | Peptide |
| 1 | 132-A | 52 | ARG | Peptide |
| 1 | 133-A | 118 | GLU | Peptide |
| 1 | 133-A | 51 | GLY | Peptide |
| 1 | 133-A | 52 | ARG | Peptide |
| 1 | 134-A | 52 | ARG | Peptide |
| 1 | 136-A | 18 | ASN | Peptide |
| 1 | 136-A | 51 | GLY | Peptide |
| 1 | 137-A | 129 | GLU | Peptide |
| 1 | 137-A | 18 | ASN | Peptide |
| 1 | 138-A | 10 | VAL | Peptide |
| 1 | 138-A | 129 | GLU | Peptide |
| 1 | 138-A | 20 | MET | Peptide |
| 1 | 139-A | 18 | ASN | Peptide |
| 1 | 14-A | 17 | GLU | Peptide |
| 1 | 14-A | 19 | ALA | Peptide |
| 1 | 14-A | 21 | PRO | Peptide |
| 1 | 140-A | 131 | ASP | Peptide |
| 1 | 140-A | 18 | ASN | Peptide |
| 1 | 141-A | 18 | ASN | Peptide |
| 1 | 143-A | 129 | GLU | Peptide |
| 1 | 143-A | 18 | ASN | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | 144-A | 129 | GLU | Peptide |
| 1 | 144-A | 18 | ASN | Peptide |
| 1 | 145-A | 128 | TYR | Peptide |
| 1 | 145-A | 129 | GLU | Peptide |
| 1 | 145-A | 130 | PRO | Peptide |
| 1 | 145-A | 18 | ASN | Peptide |
| 1 | 146-A | 128 | TYR | Peptide |
| 1 | 146-A | 130 | PRO | Peptide |
| 1 | 146-A | 20 | MET | Peptide |
| 1 | 146-A | 21 | PRO | Peptide |
| 1 | 147-A | 129 | GLU | Peptide |
| 1 | 149-A | 20 | MET | Peptide |
| 1 | 149-A | 85 | CYS | Peptide |
| 1 | 15-A | 128 | TYR | Peptide |
| 1 | 150-A | 129 | GLU | Peptide |
| 1 | 150-A | 83 | ALA | Peptide |
| 1 | 151-A | 129 | GLU | Peptide |
| 1 | 151-A | 130 | PRO | Peptide |
| 1 | 152-A | 129 | GLU | Peptide |
| 1 | 152-A | 130 | PRO | Peptide |
| 1 | 154-A | 129 | GLU | Peptide |
| 1 | 155-A | 129 | GLU | Peptide |
| 1 | 155-A | 130 | PRO | Peptide |
| 1 | 156-A | 129 | GLU | Peptide |
| 1 | 157-A | 128 | TYR | Peptide |
| 1 | 157-A | 65 | GLN | Peptide |
| 1 | 157-A | 85 | CYS | Peptide |
| 1 | 158-A | 130 | PRO | Peptide |
| 1 | 158-A | 67 | GLY | Peptide |
| 1 | 159-A | 1 | MET | Peptide |
| 1 | 159-A | 129 | GLU | Peptide |
| 1 | 159-A | 131 | ASP | Peptide |
| 1 | 159-A | 63 | SER | Peptide |
| 1 | 159-A | 86 | GLY | Peptide |
| 1 | 16-A | 128 | TYR | Peptide |
| 1 | 16-A | 16 | MET | Peptide |
| 1 | 16-A | 18 | ASN | Peptide |
| 1 | 160-A | 129 | GLU | Peptide |
| 1 | 160-A | 131 | ASP | Peptide |
| 1 | 160-A | 86 | GLY | Peptide |
| 1 | 161-A | 128 | TYR | Peptide |
| 1 | 161-A | 129 | GLU | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 161-A | 130 | PRO | Peptide |
| 1 | 162-A | 127 | ASP | Peptide |
| 1 | 162-A | 128 | TYR | Peptide |
| 1 | 162-A | 130 | PRO | Peptide |
| 1 | 162-A | 51 | GLY | Peptide |
| 1 | 162-A | 67 | GLY | Peptide |
| 1 | 163-A | 127 | ASP | Peptide |
| 1 | 163-A | 128 | TYR | Peptide |
| 1 | 163-A | 130 | PRO | Peptide |
| 1 | 163-A | 131 | ASP | Peptide |
| 1 | 163-A | 67 | GLY | Peptide |
| 1 | 164-A | 126 | PRO | Peptide |
| 1 | 164-A | 127 | ASP | Peptide |
| 1 | 164-A | 128 | TYR | Peptide |
| 1 | 164-A | 130 | PRO | Peptide |
| 1 | 164-A | 67 | GLY | Peptide |
| 1 | 165-A | 129 | GLU | Peptide |
| 1 | 166-A | 128 | TYR | Peptide |
| 1 | 166-A | 129 | GLU | Peptide |
| 1 | 167-A | 128 | TYR | Peptide |
| 1 | 17-A | 16 | MET | Peptide |
| 1 | 17-A | 17 | GLU | Peptide |
| 1 | 17-A | 18 | ASN | Peptide |
| 1 | 17-A | 20 | MET | Peptide |
| 1 | 18-A | 16 | MET | Peptide |
| 1 | 18-A | 17 | GLU | Peptide |
| 1 | 19-A | 17 | GLU | Peptide |
| 1 | 19-A | 21 | PRO | Peptide |
| 1 | 2-A | 20 | MET | Peptide |
| 1 | 20-A | 16 | MET | Peptide |
| 1 | 20-A | 87 | ASP | Peptide |
| 1 | 21-A | 17 | GLU | Peptide |
| 1 | 21-A | 87 | ASP | Peptide |
| 1 | 22-A | 87 | ASP | Peptide |
| 1 | 23-A | 17 | GLU | Peptide |
| 1 | 23-A | 18 | ASN | Peptide |
| 1 | 23-A | 87 | ASP | Peptide |
| 1 | 24-A | 128 | TYR | Peptide |
| 1 | 24-A | 18 | ASN | Peptide |
| 1 | 25-A | 1 | MET | Peptide |
| 1 | 25-A | 18 | ASN | Peptide |
| 1 | 25-A | 86 | GLY | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|--------------|
| 1 | 26-A | 1 | MET | Peptide |
| 1 | 26-A | 18 | ASN | Peptide |
| 1 | 26-A | 86 | GLY | Peptide |
| 1 | 27-A | 86 | GLY | Peptide |
| 1 | 28-A | 129 | GLU | Peptide |
| 1 | 28-A | 20 | MET | Peptide |
| 1 | 28-A | 86 | GLY | Peptide |
| 1 | 29-A | 16 | MET | Peptide |
| 1 | 3-A | 129 | GLU | Peptide |
| 1 | 30-A | 86 | GLY | Peptide |
| 1 | 31-A | 86 | GLY | Peptide |
| 1 | 31-A | 89 | PRO | Peptide |
| 1 | 32-A | 16 | MET | Peptide |
| 1 | 32-A | 18 | ASN | Peptide |
| 1 | 32-A | 87 | ASP | Peptide |
| 1 | 32-A | 89 | PRO | Peptide |
| 1 | 33-A | 118 | GLU | Peptide |
| 1 | 33-A | 127 | ASP | Peptide |
| 1 | 33-A | 141 | HIS | Peptide |
| 1 | 33-A | 18 | ASN | Peptide |
| 1 | 33-A | 22 | TRP | Peptide |
| 1 | 33-A | 88 | VAL | Peptide |
| 1 | 34-A | 128 | TYR | Peptide |
| 1 | 34-A | 86 | GLY | Peptide |
| 1 | 34-A | 88 | VAL | Peptide |
| 1 | 35-A | 19 | ALA | Peptide |
| 1 | 35-A | 88 | VAL | Peptide |
| 1 | 36-A | 23 | ASN | Peptide |
| 1 | 36-A | 67 | GLY | Peptide |
| 1 | 36-A | 87 | ASP | Peptide |
| 1 | 36-A | 88 | VAL | Peptide |
| 1 | 37-A | 141 | HIS | Peptide |
| 1 | 37-A | 87 | ASP | Peptide |
| 1 | 38-A | 19 | ALA | Peptide |
| 1 | 38-A | 87 | ASP | Peptide |
| 1 | 39-A | 87 | ASP | Peptide |
| 1 | 4-A | 127 | ASP | Peptide |
| 1 | 4-A | 129 | GLU | Peptide |
| 1 | 4-A | 86 | GLY | Peptide |
| 1 | 40-A | 18 | ASN | Peptide |
| 1 | 40-A | 87 | ASP | Peptide |
| 1 | 41-A | 121 | GLY | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | 41-A | 16 | MET | Peptide |
| 1 | 41-A | 86 | GLY | Peptide |
| 1 | 41-A | 88 | VAL | Peptide |
| 1 | 42-A | 16 | MET | Peptide |
| 1 | 42-A | 86 | GLY | Peptide |
| 1 | 43-A | 16 | MET | Peptide |
| 1 | 44-A | 16 | MET | Peptide |
| 1 | 44-A | 87 | ASP | Peptide |
| 1 | 45-A | 17 | GLU | Peptide |
| 1 | 45-A | 87 | ASP | Peptide |
| 1 | 46-A | 121 | GLY | Peptide |
| 1 | 46-A | 86 | GLY | Peptide |
| 1 | 46-A | 87 | ASP | Peptide |
| 1 | 47-A | 88 | VAL | Peptide |
| 1 | 48-A | 86 | GLY | Peptide |
| 1 | 48-A | 88 | VAL | Peptide |
| 1 | 49-A | 119 | VAL | Peptide |
| 1 | 49-A | 86 | GLY | Peptide |
| 1 | 49-A | 87 | ASP | Peptide |
| 1 | 49-A | 88 | VAL | Peptide |
| 1 | 5-A | 129 | GLU | Peptide |
| 1 | 5-A | 17 | GLU | Peptide |
| 1 | 5-A | 18 | ASN | Peptide |
| 1 | 50-A | 119 | VAL | Peptide |
| 1 | 50-A | 84 | ALA | Peptide |
| 1 | 50-A | 86 | GLY | Peptide |
| 1 | 50-A | 87 | ASP | Peptide |
| 1 | 51-A | 120 | GLU | Peptide |
| 1 | 51-A | 85 | CYS | Peptide |
| 1 | 51-A | 87 | ASP | Peptide |
| 1 | 52-A | 120 | GLU | Peptide |
| 1 | 52-A | 84 | ALA | Peptide |
| 1 | 52-A | 85 | CYS | Peptide |
| 1 | 52-A | 87 | ASP | Peptide |
| 1 | 53-A | 120 | GLU | Peptide |
| 1 | 53-A | 85 | CYS | Peptide |
| 1 | 53-A | 86 | GLY | Peptide |
| 1 | 53-A | 87 | ASP | Peptide |
| 1 | 57-A | 20 | MET | Peptide |
| 1 | 6-A | 16 | MET | Peptide |
| 1 | 6-A | 17 | GLU | Peptide |
| 1 | 61-A | 129 | GLU | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | 62-A | 126 | PRO | Peptide |
| 1 | 63-A | 20 | MET | Peptide |
| 1 | 66-A | 128 | TYR | Peptide |
| 1 | 66-A | 20 | MET | Peptide |
| 1 | 66-A | 87 | ASP | Peptide |
| 1 | 67-A | 87 | ASP | Peptide |
| 1 | 68-A | 20 | MET | Peptide |
| 1 | 68-A | 21 | PRO | Peptide |
| 1 | 69-A | 20 | MET | Peptide |
| 1 | 7-A | 127 | ASP | Peptide |
| 1 | 7-A | 16 | MET | Peptide |
| 1 | 7-A | 18 | ASN | Peptide |
| 1 | 7-A | 19 | ALA | Peptide |
| 1 | 7-A | 20 | MET | Peptide |
| 1 | 70-A | 20 | MET | Peptide |
| 1 | 71-A | 20 | MET | Peptide |
| 1 | 71-A | 21 | PRO | Peptide |
| 1 | 72-A | 17 | GLU | Peptide |
| 1 | 72-A | 18 | ASN | Peptide |
| 1 | 72-A | 21 | PRO | Peptide |
| 1 | 72-A | 65 | GLN | Peptide |
| 1 | 73-A | 19 | ALA | Peptide |
| 1 | 73-A | 65 | GLN | Peptide |
| 1 | 74-A | 65 | GLN | Peptide |
| 1 | 75-A | 128 | TYR | Peptide |
| 1 | 78-A | 127 | ASP | Peptide |
| 1 | 79-A | 126 | PRO | Peptide |
| 1 | 79-A | 127 | ASP | Peptide |
| 1 | 8-A | 119 | VAL | Peptide |
| 1 | 8-A | 127 | ASP | Peptide |
| 1 | 8-A | 16 | MET | Peptide |
| 1 | 8-A | 20 | MET | Peptide |
| 1 | 80-A | 126 | PRO | Peptide |
| 1 | 80-A | 127 | ASP | Peptide |
| 1 | 81-A | 127 | ASP | Peptide |
| 1 | 81-A | 129 | GLU | Peptide |
| 1 | 82-A | 129 | GLU | Peptide |
| 1 | 83-A | 129 | GLU | Peptide |
| 1 | 84-A | 130 | PRO | Peptide |
| 1 | 85-A | 130 | PRO | Peptide |
| 1 | 86-A | 127 | ASP | Peptide |
| 1 | 86-A | 130 | PRO | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|---------|
| 1 | 88-A | 129 | GLU | Peptide |
| 1 | 89-A | 1 | MET | Peptide |
| 1 | 89-A | 129 | GLU | Peptide |
| 1 | 9-A | 119 | VAL | Peptide |
| 1 | 9-A | 15 | GLY | Peptide |
| 1 | 9-A | 18 | ASN | Peptide |
| 1 | 9-A | 19 | ALA | Peptide |
| 1 | 9-A | 67 | GLY | Peptide |
| 1 | 90-A | 128 | TYR | Peptide |
| 1 | 90-A | 129 | GLU | Peptide |
| 1 | 91-A | 129 | GLU | Peptide |
| 1 | 94-A | 18 | ASN | Peptide |
| 1 | 95-A | 18 | ASN | Peptide |
| 1 | 97-A | 18 | ASN | Peptide |
| 1 | 98-A | 18 | ASN | Peptide |
| 1 | 99-A | 18 | ASN | 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 | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 2-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 3-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 4-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 5-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 6-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 7-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 8-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 9-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 10-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 11-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 12-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 13-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 14-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 15-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 16-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 17-A | 1268 | 1223 | 1223 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 18-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 19-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 20-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 21-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 22-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 23-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 24-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 25-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 26-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 27-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 28-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 29-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 30-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 31-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 32-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 33-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 34-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 35-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 36-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 37-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 38-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 39-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 40-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 41-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 42-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 43-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 44-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 45-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 46-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 47-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 48-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 49-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 50-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 51-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 52-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 53-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 54-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 55-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 56-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 57-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 58-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 59-A | 1268 | 1223 | 1223 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 60-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 61-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 62-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 63-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 64-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 65-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 66-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 67-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 68-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 69-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 70-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 71-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 72-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 73-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 74-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 75-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 76-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 77-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 78-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 79-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 80-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 81-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 82-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 83-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 84-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 85-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 86-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 87-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 88-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 89-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 90-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 91-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 92-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 93-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 94-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 95-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 96-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 97-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 98-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 99-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 100-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 101-A | 1268 | 1223 | 1223 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 102-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 103-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 104-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 105-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 106-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 107-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 108-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 109-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 110-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 111-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 112-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 113-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 114-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 115-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 116-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 117-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 118-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 119-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 120-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 121-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 122-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 123-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 124-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 125-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 126-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 127-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 128-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 129-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 130-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 131-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 132-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 133-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 134-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 135-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 136-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 137-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 138-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 139-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 140-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 141-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 142-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 143-A | 1268 | 1223 | 1223 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 144-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 145-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 146-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 147-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 148-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 149-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 150-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 151-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 152-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 153-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 154-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 155-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 156-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 157-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 158-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 159-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 160-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 161-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 162-A | 1268 | 1223 | 1222 | 0 | 0 |
| 1 | 163-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 164-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 165-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 166-A | 1268 | 1223 | 1223 | 0 | 0 |
| 1 | 167-A | 1268 | 1223 | 1223 | 0 | 0 |
| 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 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 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 |
| 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 |

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Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | 61-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 62-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 63-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 64-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 65-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 66-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 67-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 68-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 69-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 70-A | 32 | 17 | 17 | 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 |
| 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 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 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 |
| 2 | 126-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 127-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 128-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 129-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 130-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 131-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 132-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 133-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 134-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 135-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 136-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 137-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 138-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 139-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 140-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 141-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 142-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 143-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 144-A | 32 | 17 | 17 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | 145-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 146-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 147-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 148-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 149-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 150-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 151-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 152-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 153-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 154-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 155-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 156-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 157-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 158-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 159-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 160-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 161-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 162-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 163-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 164-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 165-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 166-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 167-A | 32 | 17 | 17 | 0 | 0 |
| 3 | 1-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 2-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 3-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 4-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 5-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 6-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 7-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 8-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 9-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 10-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 11-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 12-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 13-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 14-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 15-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 16-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 17-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 18-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 19-A | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | 20-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 21-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 22-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 23-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 24-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 25-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 26-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 27-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 28-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 29-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 30-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 31-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 32-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 33-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 34-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 35-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 36-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 37-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 38-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 39-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 40-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 41-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 42-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 43-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 44-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 45-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 46-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 47-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 48-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 49-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 50-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 51-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 52-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 53-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 54-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 55-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 56-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 57-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 58-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 59-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 60-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 61-A | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | 62-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 63-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 64-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 65-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 66-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 67-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 68-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 69-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 70-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 71-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 72-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 73-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 74-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 75-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 76-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 77-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 78-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 79-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 80-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 81-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 82-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 83-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 84-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 85-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 86-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 87-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 88-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 89-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 90-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 91-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 92-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 93-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 94-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 95-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 96-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 97-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 98-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 99-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 100-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 101-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 102-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 103-A | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | 104-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 105-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 106-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 107-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 108-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 109-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 110-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 111-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 112-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 113-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 114-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 115-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 116-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 117-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 118-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 119-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 120-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 121-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 122-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 123-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 124-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 125-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 126-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 127-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 128-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 129-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 130-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 131-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 132-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 133-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 134-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 135-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 136-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 137-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 138-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 139-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 140-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 141-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 142-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 143-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 144-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 145-A | 2 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | 146-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 147-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 148-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 149-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 150-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 151-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 152-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 153-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 154-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 155-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 156-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 157-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 158-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 159-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 160-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 161-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 162-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 163-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 164-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 165-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 166-A | 2 | 0 | 0 | 0 | 0 |
| 3 | 167-A | 2 | 0 | 0 | 0 | 0 |
| 4 | 1-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 2-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 3-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 4-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 5-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 6-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 7-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 8-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 9-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 10-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 11-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 12-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 13-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 14-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 15-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 16-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 17-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 18-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 19-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 20-A | 48 | 24 | 24 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | 21-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 22-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 23-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 24-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 25-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 26-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 27-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 28-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 29-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 30-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 31-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 32-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 33-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 34-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 35-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 36-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 37-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 38-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 39-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 40-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 41-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 42-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 43-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 44-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 45-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 46-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 47-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 48-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 49-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 50-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 51-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 52-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 53-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 54-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 55-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 56-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 57-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 58-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 59-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 60-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 61-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 62-A | 48 | 24 | 24 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | 63-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 64-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 65-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 66-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 67-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 68-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 69-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 70-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 71-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 72-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 73-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 74-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 75-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 76-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 77-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 78-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 79-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 80-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 81-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 82-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 83-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 84-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 85-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 86-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 87-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 88-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 89-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 90-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 91-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 92-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 93-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 94-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 95-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 96-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 97-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 98-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 99-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 100-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 101-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 102-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 103-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 104-A | 48 | 24 | 24 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | 105-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 106-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 107-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 108-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 109-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 110-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 111-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 112-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 113-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 114-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 115-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 116-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 117-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 118-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 119-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 120-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 121-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 122-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 123-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 124-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 125-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 126-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 127-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 128-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 129-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 130-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 131-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 132-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 133-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 134-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 135-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 136-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 137-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 138-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 139-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 140-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 141-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 142-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 143-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 144-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 145-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 146-A | 48 | 24 | 24 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | 147-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 148-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 149-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 150-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 151-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 152-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 153-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 154-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 155-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 156-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 157-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 158-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 159-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 160-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 161-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 162-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 163-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 164-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 165-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 166-A | 48 | 24 | 24 | 0 | 0 |
| 4 | 167-A | 48 | 24 | 24 | 0 | 0 |
| 5 | 1-A | 83 | 0 | 0 | 0 | 0 |
| 5 | 2-A | 83 | 0 | 0 | 0 | 0 |
| 5 | 3-A | 79 | 0 | 0 | 0 | 0 |
| 5 | 4-A | 68 | 0 | 0 | 0 | 0 |
| 5 | 5-A | 75 | 0 | 0 | 0 | 0 |
| 5 | 6-A | 80 | 0 | 0 | 0 | 0 |
| 5 | 7-A | 99 | 0 | 0 | 0 | 0 |
| 5 | 8-A | 89 | 0 | 0 | 0 | 0 |
| 5 | 9-A | 79 | 0 | 0 | 0 | 0 |
| 5 | 10-A | 79 | 0 | 0 | 0 | 0 |
| 5 | 11-A | 82 | 0 | 0 | 0 | 0 |
| 5 | 12-A | 88 | 0 | 0 | 0 | 0 |
| 5 | 13-A | 89 | 0 | 0 | 0 | 0 |
| 5 | 14-A | 96 | 0 | 0 | 0 | 0 |
| 5 | 15-A | 96 | 0 | 0 | 0 | 0 |
| 5 | 16-A | 94 | 0 | 0 | 0 | 0 |
| 5 | 17-A | 84 | 0 | 0 | 0 | 0 |
| 5 | 18-A | 89 | 0 | 0 | 0 | 0 |
| 5 | 19-A | 80 | 0 | 0 | 0 | 0 |
| 5 | 20-A | 73 | 0 | 0 | 0 | 0 |
| 5 | 21-A | 92 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | 22-A | 91 | 0 | 0 | 0 | 0 |
| 5 | 23-A | 94 | 0 | 0 | 0 | 0 |
| 5 | 24-A | 95 | 0 | 0 | 0 | 0 |
| 5 | 25-A | 76 | 0 | 0 | 0 | 0 |
| 5 | 26-A | 83 | 0 | 0 | 0 | 0 |
| 5 | 27-A | 81 | 0 | 0 | 0 | 0 |
| 5 | 28-A | 81 | 0 | 0 | 0 | 0 |
| 5 | 29-A | 83 | 0 | 0 | 0 | 0 |
| 5 | 30-A | 84 | 0 | 0 | 0 | 0 |
| 5 | 31-A | 86 | 0 | 0 | 0 | 0 |
| 5 | 32-A | 85 | 0 | 0 | 0 | 0 |
| 5 | 33-A | 86 | 0 | 0 | 0 | 0 |
| 5 | 34-A | 93 | 0 | 0 | 0 | 0 |
| 5 | 35-A | 93 | 0 | 0 | 0 | 0 |
| 5 | 36-A | 77 | 0 | 0 | 0 | 0 |
| 5 | 37-A | 82 | 0 | 0 | 0 | 0 |
| 5 | 38-A | 87 | 0 | 0 | 0 | 0 |
| 5 | 39-A | 93 | 0 | 0 | 0 | 0 |
| 5 | 40-A | 84 | 0 | 0 | 0 | 0 |
| 5 | 41-A | 82 | 0 | 0 | 0 | 0 |
| 5 | 42-A | 83 | 0 | 0 | 0 | 0 |
| 5 | 43-A | 95 | 0 | 0 | 0 | 0 |
| 5 | 44-A | 100 | 0 | 0 | 0 | 0 |
| 5 | 45-A | 93 | 0 | 0 | 0 | 0 |
| 5 | 46-A | 92 | 0 | 0 | 0 | 0 |
| 5 | 47-A | 98 | 0 | 0 | 0 | 0 |
| 5 | 48-A | 92 | 0 | 0 | 0 | 0 |
| 5 | 49-A | 89 | 0 | 0 | 0 | 0 |
| 5 | 50-A | 78 | 0 | 0 | 0 | 0 |
| 5 | 51-A | 68 | 0 | 0 | 0 | 0 |
| 5 | 52-A | 77 | 0 | 0 | 0 | 0 |
| 5 | 53-A | 87 | 0 | 0 | 0 | 0 |
| 5 | 54-A | 92 | 0 | 0 | 0 | 0 |
| 5 | 55-A | 92 | 0 | 0 | 0 | 0 |
| 5 | 56-A | 82 | 0 | 0 | 0 | 0 |
| 5 | 57-A | 86 | 0 | 0 | 0 | 0 |
| 5 | 58-A | 89 | 0 | 0 | 0 | 0 |
| 5 | 59-A | 96 | 0 | 0 | 0 | 0 |
| 5 | 60-A | 96 | 0 | 0 | 0 | 0 |
| 5 | 61-A | 98 | 0 | 0 | 0 | 0 |
| 5 | 62-A | 100 | 0 | 0 | 0 | 0 |
| 5 | 63-A | 97 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | 64-A | 87 | 0 | 0 | 0 | 0 |
| 5 | 65-A | 83 | 0 | 0 | 0 | 0 |
| 5 | 66-A | 77 | 0 | 0 | 0 | 0 |
| 5 | 67-A | 78 | 0 | 0 | 0 | 0 |
| 5 | 68-A | 79 | 0 | 0 | 0 | 0 |
| 5 | 69-A | 79 | 0 | 0 | 0 | 0 |
| 5 | 70-A | 85 | 0 | 0 | 0 | 0 |
| 5 | 71-A | 91 | 0 | 0 | 0 | 0 |
| 5 | 72-A | 101 | 0 | 0 | 0 | 0 |
| 5 | 73-A | 94 | 0 | 0 | 0 | 0 |
| 5 | 74-A | 85 | 0 | 0 | 0 | 0 |
| 5 | 75-A | 92 | 0 | 0 | 0 | 0 |
| 5 | 76-A | 82 | 0 | 0 | 0 | 0 |
| 5 | 77-A | 85 | 0 | 0 | 0 | 0 |
| 5 | 78-A | 84 | 0 | 0 | 0 | 0 |
| 5 | 79-A | 86 | 0 | 0 | 0 | 0 |
| 5 | 80-A | 85 | 0 | 0 | 0 | 0 |
| 5 | 81-A | 92 | 0 | 0 | 0 | 0 |
| 5 | 82-A | 91 | 0 | 0 | 0 | 0 |
| 5 | 83-A | 98 | 0 | 0 | 0 | 0 |
| 5 | 84-A | 94 | 0 | 0 | 0 | 0 |
| 5 | 85-A | 94 | 0 | 0 | 0 | 0 |
| 5 | 86-A | 88 | 0 | 0 | 0 | 0 |
| 5 | 87-A | 84 | 0 | 0 | 0 | 0 |
| 5 | 88-A | 82 | 0 | 0 | 0 | 0 |
| 5 | 89-A | 92 | 0 | 0 | 0 | 0 |
| 5 | 90-A | 98 | 0 | 0 | 0 | 0 |
| 5 | 91-A | 75 | 0 | 0 | 0 | 0 |
| 5 | 92-A | 77 | 0 | 0 | 0 | 0 |
| 5 | 93-A | 78 | 0 | 0 | 0 | 0 |
| 5 | 94-A | 92 | 0 | 0 | 0 | 0 |
| 5 | 95-A | 101 | 0 | 0 | 0 | 0 |
| 5 | 96-A | 106 | 0 | 0 | 0 | 0 |
| 5 | 97-A | 94 | 0 | 0 | 0 | 0 |
| 5 | 98-A | 86 | 0 | 0 | 0 | 0 |
| 5 | 99-A | 87 | 0 | 0 | 0 | 0 |
| 5 | 100-A | 80 | 0 | 0 | 0 | 0 |
| 5 | 101-A | 76 | 0 | 0 | 0 | 0 |
| 5 | 102-A | 80 | 0 | 0 | 0 | 0 |
| 5 | 103-A | 89 | 0 | 0 | 0 | 0 |
| 5 | 104-A | 88 | 0 | 0 | 0 | 0 |
| 5 | 105-A | 97 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 5 | 106-A | 85 | 0 | 0 | 0 | 0 |
| 5 | 107-A | 87 | 0 | 0 | 0 | 0 |
| 5 | 108-A | 93 | 0 | 0 | 0 | 0 |
| 5 | 109-A | 82 | 0 | 0 | 0 | 0 |
| 5 | 110-A | 82 | 0 | 0 | 0 | 0 |
| 5 | 111-A | 75 | 0 | 0 | 0 | 0 |
| 5 | 112-A | 85 | 0 | 0 | 0 | 0 |
| 5 | 113-A | 97 | 0 | 0 | 0 | 0 |
| 5 | 114-A | 98 | 0 | 0 | 0 | 0 |
| 5 | 115-A | 86 | 0 | 0 | 0 | 0 |
| 5 | 116-A | 89 | 0 | 0 | 0 | 0 |
| 5 | 117-A | 85 | 0 | 0 | 0 | 0 |
| 5 | 118-A | 89 | 0 | 0 | 0 | 0 |
| 5 | 119-A | 88 | 0 | 0 | 0 | 0 |
| 5 | 120-A | 95 | 0 | 0 | 0 | 0 |
| 5 | 121-A | 93 | 0 | 0 | 0 | 0 |
| 5 | 122-A | 90 | 0 | 0 | 0 | 0 |
| 5 | 123-A | 82 | 0 | 0 | 0 | 0 |
| 5 | 124-A | 81 | 0 | 0 | 0 | 0 |
| 5 | 125-A | 84 | 0 | 0 | 0 | 0 |
| 5 | 126-A | 101 | 0 | 0 | 0 | 0 |
| 5 | 127-A | 96 | 0 | 0 | 0 | 0 |
| 5 | 128-A | 90 | 0 | 0 | 0 | 0 |
| 5 | 129-A | 89 | 0 | 0 | 0 | 0 |
| 5 | 130-A | 81 | 0 | 0 | 0 | 0 |
| 5 | 131-A | 75 | 0 | 0 | 0 | 0 |
| 5 | 132-A | 87 | 0 | 0 | 0 | 0 |
| 5 | 133-A | 96 | 0 | 0 | 0 | 0 |
| 5 | 134-A | 89 | 0 | 0 | 0 | 0 |
| 5 | 135-A | 89 | 0 | 0 | 0 | 0 |
| 5 | 136-A | 87 | 0 | 0 | 0 | 0 |
| 5 | 137-A | 88 | 0 | 0 | 0 | 0 |
| 5 | 138-A | 88 | 0 | 0 | 0 | 0 |
| 5 | 139-A | 96 | 0 | 0 | 0 | 0 |
| 5 | 140-A | 88 | 0 | 0 | 0 | 0 |
| 5 | 141-A | 80 | 0 | 0 | 0 | 0 |
| 5 | 142-A | 80 | 0 | 0 | 0 | 0 |
| 5 | 143-A | 83 | 0 | 0 | 0 | 0 |
| 5 | 144-A | 84 | 0 | 0 | 0 | 0 |
| 5 | 145-A | 99 | 0 | 0 | 0 | 0 |
| 5 | 146-A | 101 | 0 | 0 | 0 | 0 |
| 5 | 147-A | 105 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 5 | 148-A | 103 | 0 | 0 | 0 | 0 |
| 5 | 149-A | 86 | 0 | 0 | 0 | 0 |
| 5 | 150-A | 94 | 0 | 0 | 0 | 0 |
| 5 | 151-A | 92 | 0 | 0 | 0 | 0 |
| 5 | 152-A | 89 | 0 | 0 | 0 | 0 |
| 5 | 153-A | 99 | 0 | 0 | 0 | 0 |
| 5 | 154-A | 98 | 0 | 0 | 0 | 0 |
| 5 | 155-A | 78 | 0 | 0 | 0 | 0 |
| 5 | 156-A | 79 | 0 | 0 | 0 | 0 |
| 5 | 157-A | 80 | 0 | 0 | 0 | 0 |
| 5 | 158-A | 78 | 0 | 0 | 0 | 0 |
| 5 | 159-A | 82 | 0 | 0 | 0 | 0 |
| 5 | 160-A | 82 | 0 | 0 | 0 | 0 |
| 5 | 161-A | 86 | 0 | 0 | 0 | 0 |
| 5 | 162-A | 84 | 0 | 0 | 0 | 0 |
| 5 | 163-A | 91 | 0 | 0 | 0 | 0 |
| 5 | 164-A | 92 | 0 | 0 | 0 | 0 |
| 5 | 165-A | 90 | 0 | 0 | 0 | 0 |
| 5 | 166-A | 81 | 0 | 0 | 0 | 0 |
| 5 | 167-A | 89 | 0 | 0 | 0 | 0 |
| All | All | 240066 | 211088 | 211070 | 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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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 | 157/159 (99%) | 145 (92%) | 8 (5%) | 4 (2%) | 7 0 |
| 1 | 2-A | 157/159 (99%) | 143 (91%) | 11 (7%) | 3 (2%) | 10 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|---|
| 1 | 3-A | 157/159 (99%) | 150 (96%) | 4 (2%) | 3 (2%) | 10 | 0 |
| 1 | 4-A | 157/159 (99%) | 146 (93%) | 6 (4%) | 5 (3%) | 5 | 0 |
| 1 | 5-A | 157/159 (99%) | 147 (94%) | 4 (2%) | 6 (4%) | 4 | 0 |
| 1 | 6-A | 157/159 (99%) | 144 (92%) | 9 (6%) | 4 (2%) | 7 | 0 |
| 1 | 7-A | 157/159 (99%) | 147 (94%) | 7 (4%) | 3 (2%) | 10 | 0 |
| 1 | 8-A | 157/159 (99%) | 142 (90%) | 11 (7%) | 4 (2%) | 7 | 0 |
| 1 | 9-A | 157/159 (99%) | 144 (92%) | 9 (6%) | 4 (2%) | 7 | 0 |
| 1 | 10-A | 157/159 (99%) | 146 (93%) | 3 (2%) | 8 (5%) | 2 | 0 |
| 1 | 11-A | 157/159 (99%) | 144 (92%) | 7 (4%) | 6 (4%) | 4 | 0 |
| 1 | 12-A | 157/159 (99%) | 147 (94%) | 6 (4%) | 4 (2%) | 7 | 0 |
| 1 | 13-A | 157/159 (99%) | 145 (92%) | 10 (6%) | 2 (1%) | 15 | 2 |
| 1 | 14-A | 157/159 (99%) | 146 (93%) | 8 (5%) | 3 (2%) | 10 | 0 |
| 1 | 15-A | 157/159 (99%) | 147 (94%) | 6 (4%) | 4 (2%) | 7 | 0 |
| 1 | 16-A | 157/159 (99%) | 144 (92%) | 8 (5%) | 5 (3%) | 5 | 0 |
| 1 | 17-A | 157/159 (99%) | 146 (93%) | 5 (3%) | 6 (4%) | 4 | 0 |
| 1 | 18-A | 157/159 (99%) | 142 (90%) | 10 (6%) | 5 (3%) | 5 | 0 |
| 1 | 19-A | 157/159 (99%) | 148 (94%) | 4 (2%) | 5 (3%) | 5 | 0 |
| 1 | 20-A | 157/159 (99%) | 148 (94%) | 8 (5%) | 1 (1%) | 30 | 8 |
| 1 | 21-A | 157/159 (99%) | 147 (94%) | 6 (4%) | 4 (2%) | 7 | 0 |
| 1 | 22-A | 157/159 (99%) | 145 (92%) | 9 (6%) | 3 (2%) | 10 | 0 |
| 1 | 23-A | 157/159 (99%) | 148 (94%) | 5 (3%) | 4 (2%) | 7 | 0 |
| 1 | 24-A | 157/159 (99%) | 147 (94%) | 4 (2%) | 6 (4%) | 4 | 0 |
| 1 | 25-A | 157/159 (99%) | 145 (92%) | 6 (4%) | 6 (4%) | 4 | 0 |
| 1 | 26-A | 157/159 (99%) | 142 (90%) | 9 (6%) | 6 (4%) | 4 | 0 |
| 1 | 27-A | 157/159 (99%) | 143 (91%) | 10 (6%) | 4 (2%) | 7 | 0 |
| 1 | 28-A | 157/159 (99%) | 143 (91%) | 7 (4%) | 7 (4%) | 3 | 0 |
| 1 | 29-A | 157/159 (99%) | 139 (88%) | 8 (5%) | 10 (6%) | 2 | 0 |
| 1 | 30-A | 157/159 (99%) | 138 (88%) | 10 (6%) | 9 (6%) | 2 | 0 |
| 1 | 31-A | 157/159 (99%) | 136 (87%) | 10 (6%) | 11 (7%) | 1 | 0 |
| 1 | 32-A | 157/159 (99%) | 137 (87%) | 7 (4%) | 13 (8%) | 1 | 0 |
| 1 | 33-A | 157/159 (99%) | 137 (87%) | 7 (4%) | 13 (8%) | 1 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | 34-A | 157/159 (99%) | 139 (88%) | 7 (4%) | 11 (7%) | 1 | 0 |
| 1 | 35-A | 157/159 (99%) | 141 (90%) | 7 (4%) | 9 (6%) | 2 | 0 |
| 1 | 36-A | 157/159 (99%) | 140 (89%) | 8 (5%) | 9 (6%) | 2 | 0 |
| 1 | 37-A | 157/159 (99%) | 137 (87%) | 10 (6%) | 10 (6%) | 2 | 0 |
| 1 | 38-A | 157/159 (99%) | 146 (93%) | 5 (3%) | 6 (4%) | 4 | 0 |
| 1 | 39-A | 157/159 (99%) | 142 (90%) | 9 (6%) | 6 (4%) | 4 | 0 |
| 1 | 40-A | 157/159 (99%) | 144 (92%) | 8 (5%) | 5 (3%) | 5 | 0 |
| 1 | 41-A | 157/159 (99%) | 142 (90%) | 8 (5%) | 7 (4%) | 3 | 0 |
| 1 | 42-A | 157/159 (99%) | 146 (93%) | 4 (2%) | 7 (4%) | 3 | 0 |
| 1 | 43-A | 157/159 (99%) | 142 (90%) | 9 (6%) | 6 (4%) | 4 | 0 |
| 1 | 44-A | 157/159 (99%) | 146 (93%) | 6 (4%) | 5 (3%) | 5 | 0 |
| 1 | 45-A | 157/159 (99%) | 144 (92%) | 8 (5%) | 5 (3%) | 5 | 0 |
| 1 | 46-A | 157/159 (99%) | 148 (94%) | 5 (3%) | 4 (2%) | 7 | 0 |
| 1 | 47-A | 157/159 (99%) | 147 (94%) | 4 (2%) | 6 (4%) | 4 | 0 |
| 1 | 48-A | 157/159 (99%) | 148 (94%) | 4 (2%) | 5 (3%) | 5 | 0 |
| 1 | 49-A | 157/159 (99%) | 145 (92%) | 5 (3%) | 7 (4%) | 3 | 0 |
| 1 | 50-A | 157/159 (99%) | 145 (92%) | 8 (5%) | 4 (2%) | 7 | 0 |
| 1 | 51-A | 157/159 (99%) | 146 (93%) | 4 (2%) | 7 (4%) | 3 | 0 |
| 1 | 52-A | 157/159 (99%) | 144 (92%) | 10 (6%) | 3 (2%) | 10 | 0 |
| 1 | 53-A | 157/159 (99%) | 149 (95%) | 6 (4%) | 2 (1%) | 15 | 2 |
| 1 | 54-A | 157/159 (99%) | 147 (94%) | 7 (4%) | 3 (2%) | 10 | 0 |
| 1 | 55-A | 157/159 (99%) | 149 (95%) | 6 (4%) | 2 (1%) | 15 | 2 |
| 1 | 56-A | 157/159 (99%) | 147 (94%) | 7 (4%) | 3 (2%) | 10 | 0 |
| 1 | 57-A | 157/159 (99%) | 145 (92%) | 10 (6%) | 2 (1%) | 15 | 2 |
| 1 | 58-A | 157/159 (99%) | 150 (96%) | 6 (4%) | 1 (1%) | 30 | 8 |
| 1 | 59-A | 157/159 (99%) | 148 (94%) | 9 (6%) | 0 | 100 | 100 |
| 1 | 60-A | 157/159 (99%) | 152 (97%) | 2 (1%) | 3 (2%) | 10 | 0 |
| 1 | 61-A | 157/159 (99%) | 151 (96%) | 4 (2%) | 2 (1%) | 15 | 2 |
| 1 | 62-A | 157/159 (99%) | 145 (92%) | 9 (6%) | 3 (2%) | 10 | 0 |
| 1 | 63-A | 157/159 (99%) | 150 (96%) | 5 (3%) | 2 (1%) | 15 | 2 |
| 1 | 64-A | 157/159 (99%) | 150 (96%) | 7 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | 65-A | 157/159 (99%) | 149 (95%) | 8 (5%) | 0 | 100 | 100 |
| 1 | 66-A | 157/159 (99%) | 147 (94%) | 8 (5%) | 2 (1%) | 15 | 2 |
| 1 | 67-A | 157/159 (99%) | 147 (94%) | 8 (5%) | 2 (1%) | 15 | 2 |
| 1 | 68-A | 157/159 (99%) | 144 (92%) | 9 (6%) | 4 (2%) | 7 | 0 |
| 1 | 69-A | 157/159 (99%) | 144 (92%) | 10 (6%) | 3 (2%) | 10 | 0 |
| 1 | 70-A | 157/159 (99%) | 144 (92%) | 7 (4%) | 6 (4%) | 4 | 0 |
| 1 | 71-A | 157/159 (99%) | 144 (92%) | 5 (3%) | 8 (5%) | 2 | 0 |
| 1 | 72-A | 157/159 (99%) | 144 (92%) | 6 (4%) | 7 (4%) | 3 | 0 |
| 1 | 73-A | 157/159 (99%) | 147 (94%) | 3 (2%) | 7 (4%) | 3 | 0 |
| 1 | 74-A | 157/159 (99%) | 143 (91%) | 8 (5%) | 6 (4%) | 4 | 0 |
| 1 | 75-A | 157/159 (99%) | 143 (91%) | 10 (6%) | 4 (2%) | 7 | 0 |
| 1 | 76-A | 157/159 (99%) | 143 (91%) | 10 (6%) | 4 (2%) | 7 | 0 |
| 1 | 77-A | 157/159 (99%) | 142 (90%) | 13 (8%) | 2 (1%) | 15 | 2 |
| 1 | 78-A | 157/159 (99%) | 144 (92%) | 8 (5%) | 5 (3%) | 5 | 0 |
| 1 | 79-A | 157/159 (99%) | 145 (92%) | 8 (5%) | 4 (2%) | 7 | 0 |
| 1 | 80-A | 157/159 (99%) | 145 (92%) | 8 (5%) | 4 (2%) | 7 | 0 |
| 1 | 81-A | 157/159 (99%) | 147 (94%) | 8 (5%) | 2 (1%) | 15 | 2 |
| 1 | 82-A | 157/159 (99%) | 143 (91%) | 9 (6%) | 5 (3%) | 5 | 0 |
| 1 | 83-A | 157/159 (99%) | 146 (93%) | 7 (4%) | 4 (2%) | 7 | 0 |
| 1 | 84-A | 157/159 (99%) | 147 (94%) | 7 (4%) | 3 (2%) | 10 | 0 |
| 1 | 85-A | 157/159 (99%) | 144 (92%) | 7 (4%) | 6 (4%) | 4 | 0 |
| 1 | 86-A | 157/159 (99%) | 143 (91%) | 11 (7%) | 3 (2%) | 10 | 0 |
| 1 | 87-A | 157/159 (99%) | 148 (94%) | 6 (4%) | 3 (2%) | 10 | 0 |
| 1 | 88-A | 157/159 (99%) | 149 (95%) | 8 (5%) | 0 | 100 | 100 |
| 1 | 89-A | 157/159 (99%) | 147 (94%) | 7 (4%) | 3 (2%) | 10 | 0 |
| 1 | 90-A | 157/159 (99%) | 148 (94%) | 7 (4%) | 2 (1%) | 15 | 2 |
| 1 | 91-A | 157/159 (99%) | 149 (95%) | 6 (4%) | 2 (1%) | 15 | 2 |
| 1 | 92-A | 157/159 (99%) | 146 (93%) | 7 (4%) | 4 (2%) | 7 | 0 |
| 1 | 93-A | 157/159 (99%) | 147 (94%) | 9 (6%) | 1 (1%) | 30 | 8 |
| 1 | 94-A | 157/159 (99%) | 144 (92%) | 8 (5%) | 5 (3%) | 5 | 0 |
| 1 | 95-A | 157/159 (99%) | 145 (92%) | 8 (5%) | 4 (2%) | 7 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | 96-A | 157/159 (99%) | 146 (93%) | 9 (6%) | 2 (1%) | 15 | 2 |
| 1 | 97-A | 157/159 (99%) | 149 (95%) | 7 (4%) | 1 (1%) | 30 | 8 |
| 1 | 98-A | 157/159 (99%) | 147 (94%) | 7 (4%) | 3 (2%) | 10 | 0 |
| 1 | 99-A | 157/159 (99%) | 151 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | 100-A | 157/159 (99%) | 147 (94%) | 7 (4%) | 3 (2%) | 10 | 0 |
| 1 | 101-A | 157/159 (99%) | 148 (94%) | 6 (4%) | 3 (2%) | 10 | 0 |
| 1 | 102-A | 157/159 (99%) | 151 (96%) | 4 (2%) | 2 (1%) | 15 | 2 |
| 1 | 103-A | 157/159 (99%) | 150 (96%) | 3 (2%) | 4 (2%) | 7 | 0 |
| 1 | 104-A | 157/159 (99%) | 150 (96%) | 5 (3%) | 2 (1%) | 15 | 2 |
| 1 | 105-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 30 | 8 |
| 1 | 106-A | 157/159 (99%) | 148 (94%) | 6 (4%) | 3 (2%) | 10 | 0 |
| 1 | 107-A | 157/159 (99%) | 144 (92%) | 10 (6%) | 3 (2%) | 10 | 0 |
| 1 | 108-A | 157/159 (99%) | 144 (92%) | 9 (6%) | 4 (2%) | 7 | 0 |
| 1 | 109-A | 157/159 (99%) | 143 (91%) | 9 (6%) | 5 (3%) | 5 | 0 |
| 1 | 110-A | 157/159 (99%) | 139 (88%) | 10 (6%) | 8 (5%) | 2 | 0 |
| 1 | 111-A | 157/159 (99%) | 142 (90%) | 6 (4%) | 9 (6%) | 2 | 0 |
| 1 | 112-A | 157/159 (99%) | 141 (90%) | 8 (5%) | 8 (5%) | 2 | 0 |
| 1 | 113-A | 157/159 (99%) | 141 (90%) | 5 (3%) | 11 (7%) | 1 | 0 |
| 1 | 114-A | 157/159 (99%) | 138 (88%) | 11 (7%) | 8 (5%) | 2 | 0 |
| 1 | 115-A | 157/159 (99%) | 145 (92%) | 5 (3%) | 7 (4%) | 3 | 0 |
| 1 | 116-A | 157/159 (99%) | 144 (92%) | 7 (4%) | 6 (4%) | 4 | 0 |
| 1 | 117-A | 157/159 (99%) | 145 (92%) | 8 (5%) | 4 (2%) | 7 | 0 |
| 1 | 118-A | 157/159 (99%) | 147 (94%) | 4 (2%) | 6 (4%) | 4 | 0 |
| 1 | 119-A | 157/159 (99%) | 150 (96%) | 6 (4%) | 1 (1%) | 30 | 8 |
| 1 | 120-A | 157/159 (99%) | 144 (92%) | 11 (7%) | 2 (1%) | 15 | 2 |
| 1 | 121-A | 157/159 (99%) | 148 (94%) | 4 (2%) | 5 (3%) | 5 | 0 |
| 1 | 122-A | 157/159 (99%) | 142 (90%) | 10 (6%) | 5 (3%) | 5 | 0 |
| 1 | 123-A | 157/159 (99%) | 144 (92%) | 7 (4%) | 6 (4%) | 4 | 0 |
| 1 | 124-A | 157/159 (99%) | 144 (92%) | 4 (2%) | 9 (6%) | 2 | 0 |
| 1 | 125-A | 157/159 (99%) | 142 (90%) | 7 (4%) | 8 (5%) | 2 | 0 |
| 1 | 126-A | 157/159 (99%) | 148 (94%) | 7 (4%) | 2 (1%) | 15 | 2 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|---|
| 1 | 127-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 30 | 8 |
| 1 | 128-A | 157/159 (99%) | 146 (93%) | 7 (4%) | 4 (2%) | 7 | 0 |
| 1 | 129-A | 157/159 (99%) | 149 (95%) | 7 (4%) | 1 (1%) | 30 | 8 |
| 1 | 130-A | 157/159 (99%) | 144 (92%) | 11 (7%) | 2 (1%) | 15 | 2 |
| 1 | 131-A | 157/159 (99%) | 141 (90%) | 11 (7%) | 5 (3%) | 5 | 0 |
| 1 | 132-A | 157/159 (99%) | 140 (89%) | 13 (8%) | 4 (2%) | 7 | 0 |
| 1 | 133-A | 157/159 (99%) | 146 (93%) | 8 (5%) | 3 (2%) | 10 | 0 |
| 1 | 134-A | 157/159 (99%) | 144 (92%) | 10 (6%) | 3 (2%) | 10 | 0 |
| 1 | 135-A | 157/159 (99%) | 143 (91%) | 12 (8%) | 2 (1%) | 15 | 2 |
| 1 | 136-A | 157/159 (99%) | 145 (92%) | 7 (4%) | 5 (3%) | 5 | 0 |
| 1 | 137-A | 157/159 (99%) | 144 (92%) | 5 (3%) | 8 (5%) | 2 | 0 |
| 1 | 138-A | 157/159 (99%) | 146 (93%) | 5 (3%) | 6 (4%) | 4 | 0 |
| 1 | 139-A | 157/159 (99%) | 145 (92%) | 8 (5%) | 4 (2%) | 7 | 0 |
| 1 | 140-A | 157/159 (99%) | 149 (95%) | 4 (2%) | 4 (2%) | 7 | 0 |
| 1 | 141-A | 157/159 (99%) | 145 (92%) | 7 (4%) | 5 (3%) | 5 | 0 |
| 1 | 142-A | 157/159 (99%) | 146 (93%) | 5 (3%) | 6 (4%) | 4 | 0 |
| 1 | 143-A | 157/159 (99%) | 146 (93%) | 5 (3%) | 6 (4%) | 4 | 0 |
| 1 | 144-A | 157/159 (99%) | 143 (91%) | 9 (6%) | 5 (3%) | 5 | 0 |
| 1 | 145-A | 157/159 (99%) | 141 (90%) | 11 (7%) | 5 (3%) | 5 | 0 |
| 1 | 146-A | 157/159 (99%) | 143 (91%) | 8 (5%) | 6 (4%) | 4 | 0 |
| 1 | 147-A | 157/159 (99%) | 145 (92%) | 8 (5%) | 4 (2%) | 7 | 0 |
| 1 | 148-A | 157/159 (99%) | 148 (94%) | 4 (2%) | 5 (3%) | 5 | 0 |
| 1 | 149-A | 157/159 (99%) | 146 (93%) | 9 (6%) | 2 (1%) | 15 | 2 |
| 1 | 150-A | 157/159 (99%) | 140 (89%) | 11 (7%) | 6 (4%) | 4 | 0 |
| 1 | 151-A | 157/159 (99%) | 143 (91%) | 11 (7%) | 3 (2%) | 10 | 0 |
| 1 | 152-A | 157/159 (99%) | 149 (95%) | 4 (2%) | 4 (2%) | 7 | 0 |
| 1 | 153-A | 157/159 (99%) | 150 (96%) | 3 (2%) | 4 (2%) | 7 | 0 |
| 1 | 154-A | 157/159 (99%) | 146 (93%) | 8 (5%) | 3 (2%) | 10 | 0 |
| 1 | 155-A | 157/159 (99%) | 142 (90%) | 9 (6%) | 6 (4%) | 4 | 0 |
| 1 | 156-A | 157/159 (99%) | 140 (89%) | 11 (7%) | 6 (4%) | 4 | 0 |
| 1 | 157-A | 157/159 (99%) | 142 (90%) | 10 (6%) | 5 (3%) | 5 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|----------|-------------|---|
| 1 | 158-A | 157/159 (99%) | 140 (89%) | 9 (6%) | 8 (5%) | 2 | 0 |
| 1 | 159-A | 157/159 (99%) | 140 (89%) | 11 (7%) | 6 (4%) | 4 | 0 |
| 1 | 160-A | 157/159 (99%) | 141 (90%) | 11 (7%) | 5 (3%) | 5 | 0 |
| 1 | 161-A | 157/159 (99%) | 140 (89%) | 12 (8%) | 5 (3%) | 5 | 0 |
| 1 | 162-A | 157/159 (99%) | 145 (92%) | 7 (4%) | 5 (3%) | 5 | 0 |
| 1 | 163-A | 157/159 (99%) | 147 (94%) | 6 (4%) | 4 (2%) | 7 | 0 |
| 1 | 164-A | 157/159 (99%) | 146 (93%) | 6 (4%) | 5 (3%) | 5 | 0 |
| 1 | 165-A | 157/159 (99%) | 144 (92%) | 6 (4%) | 7 (4%) | 3 | 0 |
| 1 | 166-A | 157/159 (99%) | 142 (90%) | 12 (8%) | 3 (2%) | 10 | 0 |
| 1 | 167-A | 157/159 (99%) | 145 (92%) | 5 (3%) | 7 (4%) | 3 | 0 |
| All | All | 26219/26553 (99%) | 24212 (92%) | 1237 (5%) | 770 (3%) | 6 | 0 |

All (770) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1-A | 18 | ASN |
| 1 | 1-A | 119 | VAL |
| 1 | 1-A | 130 | PRO |
| 1 | 3-A | 130 | PRO |
| 1 | 4-A | 18 | ASN |
| 1 | 4-A | 130 | PRO |
| 1 | 5-A | 18 | ASN |
| 1 | 5-A | 130 | PRO |
| 1 | 6-A | 127 | ASP |
| 1 | 7-A | 22 | TRP |
| 1 | 8-A | 21 | PRO |
| 1 | 9-A | 18 | ASN |
| 1 | 9-A | 19 | ALA |
| 1 | 9-A | 21 | PRO |
| 1 | 10-A | 18 | ASN |
| 1 | 10-A | 21 | PRO |
| 1 | 10-A | 68 | THR |
| 1 | 11-A | 18 | ASN |
| 1 | 11-A | 21 | PRO |
| 1 | 11-A | 22 | TRP |
| 1 | 12-A | 16 | MET |
| 1 | 12-A | 18 | ASN |
| 1 | 12-A | 21 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 12-A | 22 | TRP |
| 1 | 14-A | 21 | PRO |
| 1 | 14-A | 22 | TRP |
| 1 | 15-A | 17 | GLU |
| 1 | 15-A | 130 | PRO |
| 1 | 15-A | 131 | ASP |
| 1 | 16-A | 19 | ALA |
| 1 | 16-A | 130 | PRO |
| 1 | 17-A | 20 | MET |
| 1 | 17-A | 21 | PRO |
| 1 | 17-A | 129 | GLU |
| 1 | 17-A | 130 | PRO |
| 1 | 18-A | 21 | PRO |
| 1 | 18-A | 143 | ALA |
| 1 | 19-A | 17 | GLU |
| 1 | 19-A | 21 | PRO |
| 1 | 19-A | 143 | ALA |
| 1 | 20-A | 17 | GLU |
| 1 | 21-A | 18 | ASN |
| 1 | 21-A | 21 | PRO |
| 1 | 21-A | 87 | ASP |
| 1 | 22-A | 87 | ASP |
| 1 | 22-A | 88 | VAL |
| 1 | 23-A | 17 | GLU |
| 1 | 23-A | 19 | ALA |
| 1 | 23-A | 20 | MET |
| 1 | 23-A | 88 | VAL |
| 1 | 24-A | 20 | MET |
| 1 | 24-A | 85 | CYS |
| 1 | 24-A | 87 | ASP |
| 1 | 24-A | 128 | TYR |
| 1 | 25-A | 19 | ALA |
| 1 | 25-A | 20 | MET |
| 1 | 26-A | 17 | GLU |
| 1 | 26-A | 18 | ASN |
| 1 | 26-A | 19 | ALA |
| 1 | 26-A | 20 | MET |
| 1 | 26-A | 21 | PRO |
| 1 | 26-A | 88 | VAL |
| 1 | 27-A | 87 | ASP |
| 1 | 28-A | 21 | PRO |
| 1 | 28-A | 87 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 28-A | 88 | VAL |
| 1 | 29-A | 20 | MET |
| 1 | 29-A | 21 | PRO |
| 1 | 29-A | 88 | VAL |
| 1 | 29-A | 90 | GLU |
| 1 | 29-A | 137 | PHE |
| 1 | 30-A | 17 | GLU |
| 1 | 30-A | 53 | PRO |
| 1 | 30-A | 88 | VAL |
| 1 | 30-A | 90 | GLU |
| 1 | 30-A | 130 | PRO |
| 1 | 30-A | 131 | ASP |
| 1 | 31-A | 17 | GLU |
| 1 | 31-A | 53 | PRO |
| 1 | 31-A | 54 | LEU |
| 1 | 31-A | 87 | ASP |
| 1 | 31-A | 88 | VAL |
| 1 | 31-A | 130 | PRO |
| 1 | 31-A | 131 | ASP |
| 1 | 32-A | 21 | PRO |
| 1 | 32-A | 88 | VAL |
| 1 | 32-A | 90 | GLU |
| 1 | 32-A | 127 | ASP |
| 1 | 32-A | 130 | PRO |
| 1 | 32-A | 131 | ASP |
| 1 | 33-A | 22 | TRP |
| 1 | 33-A | 23 | ASN |
| 1 | 33-A | 87 | ASP |
| 1 | 33-A | 89 | PRO |
| 1 | 33-A | 119 | VAL |
| 1 | 34-A | 18 | ASN |
| 1 | 34-A | 87 | ASP |
| 1 | 34-A | 88 | VAL |
| 1 | 35-A | 18 | ASN |
| 1 | 35-A | 19 | ALA |
| 1 | 35-A | 20 | MET |
| 1 | 35-A | 23 | ASN |
| 1 | 35-A | 90 | GLU |
| 1 | 35-A | 119 | VAL |
| 1 | 36-A | 17 | GLU |
| 1 | 36-A | 19 | ALA |
| 1 | 36-A | 87 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 36-A | 89 | PRO |
| 1 | 36-A | 119 | VAL |
| 1 | 37-A | 17 | GLU |
| 1 | 37-A | 18 | ASN |
| 1 | 37-A | 89 | PRO |
| 1 | 37-A | 90 | GLU |
| 1 | 38-A | 17 | GLU |
| 1 | 38-A | 18 | ASN |
| 1 | 38-A | 89 | PRO |
| 1 | 38-A | 90 | GLU |
| 1 | 39-A | 21 | PRO |
| 1 | 39-A | 22 | TRP |
| 1 | 39-A | 89 | PRO |
| 1 | 40-A | 21 | PRO |
| 1 | 40-A | 89 | PRO |
| 1 | 41-A | 89 | PRO |
| 1 | 41-A | 120 | GLU |
| 1 | 42-A | 17 | GLU |
| 1 | 42-A | 89 | PRO |
| 1 | 42-A | 148 | SER |
| 1 | 43-A | 17 | GLU |
| 1 | 43-A | 87 | ASP |
| 1 | 43-A | 89 | PRO |
| 1 | 44-A | 88 | VAL |
| 1 | 44-A | 89 | PRO |
| 1 | 45-A | 18 | ASN |
| 1 | 45-A | 88 | VAL |
| 1 | 45-A | 89 | PRO |
| 1 | 46-A | 18 | ASN |
| 1 | 46-A | 88 | VAL |
| 1 | 47-A | 18 | ASN |
| 1 | 47-A | 85 | CYS |
| 1 | 47-A | 88 | VAL |
| 1 | 48-A | 85 | CYS |
| 1 | 48-A | 88 | VAL |
| 1 | 48-A | 119 | VAL |
| 1 | 49-A | 85 | CYS |
| 1 | 49-A | 88 | VAL |
| 1 | 49-A | 119 | VAL |
| 1 | 49-A | 120 | GLU |
| 1 | 50-A | 119 | VAL |
| 1 | 50-A | 120 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 50-A | 127 | ASP |
| 1 | 51-A | 88 | VAL |
| 1 | 52-A | 88 | VAL |
| 1 | 52-A | 119 | VAL |
| 1 | 53-A | 88 | VAL |
| 1 | 54-A | 87 | ASP |
| 1 | 54-A | 88 | VAL |
| 1 | 55-A | 87 | ASP |
| 1 | 56-A | 87 | ASP |
| 1 | 56-A | 88 | VAL |
| 1 | 56-A | 127 | ASP |
| 1 | 57-A | 87 | ASP |
| 1 | 57-A | 88 | VAL |
| 1 | 58-A | 88 | VAL |
| 1 | 61-A | 127 | ASP |
| 1 | 62-A | 127 | ASP |
| 1 | 63-A | 21 | PRO |
| 1 | 63-A | 22 | TRP |
| 1 | 67-A | 19 | ALA |
| 1 | 68-A | 18 | ASN |
| 1 | 68-A | 21 | PRO |
| 1 | 68-A | 128 | TYR |
| 1 | 69-A | 19 | ALA |
| 1 | 69-A | 67 | GLY |
| 1 | 71-A | 2 | ILE |
| 1 | 71-A | 17 | GLU |
| 1 | 71-A | 18 | ASN |
| 1 | 72-A | 2 | ILE |
| 1 | 72-A | 17 | GLU |
| 1 | 72-A | 65 | GLN |
| 1 | 72-A | 129 | GLU |
| 1 | 73-A | 17 | GLU |
| 1 | 73-A | 65 | GLN |
| 1 | 73-A | 66 | PRO |
| 1 | 74-A | 2 | ILE |
| 1 | 74-A | 17 | GLU |
| 1 | 74-A | 65 | GLN |
| 1 | 74-A | 66 | PRO |
| 1 | 74-A | 119 | VAL |
| 1 | 74-A | 127 | ASP |
| 1 | 75-A | 2 | ILE |
| 1 | 75-A | 17 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 75-A | 87 | ASP |
| 1 | 76-A | 20 | MET |
| 1 | 78-A | 20 | MET |
| 1 | 79-A | 130 | PRO |
| 1 | 80-A | 126 | PRO |
| 1 | 80-A | 128 | TYR |
| 1 | 81-A | 130 | PRO |
| 1 | 81-A | 131 | ASP |
| 1 | 82-A | 127 | ASP |
| 1 | 83-A | 129 | GLU |
| 1 | 84-A | 131 | ASP |
| 1 | 85-A | 127 | ASP |
| 1 | 85-A | 131 | ASP |
| 1 | 86-A | 127 | ASP |
| 1 | 86-A | 131 | ASP |
| 1 | 87-A | 127 | ASP |
| 1 | 91-A | 129 | GLU |
| 1 | 91-A | 130 | PRO |
| 1 | 92-A | 130 | PRO |
| 1 | 92-A | 131 | ASP |
| 1 | 93-A | 17 | GLU |
| 1 | 94-A | 18 | ASN |
| 1 | 94-A | 122 | ASP |
| 1 | 95-A | 122 | ASP |
| 1 | 96-A | 52 | ARG |
| 1 | 98-A | 143 | ALA |
| 1 | 102-A | 18 | ASN |
| 1 | 104-A | 17 | GLU |
| 1 | 106-A | 21 | PRO |
| 1 | 107-A | 21 | PRO |
| 1 | 108-A | 21 | PRO |
| 1 | 108-A | 87 | ASP |
| 1 | 110-A | 19 | ALA |
| 1 | 110-A | 20 | MET |
| 1 | 110-A | 21 | PRO |
| 1 | 110-A | 68 | THR |
| 1 | 111-A | 19 | ALA |
| 1 | 111-A | 21 | PRO |
| 1 | 111-A | 22 | TRP |
| 1 | 111-A | 121 | GLY |
| 1 | 111-A | 131 | ASP |
| 1 | 112-A | 2 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 112-A | 18 | ASN |
| 1 | 112-A | 19 | ALA |
| 1 | 112-A | 21 | PRO |
| 1 | 112-A | 121 | GLY |
| 1 | 113-A | 2 | ILE |
| 1 | 113-A | 18 | ASN |
| 1 | 113-A | 20 | MET |
| 1 | 113-A | 21 | PRO |
| 1 | 113-A | 120 | GLU |
| 1 | 113-A | 143 | ALA |
| 1 | 114-A | 20 | MET |
| 1 | 114-A | 21 | PRO |
| 1 | 114-A | 22 | TRP |
| 1 | 114-A | 23 | ASN |
| 1 | 115-A | 19 | ALA |
| 1 | 115-A | 20 | MET |
| 1 | 115-A | 21 | PRO |
| 1 | 115-A | 22 | TRP |
| 1 | 115-A | 23 | ASN |
| 1 | 115-A | 119 | VAL |
| 1 | 116-A | 18 | ASN |
| 1 | 116-A | 19 | ALA |
| 1 | 116-A | 20 | MET |
| 1 | 116-A | 21 | PRO |
| 1 | 117-A | 19 | ALA |
| 1 | 117-A | 21 | PRO |
| 1 | 117-A | 23 | ASN |
| 1 | 118-A | 17 | GLU |
| 1 | 118-A | 21 | PRO |
| 1 | 119-A | 20 | MET |
| 1 | 120-A | 23 | ASN |
| 1 | 120-A | 120 | GLU |
| 1 | 121-A | 23 | ASN |
| 1 | 121-A | 121 | GLY |
| 1 | 121-A | 130 | PRO |
| 1 | 121-A | 131 | ASP |
| 1 | 123-A | 88 | VAL |
| 1 | 123-A | 120 | GLU |
| 1 | 124-A | 21 | PRO |
| 1 | 124-A | 22 | TRP |
| 1 | 124-A | 23 | ASN |
| 1 | 124-A | 87 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 124-A | 120 | GLU |
| 1 | 124-A | 127 | ASP |
| 1 | 124-A | 130 | PRO |
| 1 | 125-A | 21 | PRO |
| 1 | 125-A | 121 | GLY |
| 1 | 125-A | 122 | ASP |
| 1 | 126-A | 88 | VAL |
| 1 | 126-A | 120 | GLU |
| 1 | 127-A | 23 | ASN |
| 1 | 128-A | 23 | ASN |
| 1 | 131-A | 52 | ARG |
| 1 | 131-A | 87 | ASP |
| 1 | 132-A | 18 | ASN |
| 1 | 132-A | 52 | ARG |
| 1 | 133-A | 50 | ILE |
| 1 | 133-A | 52 | ARG |
| 1 | 135-A | 128 | TYR |
| 1 | 136-A | 17 | GLU |
| 1 | 136-A | 128 | TYR |
| 1 | 136-A | 129 | GLU |
| 1 | 137-A | 17 | GLU |
| 1 | 137-A | 18 | ASN |
| 1 | 137-A | 51 | GLY |
| 1 | 138-A | 11 | ASP |
| 1 | 138-A | 17 | GLU |
| 1 | 138-A | 129 | GLU |
| 1 | 138-A | 132 | ASP |
| 1 | 139-A | 129 | GLU |
| 1 | 140-A | 18 | ASN |
| 1 | 140-A | 129 | GLU |
| 1 | 141-A | 17 | GLU |
| 1 | 141-A | 18 | ASN |
| 1 | 141-A | 129 | GLU |
| 1 | 142-A | 17 | GLU |
| 1 | 143-A | 17 | GLU |
| 1 | 144-A | 17 | GLU |
| 1 | 144-A | 129 | GLU |
| 1 | 145-A | 21 | PRO |
| 1 | 145-A | 130 | PRO |
| 1 | 146-A | 21 | PRO |
| 1 | 147-A | 131 | ASP |
| 1 | 148-A | 129 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 148-A | 130 | PRO |
| 1 | 148-A | 137 | PHE |
| 1 | 149-A | 130 | PRO |
| 1 | 149-A | 131 | ASP |
| 1 | 150-A | 128 | TYR |
| 1 | 150-A | 129 | GLU |
| 1 | 150-A | 131 | ASP |
| 1 | 150-A | 137 | PHE |
| 1 | 152-A | 67 | GLY |
| 1 | 154-A | 67 | GLY |
| 1 | 156-A | 65 | GLN |
| 1 | 156-A | 131 | ASP |
| 1 | 157-A | 87 | ASP |
| 1 | 157-A | 129 | GLU |
| 1 | 157-A | 131 | ASP |
| 1 | 158-A | 87 | ASP |
| 1 | 158-A | 130 | PRO |
| 1 | 159-A | 65 | GLN |
| 1 | 159-A | 66 | PRO |
| 1 | 159-A | 87 | ASP |
| 1 | 159-A | 129 | GLU |
| 1 | 159-A | 130 | PRO |
| 1 | 160-A | 65 | GLN |
| 1 | 160-A | 129 | GLU |
| 1 | 160-A | 130 | PRO |
| 1 | 160-A | 131 | ASP |
| 1 | 161-A | 18 | ASN |
| 1 | 161-A | 130 | PRO |
| 1 | 161-A | 131 | ASP |
| 1 | 162-A | 128 | TYR |
| 1 | 162-A | 130 | PRO |
| 1 | 162-A | 131 | ASP |
| 1 | 163-A | 130 | PRO |
| 1 | 163-A | 131 | ASP |
| 1 | 164-A | 128 | TYR |
| 1 | 164-A | 129 | GLU |
| 1 | 164-A | 130 | PRO |
| 1 | 164-A | 132 | ASP |
| 1 | 165-A | 68 | THR |
| 1 | 165-A | 129 | GLU |
| 1 | 165-A | 130 | PRO |
| 1 | 165-A | 131 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 165-A | 132 | ASP |
| 1 | 166-A | 68 | THR |
| 1 | 166-A | 129 | GLU |
| 1 | 166-A | 130 | PRO |
| 1 | 167-A | 68 | THR |
| 1 | 167-A | 129 | GLU |
| 1 | 167-A | 130 | PRO |
| 1 | 167-A | 131 | ASP |
| 1 | 167-A | 132 | ASP |
| 1 | 2-A | 18 | ASN |
| 1 | 2-A | 129 | GLU |
| 1 | 3-A | 17 | GLU |
| 1 | 6-A | 130 | PRO |
| 1 | 7-A | 137 | PHE |
| 1 | 8-A | 16 | MET |
| 1 | 10-A | 128 | TYR |
| 1 | 11-A | 16 | MET |
| 1 | 11-A | 68 | THR |
| 1 | 11-A | 119 | VAL |
| 1 | 13-A | 21 | PRO |
| 1 | 13-A | 22 | TRP |
| 1 | 15-A | 20 | MET |
| 1 | 16-A | 21 | PRO |
| 1 | 17-A | 120 | GLU |
| 1 | 18-A | 120 | GLU |
| 1 | 19-A | 144 | ASP |
| 1 | 25-A | 88 | VAL |
| 1 | 27-A | 18 | ASN |
| 1 | 27-A | 19 | ALA |
| 1 | 28-A | 19 | ALA |
| 1 | 28-A | 90 | GLU |
| 1 | 30-A | 50 | ILE |
| 1 | 32-A | 17 | GLU |
| 1 | 32-A | 87 | ASP |
| 1 | 32-A | 89 | PRO |
| 1 | 32-A | 119 | VAL |
| 1 | 32-A | 128 | TYR |
| 1 | 32-A | 129 | GLU |
| 1 | 33-A | 17 | GLU |
| 1 | 33-A | 18 | ASN |
| 1 | 33-A | 86 | GLY |
| 1 | 33-A | 88 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 33-A | 90 | GLU |
| 1 | 33-A | 142 | ASP |
| 1 | 34-A | 17 | GLU |
| 1 | 34-A | 86 | GLY |
| 1 | 34-A | 89 | PRO |
| 1 | 34-A | 119 | VAL |
| 1 | 34-A | 131 | ASP |
| 1 | 35-A | 88 | VAL |
| 1 | 36-A | 18 | ASN |
| 1 | 36-A | 90 | GLU |
| 1 | 37-A | 128 | TYR |
| 1 | 37-A | 143 | ALA |
| 1 | 39-A | 17 | GLU |
| 1 | 39-A | 18 | ASN |
| 1 | 40-A | 87 | ASP |
| 1 | 41-A | 17 | GLU |
| 1 | 41-A | 87 | ASP |
| 1 | 42-A | 87 | ASP |
| 1 | 43-A | 67 | GLY |
| 1 | 43-A | 88 | VAL |
| 1 | 43-A | 121 | GLY |
| 1 | 44-A | 120 | GLU |
| 1 | 45-A | 85 | CYS |
| 1 | 49-A | 69 | ASP |
| 1 | 50-A | 88 | VAL |
| 1 | 51-A | 85 | CYS |
| 1 | 51-A | 87 | ASP |
| 1 | 52-A | 87 | ASP |
| 1 | 53-A | 85 | CYS |
| 1 | 55-A | 21 | PRO |
| 1 | 60-A | 17 | GLU |
| 1 | 68-A | 19 | ALA |
| 1 | 70-A | 19 | ALA |
| 1 | 70-A | 22 | TRP |
| 1 | 71-A | 65 | GLN |
| 1 | 71-A | 66 | PRO |
| 1 | 71-A | 67 | GLY |
| 1 | 71-A | 131 | ASP |
| 1 | 72-A | 18 | ASN |
| 1 | 72-A | 19 | ALA |
| 1 | 73-A | 2 | ILE |
| 1 | 73-A | 143 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 75-A | 127 | ASP |
| 1 | 76-A | 17 | GLU |
| 1 | 77-A | 18 | ASN |
| 1 | 77-A | 21 | PRO |
| 1 | 78-A | 50 | ILE |
| 1 | 82-A | 128 | TYR |
| 1 | 83-A | 127 | ASP |
| 1 | 83-A | 128 | TYR |
| 1 | 84-A | 127 | ASP |
| 1 | 84-A | 137 | PHE |
| 1 | 85-A | 87 | ASP |
| 1 | 85-A | 120 | GLU |
| 1 | 85-A | 137 | PHE |
| 1 | 87-A | 126 | PRO |
| 1 | 89-A | 131 | ASP |
| 1 | 90-A | 130 | PRO |
| 1 | 92-A | 129 | GLU |
| 1 | 94-A | 19 | ALA |
| 1 | 94-A | 121 | GLY |
| 1 | 96-A | 17 | GLU |
| 1 | 100-A | 18 | ASN |
| 1 | 100-A | 21 | PRO |
| 1 | 101-A | 17 | GLU |
| 1 | 101-A | 18 | ASN |
| 1 | 103-A | 17 | GLU |
| 1 | 103-A | 18 | ASN |
| 1 | 104-A | 18 | ASN |
| 1 | 105-A | 18 | ASN |
| 1 | 106-A | 18 | ASN |
| 1 | 106-A | 51 | GLY |
| 1 | 108-A | 17 | GLU |
| 1 | 108-A | 86 | GLY |
| 1 | 109-A | 49 | SER |
| 1 | 109-A | 67 | GLY |
| 1 | 110-A | 17 | GLU |
| 1 | 110-A | 22 | TRP |
| 1 | 112-A | 128 | TYR |
| 1 | 113-A | 22 | TRP |
| 1 | 113-A | 23 | ASN |
| 1 | 113-A | 87 | ASP |
| 1 | 114-A | 18 | ASN |
| 1 | 114-A | 120 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 115-A | 18 | ASN |
| 1 | 122-A | 121 | GLY |
| 1 | 122-A | 136 | VAL |
| 1 | 123-A | 21 | PRO |
| 1 | 125-A | 23 | ASN |
| 1 | 125-A | 120 | GLU |
| 1 | 125-A | 130 | PRO |
| 1 | 128-A | 121 | GLY |
| 1 | 129-A | 121 | GLY |
| 1 | 130-A | 67 | GLY |
| 1 | 131-A | 121 | GLY |
| 1 | 134-A | 121 | GLY |
| 1 | 134-A | 122 | ASP |
| 1 | 136-A | 18 | ASN |
| 1 | 136-A | 130 | PRO |
| 1 | 137-A | 132 | ASP |
| 1 | 140-A | 132 | ASP |
| 1 | 142-A | 132 | ASP |
| 1 | 144-A | 18 | ASN |
| 1 | 148-A | 131 | ASP |
| 1 | 150-A | 86 | GLY |
| 1 | 151-A | 67 | GLY |
| 1 | 153-A | 67 | GLY |
| 1 | 155-A | 18 | ASN |
| 1 | 155-A | 65 | GLN |
| 1 | 155-A | 67 | GLY |
| 1 | 156-A | 119 | VAL |
| 1 | 157-A | 130 | PRO |
| 1 | 158-A | 21 | PRO |
| 1 | 158-A | 66 | PRO |
| 1 | 159-A | 67 | GLY |
| 1 | 160-A | 90 | GLU |
| 1 | 161-A | 128 | TYR |
| 1 | 164-A | 131 | ASP |
| 1 | 165-A | 21 | PRO |
| 1 | 165-A | 22 | TRP |
| 1 | 1-A | 17 | GLU |
| 1 | 2-A | 130 | PRO |
| 1 | 5-A | 127 | ASP |
| 1 | 8-A | 128 | TYR |
| 1 | 10-A | 17 | GLU |
| 1 | 14-A | 17 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 18-A | 17 | GLU |
| 1 | 22-A | 17 | GLU |
| 1 | 24-A | 19 | ALA |
| 1 | 25-A | 85 | CYS |
| 1 | 31-A | 128 | TYR |
| 1 | 35-A | 89 | PRO |
| 1 | 36-A | 23 | ASN |
| 1 | 38-A | 145 | ALA |
| 1 | 40-A | 137 | PHE |
| 1 | 41-A | 19 | ALA |
| 1 | 42-A | 120 | GLU |
| 1 | 46-A | 21 | PRO |
| 1 | 46-A | 89 | PRO |
| 1 | 47-A | 87 | ASP |
| 1 | 48-A | 131 | ASP |
| 1 | 62-A | 67 | GLY |
| 1 | 67-A | 18 | ASN |
| 1 | 70-A | 21 | PRO |
| 1 | 71-A | 21 | PRO |
| 1 | 76-A | 87 | ASP |
| 1 | 78-A | 128 | TYR |
| 1 | 78-A | 130 | PRO |
| 1 | 79-A | 126 | PRO |
| 1 | 79-A | 128 | TYR |
| 1 | 82-A | 131 | ASP |
| 1 | 87-A | 130 | PRO |
| 1 | 92-A | 21 | PRO |
| 1 | 95-A | 18 | ASN |
| 1 | 95-A | 19 | ALA |
| 1 | 101-A | 22 | TRP |
| 1 | 109-A | 22 | TRP |
| 1 | 110-A | 66 | PRO |
| 1 | 110-A | 139 | GLU |
| 1 | 113-A | 19 | ALA |
| 1 | 118-A | 18 | ASN |
| 1 | 118-A | 23 | ASN |
| 1 | 121-A | 21 | PRO |
| 1 | 122-A | 21 | PRO |
| 1 | 122-A | 23 | ASN |
| 1 | 123-A | 130 | PRO |
| 1 | 125-A | 87 | ASP |
| 1 | 128-A | 66 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 132-A | 128 | TYR |
| 1 | 137-A | 11 | ASP |
| 1 | 137-A | 130 | PRO |
| 1 | 138-A | 137 | PHE |
| 1 | 141-A | 130 | PRO |
| 1 | 144-A | 130 | PRO |
| 1 | 145-A | 18 | ASN |
| 1 | 146-A | 66 | PRO |
| 1 | 146-A | 120 | GLU |
| 1 | 147-A | 137 | PHE |
| 1 | 153-A | 18 | ASN |
| 1 | 154-A | 18 | ASN |
| 1 | 157-A | 66 | PRO |
| 1 | 158-A | 69 | ASP |
| 1 | 158-A | 129 | GLU |
| 1 | 163-A | 129 | GLU |
| 1 | 167-A | 66 | PRO |
| 1 | 5-A | 87 | ASP |
| 1 | 10-A | 16 | MET |
| 1 | 18-A | 137 | PHE |
| 1 | 25-A | 16 | MET |
| 1 | 28-A | 17 | GLU |
| 1 | 29-A | 50 | ILE |
| 1 | 29-A | 53 | PRO |
| 1 | 30-A | 18 | ASN |
| 1 | 31-A | 86 | GLY |
| 1 | 31-A | 90 | GLU |
| 1 | 32-A | 20 | MET |
| 1 | 34-A | 90 | GLU |
| 1 | 36-A | 21 | PRO |
| 1 | 37-A | 19 | ALA |
| 1 | 37-A | 88 | VAL |
| 1 | 37-A | 142 | ASP |
| 1 | 39-A | 88 | VAL |
| 1 | 44-A | 17 | GLU |
| 1 | 45-A | 21 | PRO |
| 1 | 47-A | 17 | GLU |
| 1 | 47-A | 119 | VAL |
| 1 | 51-A | 21 | PRO |
| 1 | 51-A | 120 | GLU |
| 1 | 61-A | 137 | PHE |
| 1 | 66-A | 128 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 70-A | 18 | ASN |
| 1 | 73-A | 18 | ASN |
| 1 | 73-A | 21 | PRO |
| 1 | 80-A | 21 | PRO |
| 1 | 82-A | 129 | GLU |
| 1 | 83-A | 131 | ASP |
| 1 | 85-A | 21 | PRO |
| 1 | 97-A | 21 | PRO |
| 1 | 102-A | 17 | GLU |
| 1 | 107-A | 17 | GLU |
| 1 | 109-A | 89 | PRO |
| 1 | 112-A | 20 | MET |
| 1 | 114-A | 2 | ILE |
| 1 | 116-A | 22 | TRP |
| 1 | 116-A | 24 | LEU |
| 1 | 123-A | 127 | ASP |
| 1 | 124-A | 88 | VAL |
| 1 | 128-A | 22 | TRP |
| 1 | 131-A | 129 | GLU |
| 1 | 138-A | 130 | PRO |
| 1 | 139-A | 130 | PRO |
| 1 | 140-A | 130 | PRO |
| 1 | 141-A | 132 | ASP |
| 1 | 142-A | 18 | ASN |
| 1 | 142-A | 49 | SER |
| 1 | 142-A | 129 | GLU |
| 1 | 143-A | 132 | ASP |
| 1 | 144-A | 19 | ALA |
| 1 | 145-A | 19 | ALA |
| 1 | 146-A | 130 | PRO |
| 1 | 147-A | 129 | GLU |
| 1 | 152-A | 21 | PRO |
| 1 | 152-A | 22 | TRP |
| 1 | 152-A | 131 | ASP |
| 1 | 153-A | 22 | TRP |
| 1 | 153-A | 129 | GLU |
| 1 | 156-A | 18 | ASN |
| 1 | 158-A | 22 | TRP |
| 1 | 163-A | 18 | ASN |
| 1 | 167-A | 50 | ILE |
| 1 | 4-A | 21 | PRO |
| 1 | 7-A | 20 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 9-A | 16 | MET |
| 1 | 10-A | 20 | MET |
| 1 | 16-A | 129 | GLU |
| 1 | 21-A | 127 | ASP |
| 1 | 25-A | 21 | PRO |
| 1 | 27-A | 88 | VAL |
| 1 | 28-A | 20 | MET |
| 1 | 29-A | 69 | ASP |
| 1 | 29-A | 129 | GLU |
| 1 | 30-A | 54 | LEU |
| 1 | 33-A | 129 | GLU |
| 1 | 34-A | 129 | GLU |
| 1 | 37-A | 21 | PRO |
| 1 | 41-A | 88 | VAL |
| 1 | 41-A | 122 | ASP |
| 1 | 42-A | 69 | ASP |
| 1 | 48-A | 86 | GLY |
| 1 | 49-A | 86 | GLY |
| 1 | 49-A | 127 | ASP |
| 1 | 54-A | 21 | PRO |
| 1 | 69-A | 127 | ASP |
| 1 | 70-A | 17 | GLU |
| 1 | 72-A | 66 | PRO |
| 1 | 78-A | 19 | ALA |
| 1 | 80-A | 16 | MET |
| 1 | 82-A | 130 | PRO |
| 1 | 90-A | 18 | ASN |
| 1 | 94-A | 128 | TYR |
| 1 | 98-A | 144 | ASP |
| 1 | 107-A | 137 | PHE |
| 1 | 114-A | 19 | ALA |
| 1 | 134-A | 54 | LEU |
| 1 | 143-A | 16 | MET |
| 1 | 143-A | 21 | PRO |
| 1 | 143-A | 130 | PRO |
| 1 | 145-A | 66 | PRO |
| 1 | 146-A | 20 | MET |
| 1 | 146-A | 129 | GLU |
| 1 | 156-A | 66 | PRO |
| 1 | 156-A | 130 | PRO |
| 1 | 158-A | 65 | GLN |
| 1 | 4-A | 137 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 17-A | 16 | MET |
| 1 | 24-A | 18 | ASN |
| 1 | 31-A | 129 | GLU |
| 1 | 33-A | 20 | MET |
| 1 | 34-A | 21 | PRO |
| 1 | 35-A | 17 | GLU |
| 1 | 38-A | 20 | MET |
| 1 | 60-A | 129 | GLU |
| 1 | 62-A | 22 | TRP |
| 1 | 70-A | 67 | GLY |
| 1 | 89-A | 130 | PRO |
| 1 | 98-A | 21 | PRO |
| 1 | 100-A | 87 | ASP |
| 1 | 111-A | 17 | GLU |
| 1 | 111-A | 18 | ASN |
| 1 | 111-A | 130 | PRO |
| 1 | 113-A | 126 | PRO |
| 1 | 122-A | 22 | TRP |
| 1 | 123-A | 11 | ASP |
| 1 | 124-A | 129 | GLU |
| 1 | 125-A | 88 | VAL |
| 1 | 131-A | 51 | GLY |
| 1 | 137-A | 50 | ILE |
| 1 | 139-A | 17 | GLU |
| 1 | 147-A | 136 | VAL |
| 1 | 148-A | 50 | ILE |
| 1 | 4-A | 129 | GLU |
| 1 | 5-A | 52 | ARG |
| 1 | 40-A | 88 | VAL |
| 1 | 76-A | 21 | PRO |
| 1 | 103-A | 21 | PRO |
| 1 | 103-A | 86 | GLY |
| 1 | 109-A | 21 | PRO |
| 1 | 132-A | 121 | GLY |
| 1 | 142-A | 21 | PRO |
| 1 | 143-A | 129 | GLU |
| 1 | 151-A | 21 | PRO |
| 1 | 151-A | 136 | VAL |
| 1 | 154-A | 130 | PRO |
| 1 | 155-A | 21 | PRO |
| 1 | 155-A | 66 | PRO |
| 1 | 161-A | 129 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 3-A | 129 | GLU |
| 1 | 6-A | 20 | MET |
| 1 | 16-A | 20 | MET |
| 1 | 19-A | 136 | VAL |
| 1 | 29-A | 67 | GLY |
| 1 | 60-A | 130 | PRO |
| 1 | 66-A | 119 | VAL |
| 1 | 89-A | 129 | GLU |
| 1 | 111-A | 20 | MET |
| 1 | 118-A | 20 | MET |
| 1 | 155-A | 130 | PRO |
| 1 | 8-A | 67 | GLY |
| 1 | 10-A | 66 | PRO |
| 1 | 44-A | 129 | GLU |
| 1 | 51-A | 119 | VAL |
| 1 | 51-A | 129 | GLU |
| 1 | 79-A | 129 | GLU |
| 1 | 86-A | 21 | PRO |
| 1 | 95-A | 121 | GLY |
| 1 | 117-A | 20 | MET |
| 1 | 130-A | 21 | PRO |
| 1 | 133-A | 51 | GLY |
| 1 | 137-A | 129 | GLU |
| 1 | 150-A | 21 | PRO |
| 1 | 162-A | 66 | PRO |
| 1 | 5-A | 129 | GLU |
| 1 | 6-A | 129 | GLU |
| 1 | 42-A | 88 | VAL |
| 1 | 118-A | 136 | VAL |
| 1 | 139-A | 21 | PRO |
| 1 | 112-A | 126 | PRO |
| 1 | 135-A | 52 | ARG |
| 1 | 162-A | 129 | GLU |

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 | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 2-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 3-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 4-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 5-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 21 | 1 |
| 1 | 6-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 7-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 8-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 9-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 10-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 17 | 1 |
| 1 | 11-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 12-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 13-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 21 | 1 |
| 1 | 14-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 15-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 16-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 17-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 15 | 1 |
| 1 | 18-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 24 | 2 |
| 1 | 19-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 15 | 1 |
| 1 | 20-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 21-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 17 | 1 |
| 1 | 22-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 12 | 0 |
| 1 | 23-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 24-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 12 | 0 |
| 1 | 25-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 26-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 12 | 0 |
| 1 | 27-A | 136/136 (100%) | 117 (86%) | 19 (14%) | 4 | 0 |
| 1 | 28-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 29-A | 136/136 (100%) | 116 (85%) | 20 (15%) | 4 | 0 |
| 1 | 30-A | 136/136 (100%) | 115 (85%) | 21 (15%) | 3 | 0 |
| 1 | 31-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 32-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 33-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 34-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 35-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 36-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 37-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 38-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 39-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 40-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 41-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 42-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 15 | 1 |
| 1 | 43-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 15 | 1 |
| 1 | 44-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 45-A | 136/136 (100%) | 118 (87%) | 18 (13%) | 5 | 0 |
| 1 | 46-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 47-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 48-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 12 | 0 |
| 1 | 49-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 15 | 1 |
| 1 | 50-A | 136/136 (100%) | 115 (85%) | 21 (15%) | 3 | 0 |
| 1 | 51-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 52-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 53-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 54-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 55-A | 136/136 (100%) | 118 (87%) | 18 (13%) | 5 | 0 |
| 1 | 56-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 57-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 58-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 15 | 1 |
| 1 | 59-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 21 | 1 |
| 1 | 60-A | 136/136 (100%) | 114 (84%) | 22 (16%) | 3 | 0 |
| 1 | 61-A | 136/136 (100%) | 118 (87%) | 18 (13%) | 5 | 0 |
| 1 | 62-A | 136/136 (100%) | 118 (87%) | 18 (13%) | 5 | 0 |
| 1 | 63-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 17 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 64-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 65-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 66-A | 136/136 (100%) | 118 (87%) | 18 (13%) | 5 | 0 |
| 1 | 67-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 68-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 12 | 0 |
| 1 | 69-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 70-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 71-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 21 | 1 |
| 1 | 72-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 73-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 74-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 75-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 76-A | 136/136 (100%) | 118 (87%) | 18 (13%) | 5 | 0 |
| 1 | 77-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 78-A | 136/136 (100%) | 118 (87%) | 18 (13%) | 5 | 0 |
| 1 | 79-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 80-A | 136/136 (100%) | 115 (85%) | 21 (15%) | 3 | 0 |
| 1 | 81-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 82-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 83-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 21 | 1 |
| 1 | 84-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 21 | 1 |
| 1 | 85-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 12 | 0 |
| 1 | 86-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 87-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 15 | 1 |
| 1 | 88-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 89-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 90-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 91-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 92-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 12 | 0 |
| 1 | 93-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 94-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 95-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 96-A | 136/136 (100%) | 117 (86%) | 19 (14%) | 4 | 0 |
| 1 | 97-A | 136/136 (100%) | 118 (87%) | 18 (13%) | 5 | 0 |
| 1 | 98-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 99-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 100-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 101-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 21 | 1 |
| 1 | 102-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 103-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 104-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 15 | 1 |
| 1 | 105-A | 136/136 (100%) | 118 (87%) | 18 (13%) | 5 | 0 |
| 1 | 106-A | 136/136 (100%) | 114 (84%) | 22 (16%) | 3 | 0 |
| 1 | 107-A | 136/136 (100%) | 114 (84%) | 22 (16%) | 3 | 0 |
| 1 | 108-A | 136/136 (100%) | 118 (87%) | 18 (13%) | 5 | 0 |
| 1 | 109-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 110-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 111-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 12 | 0 |
| 1 | 112-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 113-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 114-A | 136/136 (100%) | 116 (85%) | 20 (15%) | 4 | 0 |
| 1 | 115-A | 136/136 (100%) | 115 (85%) | 21 (15%) | 3 | 0 |
| 1 | 116-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 117-A | 136/136 (100%) | 118 (87%) | 18 (13%) | 5 | 0 |
| 1 | 118-A | 136/136 (100%) | 116 (85%) | 20 (15%) | 4 | 0 |
| 1 | 119-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 120-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 17 | 1 |
| 1 | 121-A | 136/136 (100%) | 118 (87%) | 18 (13%) | 5 | 0 |
| 1 | 122-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 123-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 124-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 12 | 0 |
| 1 | 125-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 12 | 0 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 126-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 15 | 1 |
| 1 | 127-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 15 | 1 |
| 1 | 128-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 129-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 17 | 1 |
| 1 | 130-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 24 | 2 |
| 1 | 131-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 12 | 0 |
| 1 | 132-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 17 | 1 |
| 1 | 133-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 15 | 1 |
| 1 | 134-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 135-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 15 | 1 |
| 1 | 136-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 9 | 0 |
| 1 | 137-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 138-A | 136/136 (100%) | 117 (86%) | 19 (14%) | 4 | 0 |
| 1 | 139-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 140-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 141-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 142-A | 136/136 (100%) | 117 (86%) | 19 (14%) | 4 | 0 |
| 1 | 143-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 144-A | 136/136 (100%) | 113 (83%) | 23 (17%) | 2 | 0 |
| 1 | 145-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 146-A | 136/136 (100%) | 117 (86%) | 19 (14%) | 4 | 0 |
| 1 | 147-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 148-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 149-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 12 | 0 |
| 1 | 150-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 6 | 0 |
| 1 | 151-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 152-A | 136/136 (100%) | 130 (96%) | 6 (4%) | 35 | 5 |
| 1 | 153-A | 136/136 (100%) | 116 (85%) | 20 (15%) | 4 | 0 |
| 1 | 154-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 155-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 156-A | 136/136 (100%) | 117 (86%) | 19 (14%) | 4 | 0 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|--------------------|-------------|------------|-------------|---|
| 1 | 157-A | 136/136 (100%) | 116 (85%) | 20 (15%) | 4 | 0 |
| 1 | 158-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 159-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 160-A | 136/136 (100%) | 118 (87%) | 18 (13%) | 5 | 0 |
| 1 | 161-A | 136/136 (100%) | 116 (85%) | 20 (15%) | 4 | 0 |
| 1 | 162-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 8 | 0 |
| 1 | 163-A | 136/136 (100%) | 118 (87%) | 18 (13%) | 5 | 0 |
| 1 | 164-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 6 | 0 |
| 1 | 165-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 10 | 0 |
| 1 | 166-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 12 | 0 |
| 1 | 167-A | 136/136 (100%) | 115 (85%) | 21 (15%) | 3 | 0 |
| All | All | 22712/22712 (100%) | 20232 (89%) | 2480 (11%) | 8 | 0 |

All (2480) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1-A | 4 | LEU |
| 1 | 1-A | 20 | MET |
| 1 | 1-A | 23 | ASN |
| 1 | 1-A | 24 | LEU |
| 1 | 1-A | 52 | ARG |
| 1 | 1-A | 106 | LYS |
| 1 | 1-A | 109 | LYS |
| 1 | 1-A | 111 | TYR |
| 1 | 1-A | 119 | VAL |
| 1 | 1-A | 129 | GLU |
| 1 | 1-A | 138 | SER |
| 1 | 1-A | 148 | SER |
| 1 | 1-A | 156 | LEU |
| 1 | 1-A | 157 | GLU |
| 1 | 2-A | 16 | MET |
| 1 | 2-A | 17 | GLU |
| 1 | 2-A | 33 | ARG |
| 1 | 2-A | 38 | LYS |
| 1 | 2-A | 52 | ARG |
| 1 | 2-A | 106 | LYS |
| 1 | 2-A | 109 | LYS |
| 1 | 2-A | 119 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 2-A | 128 | TYR |
| 1 | 2-A | 129 | GLU |
| 1 | 2-A | 134 | GLU |
| 1 | 2-A | 148 | SER |
| 1 | 2-A | 156 | LEU |
| 1 | 2-A | 159 | ARG |
| 1 | 3-A | 1 | MET |
| 1 | 3-A | 2 | ILE |
| 1 | 3-A | 16 | MET |
| 1 | 3-A | 17 | GLU |
| 1 | 3-A | 20 | MET |
| 1 | 3-A | 33 | ARG |
| 1 | 3-A | 44 | ARG |
| 1 | 3-A | 49 | SER |
| 1 | 3-A | 52 | ARG |
| 1 | 3-A | 59 | ASN |
| 1 | 3-A | 106 | LYS |
| 1 | 3-A | 118 | GLU |
| 1 | 3-A | 119 | VAL |
| 1 | 3-A | 128 | TYR |
| 1 | 3-A | 129 | GLU |
| 1 | 3-A | 135 | SER |
| 1 | 3-A | 148 | SER |
| 1 | 4-A | 4 | LEU |
| 1 | 4-A | 11 | ASP |
| 1 | 4-A | 17 | GLU |
| 1 | 4-A | 20 | MET |
| 1 | 4-A | 23 | ASN |
| 1 | 4-A | 24 | LEU |
| 1 | 4-A | 33 | ARG |
| 1 | 4-A | 52 | ARG |
| 1 | 4-A | 60 | ILE |
| 1 | 4-A | 70 | ASP |
| 1 | 4-A | 108 | GLN |
| 1 | 4-A | 109 | LYS |
| 1 | 4-A | 118 | GLU |
| 1 | 4-A | 123 | THR |
| 1 | 4-A | 132 | ASP |
| 1 | 5-A | 17 | GLU |
| 1 | 5-A | 20 | MET |
| 1 | 5-A | 33 | ARG |
| 1 | 5-A | 38 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 5-A | 60 | ILE |
| 1 | 5-A | 70 | ASP |
| 1 | 5-A | 108 | GLN |
| 1 | 5-A | 128 | TYR |
| 1 | 5-A | 129 | GLU |
| 1 | 6-A | 1 | MET |
| 1 | 6-A | 18 | ASN |
| 1 | 6-A | 20 | MET |
| 1 | 6-A | 24 | LEU |
| 1 | 6-A | 33 | ARG |
| 1 | 6-A | 36 | LEU |
| 1 | 6-A | 37 | ASN |
| 1 | 6-A | 52 | ARG |
| 1 | 6-A | 70 | ASP |
| 1 | 6-A | 79 | ASP |
| 1 | 6-A | 108 | GLN |
| 1 | 6-A | 118 | GLU |
| 1 | 6-A | 123 | THR |
| 1 | 6-A | 128 | TYR |
| 1 | 6-A | 129 | GLU |
| 1 | 6-A | 136 | VAL |
| 1 | 6-A | 152 | CYS |
| 1 | 7-A | 10 | VAL |
| 1 | 7-A | 17 | GLU |
| 1 | 7-A | 18 | ASN |
| 1 | 7-A | 20 | MET |
| 1 | 7-A | 33 | ARG |
| 1 | 7-A | 36 | LEU |
| 1 | 7-A | 38 | LYS |
| 1 | 7-A | 52 | ARG |
| 1 | 7-A | 70 | ASP |
| 1 | 7-A | 79 | ASP |
| 1 | 7-A | 87 | ASP |
| 1 | 7-A | 108 | GLN |
| 1 | 7-A | 123 | THR |
| 1 | 7-A | 128 | TYR |
| 1 | 7-A | 142 | ASP |
| 1 | 7-A | 148 | SER |
| 1 | 7-A | 156 | LEU |
| 1 | 8-A | 1 | MET |
| 1 | 8-A | 4 | LEU |
| 1 | 8-A | 17 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 8-A | 18 | ASN |
| 1 | 8-A | 20 | MET |
| 1 | 8-A | 24 | LEU |
| 1 | 8-A | 38 | LYS |
| 1 | 8-A | 59 | ASN |
| 1 | 8-A | 60 | ILE |
| 1 | 8-A | 87 | ASP |
| 1 | 8-A | 104 | LEU |
| 1 | 8-A | 128 | TYR |
| 1 | 8-A | 156 | LEU |
| 1 | 9-A | 1 | MET |
| 1 | 9-A | 16 | MET |
| 1 | 9-A | 24 | LEU |
| 1 | 9-A | 30 | TRP |
| 1 | 9-A | 65 | GLN |
| 1 | 9-A | 76 | LYS |
| 1 | 9-A | 87 | ASP |
| 1 | 9-A | 104 | LEU |
| 1 | 9-A | 108 | GLN |
| 1 | 9-A | 127 | ASP |
| 1 | 9-A | 129 | GLU |
| 1 | 9-A | 138 | SER |
| 1 | 9-A | 156 | LEU |
| 1 | 10-A | 1 | MET |
| 1 | 10-A | 17 | GLU |
| 1 | 10-A | 20 | MET |
| 1 | 10-A | 59 | ASN |
| 1 | 10-A | 104 | LEU |
| 1 | 10-A | 106 | LYS |
| 1 | 10-A | 118 | GLU |
| 1 | 10-A | 126 | PRO |
| 1 | 10-A | 127 | ASP |
| 1 | 10-A | 156 | LEU |
| 1 | 11-A | 1 | MET |
| 1 | 11-A | 8 | LEU |
| 1 | 11-A | 16 | MET |
| 1 | 11-A | 17 | GLU |
| 1 | 11-A | 18 | ASN |
| 1 | 11-A | 20 | MET |
| 1 | 11-A | 24 | LEU |
| 1 | 11-A | 38 | LYS |
| 1 | 11-A | 45 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 11-A | 87 | ASP |
| 1 | 11-A | 104 | LEU |
| 1 | 11-A | 106 | LYS |
| 1 | 11-A | 120 | GLU |
| 1 | 11-A | 129 | GLU |
| 1 | 11-A | 139 | GLU |
| 1 | 11-A | 156 | LEU |
| 1 | 12-A | 1 | MET |
| 1 | 12-A | 17 | GLU |
| 1 | 12-A | 18 | ASN |
| 1 | 12-A | 33 | ARG |
| 1 | 12-A | 38 | LYS |
| 1 | 12-A | 52 | ARG |
| 1 | 12-A | 61 | ILE |
| 1 | 12-A | 68 | THR |
| 1 | 12-A | 88 | VAL |
| 1 | 12-A | 104 | LEU |
| 1 | 12-A | 106 | LYS |
| 1 | 12-A | 118 | GLU |
| 1 | 12-A | 128 | TYR |
| 1 | 12-A | 129 | GLU |
| 1 | 12-A | 134 | GLU |
| 1 | 12-A | 138 | SER |
| 1 | 12-A | 156 | LEU |
| 1 | 13-A | 1 | MET |
| 1 | 13-A | 10 | VAL |
| 1 | 13-A | 18 | ASN |
| 1 | 13-A | 58 | LYS |
| 1 | 13-A | 104 | LEU |
| 1 | 13-A | 106 | LYS |
| 1 | 13-A | 118 | GLU |
| 1 | 13-A | 128 | TYR |
| 1 | 13-A | 129 | GLU |
| 1 | 14-A | 1 | MET |
| 1 | 14-A | 17 | GLU |
| 1 | 14-A | 20 | MET |
| 1 | 14-A | 24 | LEU |
| 1 | 14-A | 33 | ARG |
| 1 | 14-A | 37 | ASN |
| 1 | 14-A | 44 | ARG |
| 1 | 14-A | 61 | ILE |
| 1 | 14-A | 65 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 14-A | 101 | GLU |
| 1 | 14-A | 104 | LEU |
| 1 | 14-A | 115 | ILE |
| 1 | 14-A | 128 | TYR |
| 1 | 14-A | 129 | GLU |
| 1 | 14-A | 134 | GLU |
| 1 | 15-A | 4 | LEU |
| 1 | 15-A | 17 | GLU |
| 1 | 15-A | 20 | MET |
| 1 | 15-A | 33 | ARG |
| 1 | 15-A | 38 | LYS |
| 1 | 15-A | 52 | ARG |
| 1 | 15-A | 61 | ILE |
| 1 | 15-A | 65 | GLN |
| 1 | 15-A | 87 | ASP |
| 1 | 15-A | 101 | GLU |
| 1 | 15-A | 104 | LEU |
| 1 | 15-A | 109 | LYS |
| 1 | 15-A | 118 | GLU |
| 1 | 15-A | 129 | GLU |
| 1 | 15-A | 148 | SER |
| 1 | 15-A | 158 | ARG |
| 1 | 16-A | 4 | LEU |
| 1 | 16-A | 17 | GLU |
| 1 | 16-A | 20 | MET |
| 1 | 16-A | 22 | TRP |
| 1 | 16-A | 28 | LEU |
| 1 | 16-A | 32 | LYS |
| 1 | 16-A | 33 | ARG |
| 1 | 16-A | 52 | ARG |
| 1 | 16-A | 59 | ASN |
| 1 | 16-A | 61 | ILE |
| 1 | 16-A | 118 | GLU |
| 1 | 16-A | 129 | GLU |
| 1 | 16-A | 134 | GLU |
| 1 | 16-A | 158 | ARG |
| 1 | 17-A | 16 | MET |
| 1 | 17-A | 17 | GLU |
| 1 | 17-A | 20 | MET |
| 1 | 17-A | 33 | ARG |
| 1 | 17-A | 52 | ARG |
| 1 | 17-A | 61 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 17-A | 65 | GLN |
| 1 | 17-A | 119 | VAL |
| 1 | 17-A | 128 | TYR |
| 1 | 17-A | 132 | ASP |
| 1 | 17-A | 138 | SER |
| 1 | 18-A | 10 | VAL |
| 1 | 18-A | 18 | ASN |
| 1 | 18-A | 23 | ASN |
| 1 | 18-A | 61 | ILE |
| 1 | 18-A | 104 | LEU |
| 1 | 18-A | 119 | VAL |
| 1 | 18-A | 138 | SER |
| 1 | 18-A | 152 | CYS |
| 1 | 19-A | 1 | MET |
| 1 | 19-A | 8 | LEU |
| 1 | 19-A | 18 | ASN |
| 1 | 19-A | 22 | TRP |
| 1 | 19-A | 32 | LYS |
| 1 | 19-A | 36 | LEU |
| 1 | 19-A | 52 | ARG |
| 1 | 19-A | 76 | LYS |
| 1 | 19-A | 134 | GLU |
| 1 | 19-A | 135 | SER |
| 1 | 19-A | 154 | GLU |
| 1 | 20-A | 1 | MET |
| 1 | 20-A | 8 | LEU |
| 1 | 20-A | 20 | MET |
| 1 | 20-A | 52 | ARG |
| 1 | 20-A | 59 | ASN |
| 1 | 20-A | 65 | GLN |
| 1 | 20-A | 79 | ASP |
| 1 | 20-A | 108 | GLN |
| 1 | 20-A | 111 | TYR |
| 1 | 20-A | 119 | VAL |
| 1 | 20-A | 122 | ASP |
| 1 | 20-A | 129 | GLU |
| 1 | 20-A | 148 | SER |
| 1 | 20-A | 152 | CYS |
| 1 | 20-A | 157 | GLU |
| 1 | 21-A | 24 | LEU |
| 1 | 21-A | 28 | LEU |
| 1 | 21-A | 32 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 21-A | 49 | SER |
| 1 | 21-A | 65 | GLN |
| 1 | 21-A | 70 | ASP |
| 1 | 21-A | 106 | LYS |
| 1 | 21-A | 119 | VAL |
| 1 | 21-A | 128 | TYR |
| 1 | 21-A | 157 | GLU |
| 1 | 22-A | 16 | MET |
| 1 | 22-A | 18 | ASN |
| 1 | 22-A | 24 | LEU |
| 1 | 22-A | 28 | LEU |
| 1 | 22-A | 48 | GLU |
| 1 | 22-A | 50 | ILE |
| 1 | 22-A | 52 | ARG |
| 1 | 22-A | 106 | LYS |
| 1 | 22-A | 108 | GLN |
| 1 | 22-A | 128 | TYR |
| 1 | 22-A | 138 | SER |
| 1 | 22-A | 157 | GLU |
| 1 | 23-A | 1 | MET |
| 1 | 23-A | 16 | MET |
| 1 | 23-A | 18 | ASN |
| 1 | 23-A | 23 | ASN |
| 1 | 23-A | 28 | LEU |
| 1 | 23-A | 50 | ILE |
| 1 | 23-A | 52 | ARG |
| 1 | 23-A | 59 | ASN |
| 1 | 23-A | 62 | LEU |
| 1 | 23-A | 119 | VAL |
| 1 | 23-A | 128 | TYR |
| 1 | 23-A | 148 | SER |
| 1 | 23-A | 156 | LEU |
| 1 | 23-A | 157 | GLU |
| 1 | 24-A | 23 | ASN |
| 1 | 24-A | 28 | LEU |
| 1 | 24-A | 33 | ARG |
| 1 | 24-A | 45 | HIS |
| 1 | 24-A | 52 | ARG |
| 1 | 24-A | 76 | LYS |
| 1 | 24-A | 108 | GLN |
| 1 | 24-A | 119 | VAL |
| 1 | 24-A | 122 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 24-A | 127 | ASP |
| 1 | 24-A | 148 | SER |
| 1 | 24-A | 157 | GLU |
| 1 | 25-A | 1 | MET |
| 1 | 25-A | 11 | ASP |
| 1 | 25-A | 23 | ASN |
| 1 | 25-A | 28 | LEU |
| 1 | 25-A | 52 | ARG |
| 1 | 25-A | 76 | LYS |
| 1 | 25-A | 88 | VAL |
| 1 | 25-A | 106 | LYS |
| 1 | 25-A | 119 | VAL |
| 1 | 25-A | 120 | GLU |
| 1 | 25-A | 129 | GLU |
| 1 | 25-A | 139 | GLU |
| 1 | 25-A | 142 | ASP |
| 1 | 25-A | 148 | SER |
| 1 | 25-A | 157 | GLU |
| 1 | 25-A | 158 | ARG |
| 1 | 26-A | 1 | MET |
| 1 | 26-A | 18 | ASN |
| 1 | 26-A | 23 | ASN |
| 1 | 26-A | 24 | LEU |
| 1 | 26-A | 28 | LEU |
| 1 | 26-A | 33 | ARG |
| 1 | 26-A | 52 | ARG |
| 1 | 26-A | 60 | ILE |
| 1 | 26-A | 76 | LYS |
| 1 | 26-A | 87 | ASP |
| 1 | 26-A | 106 | LYS |
| 1 | 26-A | 108 | GLN |
| 1 | 27-A | 1 | MET |
| 1 | 27-A | 20 | MET |
| 1 | 27-A | 21 | PRO |
| 1 | 27-A | 24 | LEU |
| 1 | 27-A | 28 | LEU |
| 1 | 27-A | 33 | ARG |
| 1 | 27-A | 52 | ARG |
| 1 | 27-A | 58 | LYS |
| 1 | 27-A | 60 | ILE |
| 1 | 27-A | 76 | LYS |
| 1 | 27-A | 87 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 27-A | 98 | ARG |
| 1 | 27-A | 104 | LEU |
| 1 | 27-A | 106 | LYS |
| 1 | 27-A | 108 | GLN |
| 1 | 27-A | 119 | VAL |
| 1 | 27-A | 120 | GLU |
| 1 | 27-A | 142 | ASP |
| 1 | 27-A | 159 | ARG |
| 1 | 28-A | 1 | MET |
| 1 | 28-A | 18 | ASN |
| 1 | 28-A | 49 | SER |
| 1 | 28-A | 52 | ARG |
| 1 | 28-A | 65 | GLN |
| 1 | 28-A | 76 | LYS |
| 1 | 28-A | 79 | ASP |
| 1 | 28-A | 87 | ASP |
| 1 | 28-A | 88 | VAL |
| 1 | 28-A | 104 | LEU |
| 1 | 28-A | 106 | LYS |
| 1 | 28-A | 108 | GLN |
| 1 | 28-A | 119 | VAL |
| 1 | 28-A | 120 | GLU |
| 1 | 28-A | 138 | SER |
| 1 | 28-A | 148 | SER |
| 1 | 28-A | 159 | ARG |
| 1 | 29-A | 16 | MET |
| 1 | 29-A | 18 | ASN |
| 1 | 29-A | 20 | MET |
| 1 | 29-A | 33 | ARG |
| 1 | 29-A | 52 | ARG |
| 1 | 29-A | 61 | ILE |
| 1 | 29-A | 65 | GLN |
| 1 | 29-A | 68 | THR |
| 1 | 29-A | 76 | LYS |
| 1 | 29-A | 88 | VAL |
| 1 | 29-A | 104 | LEU |
| 1 | 29-A | 106 | LYS |
| 1 | 29-A | 108 | GLN |
| 1 | 29-A | 118 | GLU |
| 1 | 29-A | 119 | VAL |
| 1 | 29-A | 120 | GLU |
| 1 | 29-A | 127 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 29-A | 128 | TYR |
| 1 | 29-A | 135 | SER |
| 1 | 29-A | 142 | ASP |
| 1 | 30-A | 2 | ILE |
| 1 | 30-A | 10 | VAL |
| 1 | 30-A | 17 | GLU |
| 1 | 30-A | 18 | ASN |
| 1 | 30-A | 33 | ARG |
| 1 | 30-A | 49 | SER |
| 1 | 30-A | 50 | ILE |
| 1 | 30-A | 52 | ARG |
| 1 | 30-A | 53 | PRO |
| 1 | 30-A | 54 | LEU |
| 1 | 30-A | 76 | LYS |
| 1 | 30-A | 88 | VAL |
| 1 | 30-A | 98 | ARG |
| 1 | 30-A | 104 | LEU |
| 1 | 30-A | 106 | LYS |
| 1 | 30-A | 108 | GLN |
| 1 | 30-A | 119 | VAL |
| 1 | 30-A | 128 | TYR |
| 1 | 30-A | 142 | ASP |
| 1 | 30-A | 157 | GLU |
| 1 | 30-A | 158 | ARG |
| 1 | 31-A | 16 | MET |
| 1 | 31-A | 23 | ASN |
| 1 | 31-A | 33 | ARG |
| 1 | 31-A | 54 | LEU |
| 1 | 31-A | 65 | GLN |
| 1 | 31-A | 76 | LYS |
| 1 | 31-A | 87 | ASP |
| 1 | 31-A | 98 | ARG |
| 1 | 31-A | 104 | LEU |
| 1 | 31-A | 106 | LYS |
| 1 | 31-A | 109 | LYS |
| 1 | 31-A | 129 | GLU |
| 1 | 31-A | 142 | ASP |
| 1 | 31-A | 156 | LEU |
| 1 | 32-A | 1 | MET |
| 1 | 32-A | 10 | VAL |
| 1 | 32-A | 16 | MET |
| 1 | 32-A | 17 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 32-A | 24 | LEU |
| 1 | 32-A | 33 | ARG |
| 1 | 32-A | 52 | ARG |
| 1 | 32-A | 54 | LEU |
| 1 | 32-A | 65 | GLN |
| 1 | 32-A | 87 | ASP |
| 1 | 32-A | 98 | ARG |
| 1 | 32-A | 106 | LYS |
| 1 | 32-A | 118 | GLU |
| 1 | 32-A | 120 | GLU |
| 1 | 32-A | 128 | TYR |
| 1 | 32-A | 142 | ASP |
| 1 | 33-A | 1 | MET |
| 1 | 33-A | 2 | ILE |
| 1 | 33-A | 16 | MET |
| 1 | 33-A | 17 | GLU |
| 1 | 33-A | 20 | MET |
| 1 | 33-A | 33 | ARG |
| 1 | 33-A | 88 | VAL |
| 1 | 33-A | 89 | PRO |
| 1 | 33-A | 106 | LYS |
| 1 | 33-A | 131 | ASP |
| 1 | 33-A | 139 | GLU |
| 1 | 33-A | 142 | ASP |
| 1 | 33-A | 158 | ARG |
| 1 | 34-A | 2 | ILE |
| 1 | 34-A | 16 | MET |
| 1 | 34-A | 33 | ARG |
| 1 | 34-A | 52 | ARG |
| 1 | 34-A | 59 | ASN |
| 1 | 34-A | 104 | LEU |
| 1 | 34-A | 106 | LYS |
| 1 | 34-A | 119 | VAL |
| 1 | 34-A | 120 | GLU |
| 1 | 34-A | 127 | ASP |
| 1 | 34-A | 128 | TYR |
| 1 | 34-A | 132 | ASP |
| 1 | 34-A | 134 | GLU |
| 1 | 34-A | 136 | VAL |
| 1 | 34-A | 139 | GLU |
| 1 | 34-A | 156 | LEU |
| 1 | 35-A | 1 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 35-A | 2 | ILE |
| 1 | 35-A | 22 | TRP |
| 1 | 35-A | 33 | ARG |
| 1 | 35-A | 50 | ILE |
| 1 | 35-A | 52 | ARG |
| 1 | 35-A | 60 | ILE |
| 1 | 35-A | 68 | THR |
| 1 | 35-A | 79 | ASP |
| 1 | 35-A | 104 | LEU |
| 1 | 35-A | 106 | LYS |
| 1 | 35-A | 108 | GLN |
| 1 | 35-A | 127 | ASP |
| 1 | 35-A | 148 | SER |
| 1 | 36-A | 4 | LEU |
| 1 | 36-A | 17 | GLU |
| 1 | 36-A | 22 | TRP |
| 1 | 36-A | 23 | ASN |
| 1 | 36-A | 24 | LEU |
| 1 | 36-A | 33 | ARG |
| 1 | 36-A | 59 | ASN |
| 1 | 36-A | 62 | LEU |
| 1 | 36-A | 65 | GLN |
| 1 | 36-A | 104 | LEU |
| 1 | 36-A | 106 | LYS |
| 1 | 36-A | 122 | ASP |
| 1 | 36-A | 131 | ASP |
| 1 | 37-A | 1 | MET |
| 1 | 37-A | 17 | GLU |
| 1 | 37-A | 21 | PRO |
| 1 | 37-A | 23 | ASN |
| 1 | 37-A | 33 | ARG |
| 1 | 37-A | 36 | LEU |
| 1 | 37-A | 65 | GLN |
| 1 | 37-A | 79 | ASP |
| 1 | 37-A | 98 | ARG |
| 1 | 37-A | 108 | GLN |
| 1 | 37-A | 118 | GLU |
| 1 | 37-A | 122 | ASP |
| 1 | 37-A | 131 | ASP |
| 1 | 37-A | 142 | ASP |
| 1 | 37-A | 156 | LEU |
| 1 | 38-A | 1 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 38-A | 10 | VAL |
| 1 | 38-A | 17 | GLU |
| 1 | 38-A | 20 | MET |
| 1 | 38-A | 23 | ASN |
| 1 | 38-A | 36 | LEU |
| 1 | 38-A | 45 | HIS |
| 1 | 38-A | 59 | ASN |
| 1 | 38-A | 65 | GLN |
| 1 | 38-A | 79 | ASP |
| 1 | 38-A | 88 | VAL |
| 1 | 38-A | 101 | GLU |
| 1 | 38-A | 104 | LEU |
| 1 | 38-A | 122 | ASP |
| 1 | 38-A | 142 | ASP |
| 1 | 38-A | 156 | LEU |
| 1 | 38-A | 157 | GLU |
| 1 | 39-A | 4 | LEU |
| 1 | 39-A | 10 | VAL |
| 1 | 39-A | 11 | ASP |
| 1 | 39-A | 16 | MET |
| 1 | 39-A | 23 | ASN |
| 1 | 39-A | 32 | LYS |
| 1 | 39-A | 65 | GLN |
| 1 | 39-A | 70 | ASP |
| 1 | 39-A | 79 | ASP |
| 1 | 39-A | 88 | VAL |
| 1 | 39-A | 119 | VAL |
| 1 | 39-A | 120 | GLU |
| 1 | 39-A | 123 | THR |
| 1 | 39-A | 129 | GLU |
| 1 | 39-A | 139 | GLU |
| 1 | 39-A | 142 | ASP |
| 1 | 39-A | 157 | GLU |
| 1 | 40-A | 1 | MET |
| 1 | 40-A | 16 | MET |
| 1 | 40-A | 18 | ASN |
| 1 | 40-A | 21 | PRO |
| 1 | 40-A | 22 | TRP |
| 1 | 40-A | 23 | ASN |
| 1 | 40-A | 52 | ARG |
| 1 | 40-A | 59 | ASN |
| 1 | 40-A | 62 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 40-A | 88 | VAL |
| 1 | 40-A | 104 | LEU |
| 1 | 40-A | 120 | GLU |
| 1 | 40-A | 122 | ASP |
| 1 | 40-A | 129 | GLU |
| 1 | 40-A | 157 | GLU |
| 1 | 40-A | 158 | ARG |
| 1 | 41-A | 8 | LEU |
| 1 | 41-A | 16 | MET |
| 1 | 41-A | 20 | MET |
| 1 | 41-A | 23 | ASN |
| 1 | 41-A | 32 | LYS |
| 1 | 41-A | 44 | ARG |
| 1 | 41-A | 48 | GLU |
| 1 | 41-A | 62 | LEU |
| 1 | 41-A | 66 | PRO |
| 1 | 41-A | 79 | ASP |
| 1 | 41-A | 87 | ASP |
| 1 | 41-A | 106 | LYS |
| 1 | 41-A | 108 | GLN |
| 1 | 41-A | 119 | VAL |
| 1 | 41-A | 120 | GLU |
| 1 | 41-A | 158 | ARG |
| 1 | 42-A | 1 | MET |
| 1 | 42-A | 48 | GLU |
| 1 | 42-A | 52 | ARG |
| 1 | 42-A | 59 | ASN |
| 1 | 42-A | 79 | ASP |
| 1 | 42-A | 87 | ASP |
| 1 | 42-A | 108 | GLN |
| 1 | 42-A | 118 | GLU |
| 1 | 42-A | 120 | GLU |
| 1 | 42-A | 155 | ILE |
| 1 | 42-A | 156 | LEU |
| 1 | 43-A | 10 | VAL |
| 1 | 43-A | 17 | GLU |
| 1 | 43-A | 24 | LEU |
| 1 | 43-A | 65 | GLN |
| 1 | 43-A | 68 | THR |
| 1 | 43-A | 87 | ASP |
| 1 | 43-A | 118 | GLU |
| 1 | 43-A | 119 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 43-A | 120 | GLU |
| 1 | 43-A | 135 | SER |
| 1 | 43-A | 156 | LEU |
| 1 | 44-A | 16 | MET |
| 1 | 44-A | 24 | LEU |
| 1 | 44-A | 36 | LEU |
| 1 | 44-A | 52 | ARG |
| 1 | 44-A | 58 | LYS |
| 1 | 44-A | 62 | LEU |
| 1 | 44-A | 65 | GLN |
| 1 | 44-A | 87 | ASP |
| 1 | 44-A | 101 | GLU |
| 1 | 44-A | 118 | GLU |
| 1 | 44-A | 120 | GLU |
| 1 | 44-A | 134 | GLU |
| 1 | 44-A | 156 | LEU |
| 1 | 45-A | 16 | MET |
| 1 | 45-A | 17 | GLU |
| 1 | 45-A | 24 | LEU |
| 1 | 45-A | 33 | ARG |
| 1 | 45-A | 36 | LEU |
| 1 | 45-A | 44 | ARG |
| 1 | 45-A | 52 | ARG |
| 1 | 45-A | 58 | LYS |
| 1 | 45-A | 65 | GLN |
| 1 | 45-A | 87 | ASP |
| 1 | 45-A | 98 | ARG |
| 1 | 45-A | 106 | LYS |
| 1 | 45-A | 118 | GLU |
| 1 | 45-A | 120 | GLU |
| 1 | 45-A | 132 | ASP |
| 1 | 45-A | 135 | SER |
| 1 | 45-A | 156 | LEU |
| 1 | 45-A | 159 | ARG |
| 1 | 46-A | 17 | GLU |
| 1 | 46-A | 33 | ARG |
| 1 | 46-A | 58 | LYS |
| 1 | 46-A | 59 | ASN |
| 1 | 46-A | 79 | ASP |
| 1 | 46-A | 87 | ASP |
| 1 | 46-A | 98 | ARG |
| 1 | 46-A | 118 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 46-A | 120 | GLU |
| 1 | 46-A | 129 | GLU |
| 1 | 46-A | 132 | ASP |
| 1 | 46-A | 138 | SER |
| 1 | 46-A | 148 | SER |
| 1 | 46-A | 156 | LEU |
| 1 | 46-A | 159 | ARG |
| 1 | 47-A | 4 | LEU |
| 1 | 47-A | 23 | ASN |
| 1 | 47-A | 33 | ARG |
| 1 | 47-A | 36 | LEU |
| 1 | 47-A | 45 | HIS |
| 1 | 47-A | 52 | ARG |
| 1 | 47-A | 58 | LYS |
| 1 | 47-A | 59 | ASN |
| 1 | 47-A | 85 | CYS |
| 1 | 47-A | 98 | ARG |
| 1 | 47-A | 118 | GLU |
| 1 | 47-A | 148 | SER |
| 1 | 47-A | 152 | CYS |
| 1 | 47-A | 156 | LEU |
| 1 | 47-A | 159 | ARG |
| 1 | 48-A | 1 | MET |
| 1 | 48-A | 20 | MET |
| 1 | 48-A | 33 | ARG |
| 1 | 48-A | 36 | LEU |
| 1 | 48-A | 44 | ARG |
| 1 | 48-A | 52 | ARG |
| 1 | 48-A | 98 | ARG |
| 1 | 48-A | 108 | GLN |
| 1 | 48-A | 118 | GLU |
| 1 | 48-A | 119 | VAL |
| 1 | 48-A | 148 | SER |
| 1 | 48-A | 156 | LEU |
| 1 | 49-A | 20 | MET |
| 1 | 49-A | 33 | ARG |
| 1 | 49-A | 44 | ARG |
| 1 | 49-A | 52 | ARG |
| 1 | 49-A | 65 | GLN |
| 1 | 49-A | 68 | THR |
| 1 | 49-A | 88 | VAL |
| 1 | 49-A | 118 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 49-A | 135 | SER |
| 1 | 49-A | 144 | ASP |
| 1 | 49-A | 158 | ARG |
| 1 | 50-A | 1 | MET |
| 1 | 50-A | 18 | ASN |
| 1 | 50-A | 23 | ASN |
| 1 | 50-A | 28 | LEU |
| 1 | 50-A | 33 | ARG |
| 1 | 50-A | 36 | LEU |
| 1 | 50-A | 44 | ARG |
| 1 | 50-A | 52 | ARG |
| 1 | 50-A | 58 | LYS |
| 1 | 50-A | 65 | GLN |
| 1 | 50-A | 85 | CYS |
| 1 | 50-A | 87 | ASP |
| 1 | 50-A | 88 | VAL |
| 1 | 50-A | 98 | ARG |
| 1 | 50-A | 119 | VAL |
| 1 | 50-A | 120 | GLU |
| 1 | 50-A | 128 | TYR |
| 1 | 50-A | 129 | GLU |
| 1 | 50-A | 142 | ASP |
| 1 | 50-A | 144 | ASP |
| 1 | 50-A | 156 | LEU |
| 1 | 51-A | 11 | ASP |
| 1 | 51-A | 33 | ARG |
| 1 | 51-A | 36 | LEU |
| 1 | 51-A | 44 | ARG |
| 1 | 51-A | 52 | ARG |
| 1 | 51-A | 59 | ASN |
| 1 | 51-A | 70 | ASP |
| 1 | 51-A | 76 | LYS |
| 1 | 51-A | 98 | ARG |
| 1 | 51-A | 109 | LYS |
| 1 | 51-A | 119 | VAL |
| 1 | 51-A | 120 | GLU |
| 1 | 51-A | 127 | ASP |
| 1 | 51-A | 128 | TYR |
| 1 | 51-A | 156 | LEU |
| 1 | 52-A | 11 | ASP |
| 1 | 52-A | 16 | MET |
| 1 | 52-A | 18 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 52-A | 23 | ASN |
| 1 | 52-A | 33 | ARG |
| 1 | 52-A | 65 | GLN |
| 1 | 52-A | 70 | ASP |
| 1 | 52-A | 85 | CYS |
| 1 | 52-A | 88 | VAL |
| 1 | 52-A | 98 | ARG |
| 1 | 52-A | 104 | LEU |
| 1 | 52-A | 129 | GLU |
| 1 | 52-A | 132 | ASP |
| 1 | 52-A | 139 | GLU |
| 1 | 53-A | 1 | MET |
| 1 | 53-A | 11 | ASP |
| 1 | 53-A | 24 | LEU |
| 1 | 53-A | 33 | ARG |
| 1 | 53-A | 52 | ARG |
| 1 | 53-A | 59 | ASN |
| 1 | 53-A | 87 | ASP |
| 1 | 53-A | 88 | VAL |
| 1 | 53-A | 101 | GLU |
| 1 | 53-A | 104 | LEU |
| 1 | 53-A | 118 | GLU |
| 1 | 53-A | 127 | ASP |
| 1 | 53-A | 128 | TYR |
| 1 | 53-A | 138 | SER |
| 1 | 53-A | 139 | GLU |
| 1 | 53-A | 156 | LEU |
| 1 | 53-A | 157 | GLU |
| 1 | 54-A | 1 | MET |
| 1 | 54-A | 17 | GLU |
| 1 | 54-A | 23 | ASN |
| 1 | 54-A | 24 | LEU |
| 1 | 54-A | 33 | ARG |
| 1 | 54-A | 48 | GLU |
| 1 | 54-A | 58 | LYS |
| 1 | 54-A | 59 | ASN |
| 1 | 54-A | 76 | LYS |
| 1 | 54-A | 104 | LEU |
| 1 | 54-A | 106 | LYS |
| 1 | 54-A | 122 | ASP |
| 1 | 54-A | 127 | ASP |
| 1 | 54-A | 128 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 54-A | 139 | GLU |
| 1 | 54-A | 154 | GLU |
| 1 | 54-A | 156 | LEU |
| 1 | 55-A | 4 | LEU |
| 1 | 55-A | 16 | MET |
| 1 | 55-A | 18 | ASN |
| 1 | 55-A | 23 | ASN |
| 1 | 55-A | 24 | LEU |
| 1 | 55-A | 33 | ARG |
| 1 | 55-A | 52 | ARG |
| 1 | 55-A | 70 | ASP |
| 1 | 55-A | 98 | ARG |
| 1 | 55-A | 104 | LEU |
| 1 | 55-A | 106 | LYS |
| 1 | 55-A | 108 | GLN |
| 1 | 55-A | 118 | GLU |
| 1 | 55-A | 122 | ASP |
| 1 | 55-A | 132 | ASP |
| 1 | 55-A | 138 | SER |
| 1 | 55-A | 152 | CYS |
| 1 | 55-A | 156 | LEU |
| 1 | 56-A | 1 | MET |
| 1 | 56-A | 17 | GLU |
| 1 | 56-A | 18 | ASN |
| 1 | 56-A | 23 | ASN |
| 1 | 56-A | 24 | LEU |
| 1 | 56-A | 33 | ARG |
| 1 | 56-A | 59 | ASN |
| 1 | 56-A | 79 | ASP |
| 1 | 56-A | 98 | ARG |
| 1 | 56-A | 106 | LYS |
| 1 | 56-A | 108 | GLN |
| 1 | 56-A | 118 | GLU |
| 1 | 56-A | 127 | ASP |
| 1 | 57-A | 1 | MET |
| 1 | 57-A | 18 | ASN |
| 1 | 57-A | 20 | MET |
| 1 | 57-A | 24 | LEU |
| 1 | 57-A | 30 | TRP |
| 1 | 57-A | 33 | ARG |
| 1 | 57-A | 54 | LEU |
| 1 | 57-A | 61 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 57-A | 62 | LEU |
| 1 | 57-A | 65 | GLN |
| 1 | 57-A | 79 | ASP |
| 1 | 57-A | 87 | ASP |
| 1 | 57-A | 88 | VAL |
| 1 | 57-A | 108 | GLN |
| 1 | 57-A | 128 | TYR |
| 1 | 57-A | 156 | LEU |
| 1 | 58-A | 1 | MET |
| 1 | 58-A | 8 | LEU |
| 1 | 58-A | 16 | MET |
| 1 | 58-A | 28 | LEU |
| 1 | 58-A | 52 | ARG |
| 1 | 58-A | 54 | LEU |
| 1 | 58-A | 88 | VAL |
| 1 | 58-A | 108 | GLN |
| 1 | 58-A | 156 | LEU |
| 1 | 58-A | 157 | GLU |
| 1 | 58-A | 158 | ARG |
| 1 | 59-A | 20 | MET |
| 1 | 59-A | 23 | ASN |
| 1 | 59-A | 37 | ASN |
| 1 | 59-A | 52 | ARG |
| 1 | 59-A | 101 | GLU |
| 1 | 59-A | 104 | LEU |
| 1 | 59-A | 108 | GLN |
| 1 | 59-A | 138 | SER |
| 1 | 59-A | 156 | LEU |
| 1 | 60-A | 16 | MET |
| 1 | 60-A | 18 | ASN |
| 1 | 60-A | 20 | MET |
| 1 | 60-A | 24 | LEU |
| 1 | 60-A | 33 | ARG |
| 1 | 60-A | 52 | ARG |
| 1 | 60-A | 89 | PRO |
| 1 | 60-A | 98 | ARG |
| 1 | 60-A | 104 | LEU |
| 1 | 60-A | 108 | GLN |
| 1 | 60-A | 122 | ASP |
| 1 | 60-A | 127 | ASP |
| 1 | 60-A | 128 | TYR |
| 1 | 60-A | 130 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 60-A | 138 | SER |
| 1 | 60-A | 144 | ASP |
| 1 | 60-A | 147 | ASN |
| 1 | 60-A | 148 | SER |
| 1 | 60-A | 156 | LEU |
| 1 | 60-A | 157 | GLU |
| 1 | 60-A | 158 | ARG |
| 1 | 60-A | 159 | ARG |
| 1 | 61-A | 16 | MET |
| 1 | 61-A | 20 | MET |
| 1 | 61-A | 28 | LEU |
| 1 | 61-A | 33 | ARG |
| 1 | 61-A | 49 | SER |
| 1 | 61-A | 52 | ARG |
| 1 | 61-A | 54 | LEU |
| 1 | 61-A | 65 | GLN |
| 1 | 61-A | 79 | ASP |
| 1 | 61-A | 108 | GLN |
| 1 | 61-A | 119 | VAL |
| 1 | 61-A | 127 | ASP |
| 1 | 61-A | 128 | TYR |
| 1 | 61-A | 129 | GLU |
| 1 | 61-A | 139 | GLU |
| 1 | 61-A | 156 | LEU |
| 1 | 61-A | 157 | GLU |
| 1 | 61-A | 158 | ARG |
| 1 | 62-A | 1 | MET |
| 1 | 62-A | 20 | MET |
| 1 | 62-A | 23 | ASN |
| 1 | 62-A | 24 | LEU |
| 1 | 62-A | 28 | LEU |
| 1 | 62-A | 33 | ARG |
| 1 | 62-A | 52 | ARG |
| 1 | 62-A | 59 | ASN |
| 1 | 62-A | 65 | GLN |
| 1 | 62-A | 76 | LYS |
| 1 | 62-A | 87 | ASP |
| 1 | 62-A | 88 | VAL |
| 1 | 62-A | 108 | GLN |
| 1 | 62-A | 122 | ASP |
| 1 | 62-A | 127 | ASP |
| 1 | 62-A | 129 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 62-A | 139 | GLU |
| 1 | 62-A | 156 | LEU |
| 1 | 63-A | 18 | ASN |
| 1 | 63-A | 24 | LEU |
| 1 | 63-A | 33 | ARG |
| 1 | 63-A | 76 | LYS |
| 1 | 63-A | 87 | ASP |
| 1 | 63-A | 88 | VAL |
| 1 | 63-A | 108 | GLN |
| 1 | 63-A | 138 | SER |
| 1 | 63-A | 139 | GLU |
| 1 | 63-A | 159 | ARG |
| 1 | 64-A | 1 | MET |
| 1 | 64-A | 2 | ILE |
| 1 | 64-A | 20 | MET |
| 1 | 64-A | 33 | ARG |
| 1 | 64-A | 59 | ASN |
| 1 | 64-A | 87 | ASP |
| 1 | 64-A | 98 | ARG |
| 1 | 64-A | 106 | LYS |
| 1 | 64-A | 108 | GLN |
| 1 | 64-A | 127 | ASP |
| 1 | 64-A | 137 | PHE |
| 1 | 64-A | 138 | SER |
| 1 | 64-A | 148 | SER |
| 1 | 64-A | 156 | LEU |
| 1 | 65-A | 1 | MET |
| 1 | 65-A | 2 | ILE |
| 1 | 65-A | 16 | MET |
| 1 | 65-A | 33 | ARG |
| 1 | 65-A | 52 | ARG |
| 1 | 65-A | 54 | LEU |
| 1 | 65-A | 65 | GLN |
| 1 | 65-A | 79 | ASP |
| 1 | 65-A | 87 | ASP |
| 1 | 65-A | 98 | ARG |
| 1 | 65-A | 106 | LYS |
| 1 | 65-A | 108 | GLN |
| 1 | 65-A | 139 | GLU |
| 1 | 65-A | 142 | ASP |
| 1 | 65-A | 156 | LEU |
| 1 | 65-A | 157 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 66-A | 1 | MET |
| 1 | 66-A | 2 | ILE |
| 1 | 66-A | 11 | ASP |
| 1 | 66-A | 16 | MET |
| 1 | 66-A | 20 | MET |
| 1 | 66-A | 30 | TRP |
| 1 | 66-A | 33 | ARG |
| 1 | 66-A | 52 | ARG |
| 1 | 66-A | 59 | ASN |
| 1 | 66-A | 65 | GLN |
| 1 | 66-A | 79 | ASP |
| 1 | 66-A | 87 | ASP |
| 1 | 66-A | 98 | ARG |
| 1 | 66-A | 106 | LYS |
| 1 | 66-A | 118 | GLU |
| 1 | 66-A | 129 | GLU |
| 1 | 66-A | 136 | VAL |
| 1 | 66-A | 157 | GLU |
| 1 | 67-A | 2 | ILE |
| 1 | 67-A | 11 | ASP |
| 1 | 67-A | 16 | MET |
| 1 | 67-A | 18 | ASN |
| 1 | 67-A | 20 | MET |
| 1 | 67-A | 33 | ARG |
| 1 | 67-A | 65 | GLN |
| 1 | 67-A | 79 | ASP |
| 1 | 67-A | 98 | ARG |
| 1 | 67-A | 118 | GLU |
| 1 | 67-A | 134 | GLU |
| 1 | 67-A | 136 | VAL |
| 1 | 67-A | 152 | CYS |
| 1 | 67-A | 157 | GLU |
| 1 | 67-A | 159 | ARG |
| 1 | 68-A | 16 | MET |
| 1 | 68-A | 20 | MET |
| 1 | 68-A | 33 | ARG |
| 1 | 68-A | 36 | LEU |
| 1 | 68-A | 52 | ARG |
| 1 | 68-A | 62 | LEU |
| 1 | 68-A | 65 | GLN |
| 1 | 68-A | 87 | ASP |
| 1 | 68-A | 98 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 68-A | 118 | GLU |
| 1 | 68-A | 127 | ASP |
| 1 | 68-A | 159 | ARG |
| 1 | 69-A | 1 | MET |
| 1 | 69-A | 16 | MET |
| 1 | 69-A | 20 | MET |
| 1 | 69-A | 22 | TRP |
| 1 | 69-A | 23 | ASN |
| 1 | 69-A | 32 | LYS |
| 1 | 69-A | 62 | LEU |
| 1 | 69-A | 65 | GLN |
| 1 | 69-A | 79 | ASP |
| 1 | 69-A | 98 | ARG |
| 1 | 69-A | 118 | GLU |
| 1 | 69-A | 135 | SER |
| 1 | 69-A | 142 | ASP |
| 1 | 69-A | 159 | ARG |
| 1 | 70-A | 1 | MET |
| 1 | 70-A | 4 | LEU |
| 1 | 70-A | 16 | MET |
| 1 | 70-A | 18 | ASN |
| 1 | 70-A | 20 | MET |
| 1 | 70-A | 22 | TRP |
| 1 | 70-A | 23 | ASN |
| 1 | 70-A | 33 | ARG |
| 1 | 70-A | 52 | ARG |
| 1 | 70-A | 59 | ASN |
| 1 | 70-A | 98 | ARG |
| 1 | 70-A | 128 | TYR |
| 1 | 70-A | 135 | SER |
| 1 | 70-A | 138 | SER |
| 1 | 70-A | 148 | SER |
| 1 | 71-A | 18 | ASN |
| 1 | 71-A | 22 | TRP |
| 1 | 71-A | 70 | ASP |
| 1 | 71-A | 88 | VAL |
| 1 | 71-A | 98 | ARG |
| 1 | 71-A | 120 | GLU |
| 1 | 71-A | 123 | THR |
| 1 | 71-A | 128 | TYR |
| 1 | 71-A | 152 | CYS |
| 1 | 72-A | 1 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 72-A | 8 | LEU |
| 1 | 72-A | 16 | MET |
| 1 | 72-A | 18 | ASN |
| 1 | 72-A | 20 | MET |
| 1 | 72-A | 70 | ASP |
| 1 | 72-A | 88 | VAL |
| 1 | 72-A | 98 | ARG |
| 1 | 72-A | 101 | GLU |
| 1 | 72-A | 104 | LEU |
| 1 | 72-A | 108 | GLN |
| 1 | 72-A | 120 | GLU |
| 1 | 72-A | 132 | ASP |
| 1 | 72-A | 138 | SER |
| 1 | 72-A | 152 | CYS |
| 1 | 72-A | 154 | GLU |
| 1 | 73-A | 8 | LEU |
| 1 | 73-A | 10 | VAL |
| 1 | 73-A | 16 | MET |
| 1 | 73-A | 18 | ASN |
| 1 | 73-A | 20 | MET |
| 1 | 73-A | 21 | PRO |
| 1 | 73-A | 52 | ARG |
| 1 | 73-A | 65 | GLN |
| 1 | 73-A | 98 | ARG |
| 1 | 73-A | 104 | LEU |
| 1 | 73-A | 108 | GLN |
| 1 | 73-A | 118 | GLU |
| 1 | 73-A | 120 | GLU |
| 1 | 73-A | 148 | SER |
| 1 | 74-A | 1 | MET |
| 1 | 74-A | 8 | LEU |
| 1 | 74-A | 18 | ASN |
| 1 | 74-A | 20 | MET |
| 1 | 74-A | 33 | ARG |
| 1 | 74-A | 49 | SER |
| 1 | 74-A | 65 | GLN |
| 1 | 74-A | 79 | ASP |
| 1 | 74-A | 89 | PRO |
| 1 | 74-A | 104 | LEU |
| 1 | 74-A | 118 | GLU |
| 1 | 74-A | 119 | VAL |
| 1 | 74-A | 132 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 74-A | 148 | SER |
| 1 | 74-A | 152 | CYS |
| 1 | 75-A | 1 | MET |
| 1 | 75-A | 12 | ARG |
| 1 | 75-A | 16 | MET |
| 1 | 75-A | 18 | ASN |
| 1 | 75-A | 33 | ARG |
| 1 | 75-A | 52 | ARG |
| 1 | 75-A | 65 | GLN |
| 1 | 75-A | 79 | ASP |
| 1 | 75-A | 88 | VAL |
| 1 | 75-A | 108 | GLN |
| 1 | 75-A | 128 | TYR |
| 1 | 75-A | 137 | PHE |
| 1 | 75-A | 156 | LEU |
| 1 | 76-A | 12 | ARG |
| 1 | 76-A | 16 | MET |
| 1 | 76-A | 18 | ASN |
| 1 | 76-A | 52 | ARG |
| 1 | 76-A | 59 | ASN |
| 1 | 76-A | 60 | ILE |
| 1 | 76-A | 65 | GLN |
| 1 | 76-A | 79 | ASP |
| 1 | 76-A | 88 | VAL |
| 1 | 76-A | 106 | LYS |
| 1 | 76-A | 108 | GLN |
| 1 | 76-A | 109 | LYS |
| 1 | 76-A | 119 | VAL |
| 1 | 76-A | 128 | TYR |
| 1 | 76-A | 135 | SER |
| 1 | 76-A | 156 | LEU |
| 1 | 76-A | 158 | ARG |
| 1 | 76-A | 159 | ARG |
| 1 | 77-A | 12 | ARG |
| 1 | 77-A | 18 | ASN |
| 1 | 77-A | 36 | LEU |
| 1 | 77-A | 52 | ARG |
| 1 | 77-A | 59 | ASN |
| 1 | 77-A | 65 | GLN |
| 1 | 77-A | 76 | LYS |
| 1 | 77-A | 106 | LYS |
| 1 | 77-A | 108 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 77-A | 118 | GLU |
| 1 | 77-A | 128 | TYR |
| 1 | 77-A | 129 | GLU |
| 1 | 77-A | 156 | LEU |
| 1 | 78-A | 1 | MET |
| 1 | 78-A | 4 | LEU |
| 1 | 78-A | 12 | ARG |
| 1 | 78-A | 18 | ASN |
| 1 | 78-A | 33 | ARG |
| 1 | 78-A | 36 | LEU |
| 1 | 78-A | 52 | ARG |
| 1 | 78-A | 65 | GLN |
| 1 | 78-A | 76 | LYS |
| 1 | 78-A | 79 | ASP |
| 1 | 78-A | 88 | VAL |
| 1 | 78-A | 104 | LEU |
| 1 | 78-A | 106 | LYS |
| 1 | 78-A | 118 | GLU |
| 1 | 78-A | 128 | TYR |
| 1 | 78-A | 135 | SER |
| 1 | 78-A | 138 | SER |
| 1 | 78-A | 158 | ARG |
| 1 | 79-A | 1 | MET |
| 1 | 79-A | 12 | ARG |
| 1 | 79-A | 16 | MET |
| 1 | 79-A | 36 | LEU |
| 1 | 79-A | 48 | GLU |
| 1 | 79-A | 52 | ARG |
| 1 | 79-A | 59 | ASN |
| 1 | 79-A | 76 | LYS |
| 1 | 79-A | 88 | VAL |
| 1 | 79-A | 109 | LYS |
| 1 | 79-A | 123 | THR |
| 1 | 79-A | 128 | TYR |
| 1 | 79-A | 129 | GLU |
| 1 | 79-A | 158 | ARG |
| 1 | 80-A | 12 | ARG |
| 1 | 80-A | 16 | MET |
| 1 | 80-A | 17 | GLU |
| 1 | 80-A | 18 | ASN |
| 1 | 80-A | 33 | ARG |
| 1 | 80-A | 44 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 80-A | 48 | GLU |
| 1 | 80-A | 52 | ARG |
| 1 | 80-A | 59 | ASN |
| 1 | 80-A | 76 | LYS |
| 1 | 80-A | 79 | ASP |
| 1 | 80-A | 88 | VAL |
| 1 | 80-A | 104 | LEU |
| 1 | 80-A | 106 | LYS |
| 1 | 80-A | 108 | GLN |
| 1 | 80-A | 109 | LYS |
| 1 | 80-A | 127 | ASP |
| 1 | 80-A | 128 | TYR |
| 1 | 80-A | 138 | SER |
| 1 | 80-A | 142 | ASP |
| 1 | 80-A | 148 | SER |
| 1 | 81-A | 1 | MET |
| 1 | 81-A | 16 | MET |
| 1 | 81-A | 33 | ARG |
| 1 | 81-A | 48 | GLU |
| 1 | 81-A | 76 | LYS |
| 1 | 81-A | 104 | LEU |
| 1 | 81-A | 109 | LYS |
| 1 | 81-A | 118 | GLU |
| 1 | 81-A | 119 | VAL |
| 1 | 81-A | 127 | ASP |
| 1 | 81-A | 131 | ASP |
| 1 | 81-A | 132 | ASP |
| 1 | 81-A | 158 | ARG |
| 1 | 82-A | 1 | MET |
| 1 | 82-A | 2 | ILE |
| 1 | 82-A | 10 | VAL |
| 1 | 82-A | 16 | MET |
| 1 | 82-A | 18 | ASN |
| 1 | 82-A | 33 | ARG |
| 1 | 82-A | 52 | ARG |
| 1 | 82-A | 58 | LYS |
| 1 | 82-A | 59 | ASN |
| 1 | 82-A | 119 | VAL |
| 1 | 82-A | 127 | ASP |
| 1 | 82-A | 128 | TYR |
| 1 | 82-A | 131 | ASP |
| 1 | 82-A | 154 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 83-A | 1 | MET |
| 1 | 83-A | 23 | ASN |
| 1 | 83-A | 30 | TRP |
| 1 | 83-A | 33 | ARG |
| 1 | 83-A | 36 | LEU |
| 1 | 83-A | 44 | ARG |
| 1 | 83-A | 52 | ARG |
| 1 | 83-A | 128 | TYR |
| 1 | 83-A | 129 | GLU |
| 1 | 84-A | 1 | MET |
| 1 | 84-A | 18 | ASN |
| 1 | 84-A | 23 | ASN |
| 1 | 84-A | 36 | LEU |
| 1 | 84-A | 58 | LYS |
| 1 | 84-A | 65 | GLN |
| 1 | 84-A | 118 | GLU |
| 1 | 84-A | 127 | ASP |
| 1 | 84-A | 129 | GLU |
| 1 | 85-A | 1 | MET |
| 1 | 85-A | 16 | MET |
| 1 | 85-A | 36 | LEU |
| 1 | 85-A | 54 | LEU |
| 1 | 85-A | 58 | LYS |
| 1 | 85-A | 87 | ASP |
| 1 | 85-A | 88 | VAL |
| 1 | 85-A | 104 | LEU |
| 1 | 85-A | 106 | LYS |
| 1 | 85-A | 127 | ASP |
| 1 | 85-A | 134 | GLU |
| 1 | 85-A | 148 | SER |
| 1 | 86-A | 1 | MET |
| 1 | 86-A | 16 | MET |
| 1 | 86-A | 18 | ASN |
| 1 | 86-A | 33 | ARG |
| 1 | 86-A | 36 | LEU |
| 1 | 86-A | 49 | SER |
| 1 | 86-A | 54 | LEU |
| 1 | 86-A | 65 | GLN |
| 1 | 86-A | 104 | LEU |
| 1 | 86-A | 120 | GLU |
| 1 | 86-A | 127 | ASP |
| 1 | 86-A | 129 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 86-A | 155 | ILE |
| 1 | 87-A | 1 | MET |
| 1 | 87-A | 18 | ASN |
| 1 | 87-A | 23 | ASN |
| 1 | 87-A | 36 | LEU |
| 1 | 87-A | 54 | LEU |
| 1 | 87-A | 58 | LYS |
| 1 | 87-A | 98 | ARG |
| 1 | 87-A | 104 | LEU |
| 1 | 87-A | 119 | VAL |
| 1 | 87-A | 122 | ASP |
| 1 | 87-A | 127 | ASP |
| 1 | 88-A | 1 | MET |
| 1 | 88-A | 28 | LEU |
| 1 | 88-A | 36 | LEU |
| 1 | 88-A | 52 | ARG |
| 1 | 88-A | 58 | LYS |
| 1 | 88-A | 65 | GLN |
| 1 | 88-A | 88 | VAL |
| 1 | 88-A | 104 | LEU |
| 1 | 88-A | 119 | VAL |
| 1 | 88-A | 130 | PRO |
| 1 | 88-A | 134 | GLU |
| 1 | 88-A | 135 | SER |
| 1 | 88-A | 138 | SER |
| 1 | 88-A | 144 | ASP |
| 1 | 88-A | 148 | SER |
| 1 | 88-A | 158 | ARG |
| 1 | 89-A | 1 | MET |
| 1 | 89-A | 11 | ASP |
| 1 | 89-A | 18 | ASN |
| 1 | 89-A | 24 | LEU |
| 1 | 89-A | 33 | ARG |
| 1 | 89-A | 52 | ARG |
| 1 | 89-A | 65 | GLN |
| 1 | 89-A | 76 | LYS |
| 1 | 89-A | 101 | GLU |
| 1 | 89-A | 104 | LEU |
| 1 | 89-A | 118 | GLU |
| 1 | 89-A | 128 | TYR |
| 1 | 89-A | 130 | PRO |
| 1 | 89-A | 144 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 90-A | 1 | MET |
| 1 | 90-A | 10 | VAL |
| 1 | 90-A | 11 | ASP |
| 1 | 90-A | 20 | MET |
| 1 | 90-A | 23 | ASN |
| 1 | 90-A | 36 | LEU |
| 1 | 90-A | 52 | ARG |
| 1 | 90-A | 54 | LEU |
| 1 | 90-A | 98 | ARG |
| 1 | 90-A | 104 | LEU |
| 1 | 90-A | 120 | GLU |
| 1 | 90-A | 134 | GLU |
| 1 | 90-A | 136 | VAL |
| 1 | 90-A | 142 | ASP |
| 1 | 90-A | 144 | ASP |
| 1 | 90-A | 154 | GLU |
| 1 | 91-A | 16 | MET |
| 1 | 91-A | 20 | MET |
| 1 | 91-A | 24 | LEU |
| 1 | 91-A | 36 | LEU |
| 1 | 91-A | 54 | LEU |
| 1 | 91-A | 87 | ASP |
| 1 | 91-A | 88 | VAL |
| 1 | 91-A | 101 | GLU |
| 1 | 91-A | 104 | LEU |
| 1 | 91-A | 120 | GLU |
| 1 | 91-A | 132 | ASP |
| 1 | 91-A | 134 | GLU |
| 1 | 91-A | 142 | ASP |
| 1 | 91-A | 144 | ASP |
| 1 | 92-A | 1 | MET |
| 1 | 92-A | 10 | VAL |
| 1 | 92-A | 16 | MET |
| 1 | 92-A | 33 | ARG |
| 1 | 92-A | 36 | LEU |
| 1 | 92-A | 52 | ARG |
| 1 | 92-A | 59 | ASN |
| 1 | 92-A | 87 | ASP |
| 1 | 92-A | 88 | VAL |
| 1 | 92-A | 101 | GLU |
| 1 | 92-A | 109 | LYS |
| 1 | 92-A | 142 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 93-A | 16 | MET |
| 1 | 93-A | 17 | GLU |
| 1 | 93-A | 18 | ASN |
| 1 | 93-A | 24 | LEU |
| 1 | 93-A | 32 | LYS |
| 1 | 93-A | 33 | ARG |
| 1 | 93-A | 36 | LEU |
| 1 | 93-A | 48 | GLU |
| 1 | 93-A | 52 | ARG |
| 1 | 93-A | 87 | ASP |
| 1 | 93-A | 88 | VAL |
| 1 | 93-A | 109 | LYS |
| 1 | 93-A | 122 | ASP |
| 1 | 93-A | 128 | TYR |
| 1 | 93-A | 157 | GLU |
| 1 | 94-A | 16 | MET |
| 1 | 94-A | 17 | GLU |
| 1 | 94-A | 18 | ASN |
| 1 | 94-A | 23 | ASN |
| 1 | 94-A | 24 | LEU |
| 1 | 94-A | 32 | LYS |
| 1 | 94-A | 33 | ARG |
| 1 | 94-A | 58 | LYS |
| 1 | 94-A | 59 | ASN |
| 1 | 94-A | 60 | ILE |
| 1 | 94-A | 87 | ASP |
| 1 | 94-A | 98 | ARG |
| 1 | 94-A | 129 | GLU |
| 1 | 94-A | 132 | ASP |
| 1 | 94-A | 134 | GLU |
| 1 | 94-A | 138 | SER |
| 1 | 94-A | 156 | LEU |
| 1 | 95-A | 2 | ILE |
| 1 | 95-A | 16 | MET |
| 1 | 95-A | 17 | GLU |
| 1 | 95-A | 18 | ASN |
| 1 | 95-A | 32 | LYS |
| 1 | 95-A | 33 | ARG |
| 1 | 95-A | 52 | ARG |
| 1 | 95-A | 58 | LYS |
| 1 | 95-A | 59 | ASN |
| 1 | 95-A | 60 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 95-A | 85 | CYS |
| 1 | 95-A | 87 | ASP |
| 1 | 95-A | 89 | PRO |
| 1 | 95-A | 104 | LEU |
| 1 | 95-A | 118 | GLU |
| 1 | 95-A | 120 | GLU |
| 1 | 95-A | 129 | GLU |
| 1 | 96-A | 1 | MET |
| 1 | 96-A | 2 | ILE |
| 1 | 96-A | 16 | MET |
| 1 | 96-A | 17 | GLU |
| 1 | 96-A | 24 | LEU |
| 1 | 96-A | 33 | ARG |
| 1 | 96-A | 59 | ASN |
| 1 | 96-A | 65 | GLN |
| 1 | 96-A | 66 | PRO |
| 1 | 96-A | 87 | ASP |
| 1 | 96-A | 88 | VAL |
| 1 | 96-A | 101 | GLU |
| 1 | 96-A | 104 | LEU |
| 1 | 96-A | 106 | LYS |
| 1 | 96-A | 109 | LYS |
| 1 | 96-A | 119 | VAL |
| 1 | 96-A | 122 | ASP |
| 1 | 96-A | 157 | GLU |
| 1 | 96-A | 159 | ARG |
| 1 | 97-A | 4 | LEU |
| 1 | 97-A | 18 | ASN |
| 1 | 97-A | 20 | MET |
| 1 | 97-A | 33 | ARG |
| 1 | 97-A | 52 | ARG |
| 1 | 97-A | 58 | LYS |
| 1 | 97-A | 65 | GLN |
| 1 | 97-A | 70 | ASP |
| 1 | 97-A | 76 | LYS |
| 1 | 97-A | 79 | ASP |
| 1 | 97-A | 87 | ASP |
| 1 | 97-A | 88 | VAL |
| 1 | 97-A | 98 | ARG |
| 1 | 97-A | 101 | GLU |
| 1 | 97-A | 118 | GLU |
| 1 | 97-A | 119 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 97-A | 123 | THR |
| 1 | 97-A | 157 | GLU |
| 1 | 98-A | 1 | MET |
| 1 | 98-A | 16 | MET |
| 1 | 98-A | 18 | ASN |
| 1 | 98-A | 24 | LEU |
| 1 | 98-A | 33 | ARG |
| 1 | 98-A | 52 | ARG |
| 1 | 98-A | 58 | LYS |
| 1 | 98-A | 62 | LEU |
| 1 | 98-A | 65 | GLN |
| 1 | 98-A | 76 | LYS |
| 1 | 98-A | 101 | GLU |
| 1 | 98-A | 106 | LYS |
| 1 | 98-A | 119 | VAL |
| 1 | 98-A | 138 | SER |
| 1 | 99-A | 18 | ASN |
| 1 | 99-A | 24 | LEU |
| 1 | 99-A | 33 | ARG |
| 1 | 99-A | 52 | ARG |
| 1 | 99-A | 58 | LYS |
| 1 | 99-A | 65 | GLN |
| 1 | 99-A | 68 | THR |
| 1 | 99-A | 76 | LYS |
| 1 | 99-A | 77 | SER |
| 1 | 99-A | 87 | ASP |
| 1 | 99-A | 104 | LEU |
| 1 | 99-A | 106 | LYS |
| 1 | 99-A | 109 | LYS |
| 1 | 99-A | 128 | TYR |
| 1 | 99-A | 135 | SER |
| 1 | 99-A | 138 | SER |
| 1 | 99-A | 158 | ARG |
| 1 | 100-A | 20 | MET |
| 1 | 100-A | 24 | LEU |
| 1 | 100-A | 49 | SER |
| 1 | 100-A | 52 | ARG |
| 1 | 100-A | 58 | LYS |
| 1 | 100-A | 59 | ASN |
| 1 | 100-A | 60 | ILE |
| 1 | 100-A | 65 | GLN |
| 1 | 100-A | 79 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 100-A | 104 | LEU |
| 1 | 100-A | 106 | LYS |
| 1 | 100-A | 109 | LYS |
| 1 | 100-A | 120 | GLU |
| 1 | 100-A | 141 | HIS |
| 1 | 101-A | 8 | LEU |
| 1 | 101-A | 17 | GLU |
| 1 | 101-A | 52 | ARG |
| 1 | 101-A | 58 | LYS |
| 1 | 101-A | 104 | LEU |
| 1 | 101-A | 118 | GLU |
| 1 | 101-A | 119 | VAL |
| 1 | 101-A | 137 | PHE |
| 1 | 101-A | 148 | SER |
| 1 | 102-A | 1 | MET |
| 1 | 102-A | 8 | LEU |
| 1 | 102-A | 16 | MET |
| 1 | 102-A | 17 | GLU |
| 1 | 102-A | 18 | ASN |
| 1 | 102-A | 52 | ARG |
| 1 | 102-A | 58 | LYS |
| 1 | 102-A | 68 | THR |
| 1 | 102-A | 104 | LEU |
| 1 | 102-A | 120 | GLU |
| 1 | 102-A | 127 | ASP |
| 1 | 102-A | 134 | GLU |
| 1 | 102-A | 141 | HIS |
| 1 | 102-A | 142 | ASP |
| 1 | 103-A | 1 | MET |
| 1 | 103-A | 17 | GLU |
| 1 | 103-A | 18 | ASN |
| 1 | 103-A | 23 | ASN |
| 1 | 103-A | 36 | LEU |
| 1 | 103-A | 45 | HIS |
| 1 | 103-A | 52 | ARG |
| 1 | 103-A | 58 | LYS |
| 1 | 103-A | 65 | GLN |
| 1 | 103-A | 104 | LEU |
| 1 | 103-A | 120 | GLU |
| 1 | 103-A | 129 | GLU |
| 1 | 103-A | 139 | GLU |
| 1 | 103-A | 141 | HIS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 103-A | 152 | CYS |
| 1 | 103-A | 158 | ARG |
| 1 | 104-A | 1 | MET |
| 1 | 104-A | 23 | ASN |
| 1 | 104-A | 36 | LEU |
| 1 | 104-A | 45 | HIS |
| 1 | 104-A | 76 | LYS |
| 1 | 104-A | 87 | ASP |
| 1 | 104-A | 108 | GLN |
| 1 | 104-A | 138 | SER |
| 1 | 104-A | 139 | GLU |
| 1 | 104-A | 141 | HIS |
| 1 | 104-A | 148 | SER |
| 1 | 105-A | 1 | MET |
| 1 | 105-A | 17 | GLU |
| 1 | 105-A | 18 | ASN |
| 1 | 105-A | 20 | MET |
| 1 | 105-A | 23 | ASN |
| 1 | 105-A | 24 | LEU |
| 1 | 105-A | 36 | LEU |
| 1 | 105-A | 45 | HIS |
| 1 | 105-A | 59 | ASN |
| 1 | 105-A | 65 | GLN |
| 1 | 105-A | 79 | ASP |
| 1 | 105-A | 108 | GLN |
| 1 | 105-A | 109 | LYS |
| 1 | 105-A | 120 | GLU |
| 1 | 105-A | 128 | TYR |
| 1 | 105-A | 132 | ASP |
| 1 | 105-A | 141 | HIS |
| 1 | 105-A | 148 | SER |
| 1 | 106-A | 1 | MET |
| 1 | 106-A | 4 | LEU |
| 1 | 106-A | 17 | GLU |
| 1 | 106-A | 23 | ASN |
| 1 | 106-A | 24 | LEU |
| 1 | 106-A | 36 | LEU |
| 1 | 106-A | 49 | SER |
| 1 | 106-A | 58 | LYS |
| 1 | 106-A | 65 | GLN |
| 1 | 106-A | 79 | ASP |
| 1 | 106-A | 88 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 106-A | 106 | LYS |
| 1 | 106-A | 108 | GLN |
| 1 | 106-A | 122 | ASP |
| 1 | 106-A | 129 | GLU |
| 1 | 106-A | 132 | ASP |
| 1 | 106-A | 137 | PHE |
| 1 | 106-A | 141 | HIS |
| 1 | 106-A | 148 | SER |
| 1 | 106-A | 150 | SER |
| 1 | 106-A | 152 | CYS |
| 1 | 106-A | 159 | ARG |
| 1 | 107-A | 16 | MET |
| 1 | 107-A | 18 | ASN |
| 1 | 107-A | 20 | MET |
| 1 | 107-A | 21 | PRO |
| 1 | 107-A | 23 | ASN |
| 1 | 107-A | 24 | LEU |
| 1 | 107-A | 52 | ARG |
| 1 | 107-A | 58 | LYS |
| 1 | 107-A | 59 | ASN |
| 1 | 107-A | 60 | ILE |
| 1 | 107-A | 79 | ASP |
| 1 | 107-A | 87 | ASP |
| 1 | 107-A | 88 | VAL |
| 1 | 107-A | 104 | LEU |
| 1 | 107-A | 106 | LYS |
| 1 | 107-A | 108 | GLN |
| 1 | 107-A | 119 | VAL |
| 1 | 107-A | 129 | GLU |
| 1 | 107-A | 135 | SER |
| 1 | 107-A | 148 | SER |
| 1 | 107-A | 156 | LEU |
| 1 | 107-A | 159 | ARG |
| 1 | 108-A | 1 | MET |
| 1 | 108-A | 13 | VAL |
| 1 | 108-A | 20 | MET |
| 1 | 108-A | 23 | ASN |
| 1 | 108-A | 24 | LEU |
| 1 | 108-A | 49 | SER |
| 1 | 108-A | 52 | ARG |
| 1 | 108-A | 58 | LYS |
| 1 | 108-A | 59 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 108-A | 98 | ARG |
| 1 | 108-A | 104 | LEU |
| 1 | 108-A | 106 | LYS |
| 1 | 108-A | 108 | GLN |
| 1 | 108-A | 127 | ASP |
| 1 | 108-A | 138 | SER |
| 1 | 108-A | 152 | CYS |
| 1 | 108-A | 156 | LEU |
| 1 | 108-A | 159 | ARG |
| 1 | 109-A | 17 | GLU |
| 1 | 109-A | 18 | ASN |
| 1 | 109-A | 23 | ASN |
| 1 | 109-A | 30 | TRP |
| 1 | 109-A | 33 | ARG |
| 1 | 109-A | 45 | HIS |
| 1 | 109-A | 52 | ARG |
| 1 | 109-A | 58 | LYS |
| 1 | 109-A | 87 | ASP |
| 1 | 109-A | 98 | ARG |
| 1 | 109-A | 104 | LEU |
| 1 | 109-A | 106 | LYS |
| 1 | 109-A | 108 | GLN |
| 1 | 109-A | 129 | GLU |
| 1 | 110-A | 1 | MET |
| 1 | 110-A | 18 | ASN |
| 1 | 110-A | 20 | MET |
| 1 | 110-A | 23 | ASN |
| 1 | 110-A | 49 | SER |
| 1 | 110-A | 59 | ASN |
| 1 | 110-A | 76 | LYS |
| 1 | 110-A | 98 | ARG |
| 1 | 110-A | 106 | LYS |
| 1 | 110-A | 108 | GLN |
| 1 | 110-A | 118 | GLU |
| 1 | 110-A | 129 | GLU |
| 1 | 110-A | 135 | SER |
| 1 | 110-A | 152 | CYS |
| 1 | 110-A | 156 | LEU |
| 1 | 111-A | 13 | VAL |
| 1 | 111-A | 16 | MET |
| 1 | 111-A | 18 | ASN |
| 1 | 111-A | 65 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 111-A | 68 | THR |
| 1 | 111-A | 76 | LYS |
| 1 | 111-A | 98 | ARG |
| 1 | 111-A | 106 | LYS |
| 1 | 111-A | 108 | GLN |
| 1 | 111-A | 118 | GLU |
| 1 | 111-A | 156 | LEU |
| 1 | 111-A | 157 | GLU |
| 1 | 112-A | 16 | MET |
| 1 | 112-A | 18 | ASN |
| 1 | 112-A | 20 | MET |
| 1 | 112-A | 54 | LEU |
| 1 | 112-A | 59 | ASN |
| 1 | 112-A | 61 | ILE |
| 1 | 112-A | 68 | THR |
| 1 | 112-A | 76 | LYS |
| 1 | 112-A | 87 | ASP |
| 1 | 112-A | 98 | ARG |
| 1 | 112-A | 106 | LYS |
| 1 | 112-A | 108 | GLN |
| 1 | 112-A | 115 | ILE |
| 1 | 112-A | 118 | GLU |
| 1 | 112-A | 142 | ASP |
| 1 | 113-A | 1 | MET |
| 1 | 113-A | 2 | ILE |
| 1 | 113-A | 4 | LEU |
| 1 | 113-A | 23 | ASN |
| 1 | 113-A | 33 | ARG |
| 1 | 113-A | 52 | ARG |
| 1 | 113-A | 54 | LEU |
| 1 | 113-A | 58 | LYS |
| 1 | 113-A | 60 | ILE |
| 1 | 113-A | 65 | GLN |
| 1 | 113-A | 68 | THR |
| 1 | 113-A | 76 | LYS |
| 1 | 113-A | 106 | LYS |
| 1 | 113-A | 108 | GLN |
| 1 | 113-A | 127 | ASP |
| 1 | 113-A | 128 | TYR |
| 1 | 113-A | 142 | ASP |
| 1 | 114-A | 1 | MET |
| 1 | 114-A | 2 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 114-A | 8 | LEU |
| 1 | 114-A | 11 | ASP |
| 1 | 114-A | 18 | ASN |
| 1 | 114-A | 20 | MET |
| 1 | 114-A | 33 | ARG |
| 1 | 114-A | 52 | ARG |
| 1 | 114-A | 58 | LYS |
| 1 | 114-A | 59 | ASN |
| 1 | 114-A | 76 | LYS |
| 1 | 114-A | 87 | ASP |
| 1 | 114-A | 104 | LEU |
| 1 | 114-A | 106 | LYS |
| 1 | 114-A | 120 | GLU |
| 1 | 114-A | 122 | ASP |
| 1 | 114-A | 127 | ASP |
| 1 | 114-A | 128 | TYR |
| 1 | 114-A | 142 | ASP |
| 1 | 114-A | 158 | ARG |
| 1 | 115-A | 1 | MET |
| 1 | 115-A | 2 | ILE |
| 1 | 115-A | 8 | LEU |
| 1 | 115-A | 10 | VAL |
| 1 | 115-A | 13 | VAL |
| 1 | 115-A | 16 | MET |
| 1 | 115-A | 20 | MET |
| 1 | 115-A | 23 | ASN |
| 1 | 115-A | 24 | LEU |
| 1 | 115-A | 33 | ARG |
| 1 | 115-A | 52 | ARG |
| 1 | 115-A | 65 | GLN |
| 1 | 115-A | 68 | THR |
| 1 | 115-A | 87 | ASP |
| 1 | 115-A | 109 | LYS |
| 1 | 115-A | 119 | VAL |
| 1 | 115-A | 122 | ASP |
| 1 | 115-A | 132 | ASP |
| 1 | 115-A | 136 | VAL |
| 1 | 115-A | 157 | GLU |
| 1 | 115-A | 158 | ARG |
| 1 | 116-A | 1 | MET |
| 1 | 116-A | 2 | ILE |
| 1 | 116-A | 16 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 116-A | 20 | MET |
| 1 | 116-A | 23 | ASN |
| 1 | 116-A | 24 | LEU |
| 1 | 116-A | 27 | ASP |
| 1 | 116-A | 44 | ARG |
| 1 | 116-A | 52 | ARG |
| 1 | 116-A | 64 | SER |
| 1 | 116-A | 68 | THR |
| 1 | 116-A | 87 | ASP |
| 1 | 116-A | 109 | LYS |
| 1 | 116-A | 132 | ASP |
| 1 | 116-A | 138 | SER |
| 1 | 116-A | 152 | CYS |
| 1 | 116-A | 157 | GLU |
| 1 | 117-A | 2 | ILE |
| 1 | 117-A | 11 | ASP |
| 1 | 117-A | 16 | MET |
| 1 | 117-A | 18 | ASN |
| 1 | 117-A | 23 | ASN |
| 1 | 117-A | 24 | LEU |
| 1 | 117-A | 28 | LEU |
| 1 | 117-A | 52 | ARG |
| 1 | 117-A | 58 | LYS |
| 1 | 117-A | 68 | THR |
| 1 | 117-A | 87 | ASP |
| 1 | 117-A | 104 | LEU |
| 1 | 117-A | 106 | LYS |
| 1 | 117-A | 127 | ASP |
| 1 | 117-A | 128 | TYR |
| 1 | 117-A | 132 | ASP |
| 1 | 117-A | 138 | SER |
| 1 | 117-A | 148 | SER |
| 1 | 118-A | 1 | MET |
| 1 | 118-A | 2 | ILE |
| 1 | 118-A | 4 | LEU |
| 1 | 118-A | 16 | MET |
| 1 | 118-A | 18 | ASN |
| 1 | 118-A | 20 | MET |
| 1 | 118-A | 23 | ASN |
| 1 | 118-A | 24 | LEU |
| 1 | 118-A | 33 | ARG |
| 1 | 118-A | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 118-A | 101 | GLU |
| 1 | 118-A | 104 | LEU |
| 1 | 118-A | 109 | LYS |
| 1 | 118-A | 118 | GLU |
| 1 | 118-A | 119 | VAL |
| 1 | 118-A | 122 | ASP |
| 1 | 118-A | 127 | ASP |
| 1 | 118-A | 132 | ASP |
| 1 | 118-A | 134 | GLU |
| 1 | 118-A | 139 | GLU |
| 1 | 119-A | 1 | MET |
| 1 | 119-A | 2 | ILE |
| 1 | 119-A | 18 | ASN |
| 1 | 119-A | 22 | TRP |
| 1 | 119-A | 23 | ASN |
| 1 | 119-A | 36 | LEU |
| 1 | 119-A | 52 | ARG |
| 1 | 119-A | 65 | GLN |
| 1 | 119-A | 70 | ASP |
| 1 | 119-A | 79 | ASP |
| 1 | 119-A | 87 | ASP |
| 1 | 119-A | 101 | GLU |
| 1 | 119-A | 118 | GLU |
| 1 | 119-A | 119 | VAL |
| 1 | 119-A | 122 | ASP |
| 1 | 119-A | 157 | GLU |
| 1 | 119-A | 159 | ARG |
| 1 | 120-A | 23 | ASN |
| 1 | 120-A | 33 | ARG |
| 1 | 120-A | 36 | LEU |
| 1 | 120-A | 58 | LYS |
| 1 | 120-A | 79 | ASP |
| 1 | 120-A | 87 | ASP |
| 1 | 120-A | 108 | GLN |
| 1 | 120-A | 119 | VAL |
| 1 | 120-A | 122 | ASP |
| 1 | 120-A | 159 | ARG |
| 1 | 121-A | 1 | MET |
| 1 | 121-A | 4 | LEU |
| 1 | 121-A | 18 | ASN |
| 1 | 121-A | 20 | MET |
| 1 | 121-A | 33 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 121-A | 44 | ARG |
| 1 | 121-A | 49 | SER |
| 1 | 121-A | 52 | ARG |
| 1 | 121-A | 79 | ASP |
| 1 | 121-A | 87 | ASP |
| 1 | 121-A | 101 | GLU |
| 1 | 121-A | 108 | GLN |
| 1 | 121-A | 118 | GLU |
| 1 | 121-A | 122 | ASP |
| 1 | 121-A | 128 | TYR |
| 1 | 121-A | 129 | GLU |
| 1 | 121-A | 131 | ASP |
| 1 | 121-A | 158 | ARG |
| 1 | 122-A | 16 | MET |
| 1 | 122-A | 18 | ASN |
| 1 | 122-A | 23 | ASN |
| 1 | 122-A | 33 | ARG |
| 1 | 122-A | 60 | ILE |
| 1 | 122-A | 79 | ASP |
| 1 | 122-A | 87 | ASP |
| 1 | 122-A | 101 | GLU |
| 1 | 122-A | 118 | GLU |
| 1 | 122-A | 122 | ASP |
| 1 | 122-A | 127 | ASP |
| 1 | 122-A | 131 | ASP |
| 1 | 122-A | 159 | ARG |
| 1 | 123-A | 11 | ASP |
| 1 | 123-A | 18 | ASN |
| 1 | 123-A | 23 | ASN |
| 1 | 123-A | 33 | ARG |
| 1 | 123-A | 87 | ASP |
| 1 | 123-A | 118 | GLU |
| 1 | 123-A | 122 | ASP |
| 1 | 123-A | 127 | ASP |
| 1 | 123-A | 128 | TYR |
| 1 | 123-A | 129 | GLU |
| 1 | 123-A | 132 | ASP |
| 1 | 123-A | 135 | SER |
| 1 | 123-A | 148 | SER |
| 1 | 123-A | 156 | LEU |
| 1 | 123-A | 159 | ARG |
| 1 | 124-A | 1 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 124-A | 4 | LEU |
| 1 | 124-A | 16 | MET |
| 1 | 124-A | 33 | ARG |
| 1 | 124-A | 52 | ARG |
| 1 | 124-A | 119 | VAL |
| 1 | 124-A | 128 | TYR |
| 1 | 124-A | 132 | ASP |
| 1 | 124-A | 148 | SER |
| 1 | 124-A | 156 | LEU |
| 1 | 124-A | 158 | ARG |
| 1 | 124-A | 159 | ARG |
| 1 | 125-A | 1 | MET |
| 1 | 125-A | 8 | LEU |
| 1 | 125-A | 17 | GLU |
| 1 | 125-A | 24 | LEU |
| 1 | 125-A | 28 | LEU |
| 1 | 125-A | 33 | ARG |
| 1 | 125-A | 59 | ASN |
| 1 | 125-A | 61 | ILE |
| 1 | 125-A | 87 | ASP |
| 1 | 125-A | 118 | GLU |
| 1 | 125-A | 129 | GLU |
| 1 | 125-A | 148 | SER |
| 1 | 126-A | 17 | GLU |
| 1 | 126-A | 24 | LEU |
| 1 | 126-A | 33 | ARG |
| 1 | 126-A | 70 | ASP |
| 1 | 126-A | 87 | ASP |
| 1 | 126-A | 106 | LYS |
| 1 | 126-A | 108 | GLN |
| 1 | 126-A | 118 | GLU |
| 1 | 126-A | 120 | GLU |
| 1 | 126-A | 156 | LEU |
| 1 | 126-A | 158 | ARG |
| 1 | 127-A | 1 | MET |
| 1 | 127-A | 24 | LEU |
| 1 | 127-A | 28 | LEU |
| 1 | 127-A | 33 | ARG |
| 1 | 127-A | 65 | GLN |
| 1 | 127-A | 104 | LEU |
| 1 | 127-A | 118 | GLU |
| 1 | 127-A | 123 | THR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 127-A | 129 | GLU |
| 1 | 127-A | 132 | ASP |
| 1 | 127-A | 135 | SER |
| 1 | 128-A | 1 | MET |
| 1 | 128-A | 16 | MET |
| 1 | 128-A | 18 | ASN |
| 1 | 128-A | 20 | MET |
| 1 | 128-A | 22 | TRP |
| 1 | 128-A | 24 | LEU |
| 1 | 128-A | 33 | ARG |
| 1 | 128-A | 52 | ARG |
| 1 | 128-A | 104 | LEU |
| 1 | 128-A | 119 | VAL |
| 1 | 128-A | 120 | GLU |
| 1 | 128-A | 127 | ASP |
| 1 | 128-A | 132 | ASP |
| 1 | 128-A | 154 | GLU |
| 1 | 129-A | 1 | MET |
| 1 | 129-A | 4 | LEU |
| 1 | 129-A | 16 | MET |
| 1 | 129-A | 20 | MET |
| 1 | 129-A | 52 | ARG |
| 1 | 129-A | 118 | GLU |
| 1 | 129-A | 119 | VAL |
| 1 | 129-A | 127 | ASP |
| 1 | 129-A | 146 | GLN |
| 1 | 129-A | 159 | ARG |
| 1 | 130-A | 1 | MET |
| 1 | 130-A | 16 | MET |
| 1 | 130-A | 59 | ASN |
| 1 | 130-A | 119 | VAL |
| 1 | 130-A | 120 | GLU |
| 1 | 130-A | 129 | GLU |
| 1 | 130-A | 134 | GLU |
| 1 | 130-A | 146 | GLN |
| 1 | 131-A | 10 | VAL |
| 1 | 131-A | 16 | MET |
| 1 | 131-A | 20 | MET |
| 1 | 131-A | 24 | LEU |
| 1 | 131-A | 28 | LEU |
| 1 | 131-A | 101 | GLU |
| 1 | 131-A | 109 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 131-A | 115 | ILE |
| 1 | 131-A | 119 | VAL |
| 1 | 131-A | 129 | GLU |
| 1 | 131-A | 134 | GLU |
| 1 | 131-A | 146 | GLN |
| 1 | 132-A | 10 | VAL |
| 1 | 132-A | 16 | MET |
| 1 | 132-A | 23 | ASN |
| 1 | 132-A | 28 | LEU |
| 1 | 132-A | 59 | ASN |
| 1 | 132-A | 106 | LYS |
| 1 | 132-A | 119 | VAL |
| 1 | 132-A | 129 | GLU |
| 1 | 132-A | 142 | ASP |
| 1 | 132-A | 146 | GLN |
| 1 | 133-A | 16 | MET |
| 1 | 133-A | 18 | ASN |
| 1 | 133-A | 28 | LEU |
| 1 | 133-A | 52 | ARG |
| 1 | 133-A | 106 | LYS |
| 1 | 133-A | 109 | LYS |
| 1 | 133-A | 118 | GLU |
| 1 | 133-A | 119 | VAL |
| 1 | 133-A | 129 | GLU |
| 1 | 133-A | 142 | ASP |
| 1 | 133-A | 146 | GLN |
| 1 | 134-A | 1 | MET |
| 1 | 134-A | 8 | LEU |
| 1 | 134-A | 16 | MET |
| 1 | 134-A | 20 | MET |
| 1 | 134-A | 23 | ASN |
| 1 | 134-A | 30 | TRP |
| 1 | 134-A | 33 | ARG |
| 1 | 134-A | 87 | ASP |
| 1 | 134-A | 106 | LYS |
| 1 | 134-A | 109 | LYS |
| 1 | 134-A | 120 | GLU |
| 1 | 134-A | 129 | GLU |
| 1 | 134-A | 146 | GLN |
| 1 | 135-A | 8 | LEU |
| 1 | 135-A | 11 | ASP |
| 1 | 135-A | 16 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 135-A | 33 | ARG |
| 1 | 135-A | 44 | ARG |
| 1 | 135-A | 52 | ARG |
| 1 | 135-A | 87 | ASP |
| 1 | 135-A | 120 | GLU |
| 1 | 135-A | 129 | GLU |
| 1 | 135-A | 146 | GLN |
| 1 | 135-A | 159 | ARG |
| 1 | 136-A | 1 | MET |
| 1 | 136-A | 10 | VAL |
| 1 | 136-A | 16 | MET |
| 1 | 136-A | 28 | LEU |
| 1 | 136-A | 33 | ARG |
| 1 | 136-A | 66 | PRO |
| 1 | 136-A | 79 | ASP |
| 1 | 136-A | 87 | ASP |
| 1 | 136-A | 104 | LEU |
| 1 | 136-A | 118 | GLU |
| 1 | 136-A | 128 | TYR |
| 1 | 136-A | 129 | GLU |
| 1 | 136-A | 131 | ASP |
| 1 | 136-A | 138 | SER |
| 1 | 137-A | 13 | VAL |
| 1 | 137-A | 16 | MET |
| 1 | 137-A | 18 | ASN |
| 1 | 137-A | 23 | ASN |
| 1 | 137-A | 52 | ARG |
| 1 | 137-A | 106 | LYS |
| 1 | 137-A | 108 | GLN |
| 1 | 137-A | 127 | ASP |
| 1 | 137-A | 128 | TYR |
| 1 | 137-A | 129 | GLU |
| 1 | 137-A | 131 | ASP |
| 1 | 137-A | 146 | GLN |
| 1 | 137-A | 157 | GLU |
| 1 | 138-A | 1 | MET |
| 1 | 138-A | 2 | ILE |
| 1 | 138-A | 10 | VAL |
| 1 | 138-A | 11 | ASP |
| 1 | 138-A | 16 | MET |
| 1 | 138-A | 17 | GLU |
| 1 | 138-A | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 138-A | 59 | ASN |
| 1 | 138-A | 70 | ASP |
| 1 | 138-A | 76 | LYS |
| 1 | 138-A | 108 | GLN |
| 1 | 138-A | 118 | GLU |
| 1 | 138-A | 128 | TYR |
| 1 | 138-A | 129 | GLU |
| 1 | 138-A | 138 | SER |
| 1 | 138-A | 146 | GLN |
| 1 | 138-A | 154 | GLU |
| 1 | 138-A | 157 | GLU |
| 1 | 138-A | 158 | ARG |
| 1 | 139-A | 1 | MET |
| 1 | 139-A | 18 | ASN |
| 1 | 139-A | 23 | ASN |
| 1 | 139-A | 24 | LEU |
| 1 | 139-A | 52 | ARG |
| 1 | 139-A | 68 | THR |
| 1 | 139-A | 108 | GLN |
| 1 | 139-A | 118 | GLU |
| 1 | 139-A | 129 | GLU |
| 1 | 139-A | 131 | ASP |
| 1 | 139-A | 134 | GLU |
| 1 | 139-A | 135 | SER |
| 1 | 139-A | 152 | CYS |
| 1 | 139-A | 154 | GLU |
| 1 | 139-A | 156 | LEU |
| 1 | 139-A | 157 | GLU |
| 1 | 140-A | 1 | MET |
| 1 | 140-A | 16 | MET |
| 1 | 140-A | 18 | ASN |
| 1 | 140-A | 23 | ASN |
| 1 | 140-A | 24 | LEU |
| 1 | 140-A | 59 | ASN |
| 1 | 140-A | 87 | ASP |
| 1 | 140-A | 108 | GLN |
| 1 | 140-A | 118 | GLU |
| 1 | 140-A | 129 | GLU |
| 1 | 140-A | 131 | ASP |
| 1 | 140-A | 138 | SER |
| 1 | 140-A | 148 | SER |
| 1 | 140-A | 152 | CYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 140-A | 154 | GLU |
| 1 | 141-A | 16 | MET |
| 1 | 141-A | 24 | LEU |
| 1 | 141-A | 36 | LEU |
| 1 | 141-A | 52 | ARG |
| 1 | 141-A | 65 | GLN |
| 1 | 141-A | 68 | THR |
| 1 | 141-A | 101 | GLU |
| 1 | 141-A | 108 | GLN |
| 1 | 141-A | 119 | VAL |
| 1 | 141-A | 128 | TYR |
| 1 | 141-A | 129 | GLU |
| 1 | 141-A | 131 | ASP |
| 1 | 141-A | 132 | ASP |
| 1 | 141-A | 146 | GLN |
| 1 | 141-A | 154 | GLU |
| 1 | 141-A | 156 | LEU |
| 1 | 141-A | 157 | GLU |
| 1 | 142-A | 1 | MET |
| 1 | 142-A | 8 | LEU |
| 1 | 142-A | 10 | VAL |
| 1 | 142-A | 16 | MET |
| 1 | 142-A | 17 | GLU |
| 1 | 142-A | 18 | ASN |
| 1 | 142-A | 23 | ASN |
| 1 | 142-A | 24 | LEU |
| 1 | 142-A | 36 | LEU |
| 1 | 142-A | 52 | ARG |
| 1 | 142-A | 59 | ASN |
| 1 | 142-A | 104 | LEU |
| 1 | 142-A | 108 | GLN |
| 1 | 142-A | 119 | VAL |
| 1 | 142-A | 128 | TYR |
| 1 | 142-A | 129 | GLU |
| 1 | 142-A | 131 | ASP |
| 1 | 142-A | 152 | CYS |
| 1 | 142-A | 154 | GLU |
| 1 | 143-A | 8 | LEU |
| 1 | 143-A | 16 | MET |
| 1 | 143-A | 17 | GLU |
| 1 | 143-A | 18 | ASN |
| 1 | 143-A | 20 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 143-A | 44 | ARG |
| 1 | 143-A | 52 | ARG |
| 1 | 143-A | 87 | ASP |
| 1 | 143-A | 106 | LYS |
| 1 | 143-A | 118 | GLU |
| 1 | 143-A | 122 | ASP |
| 1 | 143-A | 128 | TYR |
| 1 | 143-A | 129 | GLU |
| 1 | 143-A | 131 | ASP |
| 1 | 143-A | 142 | ASP |
| 1 | 143-A | 154 | GLU |
| 1 | 144-A | 1 | MET |
| 1 | 144-A | 8 | LEU |
| 1 | 144-A | 13 | VAL |
| 1 | 144-A | 16 | MET |
| 1 | 144-A | 17 | GLU |
| 1 | 144-A | 36 | LEU |
| 1 | 144-A | 44 | ARG |
| 1 | 144-A | 48 | GLU |
| 1 | 144-A | 52 | ARG |
| 1 | 144-A | 79 | ASP |
| 1 | 144-A | 87 | ASP |
| 1 | 144-A | 88 | VAL |
| 1 | 144-A | 106 | LYS |
| 1 | 144-A | 108 | GLN |
| 1 | 144-A | 112 | LEU |
| 1 | 144-A | 118 | GLU |
| 1 | 144-A | 123 | THR |
| 1 | 144-A | 128 | TYR |
| 1 | 144-A | 129 | GLU |
| 1 | 144-A | 131 | ASP |
| 1 | 144-A | 142 | ASP |
| 1 | 144-A | 148 | SER |
| 1 | 144-A | 157 | GLU |
| 1 | 145-A | 4 | LEU |
| 1 | 145-A | 10 | VAL |
| 1 | 145-A | 11 | ASP |
| 1 | 145-A | 16 | MET |
| 1 | 145-A | 21 | PRO |
| 1 | 145-A | 36 | LEU |
| 1 | 145-A | 44 | ARG |
| 1 | 145-A | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 145-A | 60 | ILE |
| 1 | 145-A | 106 | LYS |
| 1 | 145-A | 108 | GLN |
| 1 | 145-A | 109 | LYS |
| 1 | 145-A | 112 | LEU |
| 1 | 145-A | 120 | GLU |
| 1 | 145-A | 122 | ASP |
| 1 | 145-A | 129 | GLU |
| 1 | 145-A | 154 | GLU |
| 1 | 146-A | 8 | LEU |
| 1 | 146-A | 10 | VAL |
| 1 | 146-A | 16 | MET |
| 1 | 146-A | 20 | MET |
| 1 | 146-A | 21 | PRO |
| 1 | 146-A | 36 | LEU |
| 1 | 146-A | 44 | ARG |
| 1 | 146-A | 52 | ARG |
| 1 | 146-A | 60 | ILE |
| 1 | 146-A | 101 | GLU |
| 1 | 146-A | 106 | LYS |
| 1 | 146-A | 109 | LYS |
| 1 | 146-A | 118 | GLU |
| 1 | 146-A | 120 | GLU |
| 1 | 146-A | 127 | ASP |
| 1 | 146-A | 129 | GLU |
| 1 | 146-A | 137 | PHE |
| 1 | 146-A | 139 | GLU |
| 1 | 146-A | 148 | SER |
| 1 | 147-A | 8 | LEU |
| 1 | 147-A | 10 | VAL |
| 1 | 147-A | 11 | ASP |
| 1 | 147-A | 18 | ASN |
| 1 | 147-A | 48 | GLU |
| 1 | 147-A | 52 | ARG |
| 1 | 147-A | 59 | ASN |
| 1 | 147-A | 101 | GLU |
| 1 | 147-A | 106 | LYS |
| 1 | 147-A | 108 | GLN |
| 1 | 147-A | 116 | ASP |
| 1 | 147-A | 127 | ASP |
| 1 | 147-A | 129 | GLU |
| 1 | 147-A | 137 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 147-A | 142 | ASP |
| 1 | 147-A | 148 | SER |
| 1 | 148-A | 13 | VAL |
| 1 | 148-A | 20 | MET |
| 1 | 148-A | 28 | LEU |
| 1 | 148-A | 52 | ARG |
| 1 | 148-A | 85 | CYS |
| 1 | 148-A | 101 | GLU |
| 1 | 148-A | 109 | LYS |
| 1 | 148-A | 118 | GLU |
| 1 | 148-A | 119 | VAL |
| 1 | 148-A | 120 | GLU |
| 1 | 148-A | 129 | GLU |
| 1 | 148-A | 131 | ASP |
| 1 | 148-A | 134 | GLU |
| 1 | 148-A | 137 | PHE |
| 1 | 148-A | 142 | ASP |
| 1 | 148-A | 157 | GLU |
| 1 | 149-A | 16 | MET |
| 1 | 149-A | 18 | ASN |
| 1 | 149-A | 28 | LEU |
| 1 | 149-A | 30 | TRP |
| 1 | 149-A | 33 | ARG |
| 1 | 149-A | 52 | ARG |
| 1 | 149-A | 68 | THR |
| 1 | 149-A | 106 | LYS |
| 1 | 149-A | 120 | GLU |
| 1 | 149-A | 129 | GLU |
| 1 | 149-A | 137 | PHE |
| 1 | 149-A | 156 | LEU |
| 1 | 150-A | 13 | VAL |
| 1 | 150-A | 16 | MET |
| 1 | 150-A | 22 | TRP |
| 1 | 150-A | 23 | ASN |
| 1 | 150-A | 24 | LEU |
| 1 | 150-A | 33 | ARG |
| 1 | 150-A | 36 | LEU |
| 1 | 150-A | 52 | ARG |
| 1 | 150-A | 62 | LEU |
| 1 | 150-A | 65 | GLN |
| 1 | 150-A | 101 | GLU |
| 1 | 150-A | 104 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 150-A | 109 | LYS |
| 1 | 150-A | 110 | LEU |
| 1 | 150-A | 118 | GLU |
| 1 | 150-A | 156 | LEU |
| 1 | 151-A | 2 | ILE |
| 1 | 151-A | 18 | ASN |
| 1 | 151-A | 23 | ASN |
| 1 | 151-A | 24 | LEU |
| 1 | 151-A | 33 | ARG |
| 1 | 151-A | 36 | LEU |
| 1 | 151-A | 48 | GLU |
| 1 | 151-A | 52 | ARG |
| 1 | 151-A | 59 | ASN |
| 1 | 151-A | 60 | ILE |
| 1 | 151-A | 65 | GLN |
| 1 | 151-A | 70 | ASP |
| 1 | 151-A | 85 | CYS |
| 1 | 151-A | 104 | LEU |
| 1 | 151-A | 137 | PHE |
| 1 | 151-A | 138 | SER |
| 1 | 151-A | 156 | LEU |
| 1 | 152-A | 33 | ARG |
| 1 | 152-A | 36 | LEU |
| 1 | 152-A | 65 | GLN |
| 1 | 152-A | 101 | GLU |
| 1 | 152-A | 104 | LEU |
| 1 | 152-A | 128 | TYR |
| 1 | 153-A | 1 | MET |
| 1 | 153-A | 16 | MET |
| 1 | 153-A | 18 | ASN |
| 1 | 153-A | 22 | TRP |
| 1 | 153-A | 33 | ARG |
| 1 | 153-A | 48 | GLU |
| 1 | 153-A | 52 | ARG |
| 1 | 153-A | 65 | GLN |
| 1 | 153-A | 76 | LYS |
| 1 | 153-A | 85 | CYS |
| 1 | 153-A | 104 | LEU |
| 1 | 153-A | 109 | LYS |
| 1 | 153-A | 120 | GLU |
| 1 | 153-A | 127 | ASP |
| 1 | 153-A | 128 | TYR |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 153-A | 129 | GLU |
| 1 | 153-A | 142 | ASP |
| 1 | 153-A | 156 | LEU |
| 1 | 153-A | 158 | ARG |
| 1 | 153-A | 159 | ARG |
| 1 | 154-A | 1 | MET |
| 1 | 154-A | 18 | ASN |
| 1 | 154-A | 33 | ARG |
| 1 | 154-A | 52 | ARG |
| 1 | 154-A | 65 | GLN |
| 1 | 154-A | 70 | ASP |
| 1 | 154-A | 76 | LYS |
| 1 | 154-A | 85 | CYS |
| 1 | 154-A | 87 | ASP |
| 1 | 154-A | 108 | GLN |
| 1 | 154-A | 127 | ASP |
| 1 | 154-A | 128 | TYR |
| 1 | 154-A | 142 | ASP |
| 1 | 155-A | 10 | VAL |
| 1 | 155-A | 18 | ASN |
| 1 | 155-A | 20 | MET |
| 1 | 155-A | 27 | ASP |
| 1 | 155-A | 52 | ARG |
| 1 | 155-A | 65 | GLN |
| 1 | 155-A | 68 | THR |
| 1 | 155-A | 70 | ASP |
| 1 | 155-A | 76 | LYS |
| 1 | 155-A | 106 | LYS |
| 1 | 155-A | 108 | GLN |
| 1 | 155-A | 142 | ASP |
| 1 | 155-A | 156 | LEU |
| 1 | 156-A | 10 | VAL |
| 1 | 156-A | 13 | VAL |
| 1 | 156-A | 18 | ASN |
| 1 | 156-A | 20 | MET |
| 1 | 156-A | 23 | ASN |
| 1 | 156-A | 27 | ASP |
| 1 | 156-A | 33 | ARG |
| 1 | 156-A | 36 | LEU |
| 1 | 156-A | 45 | HIS |
| 1 | 156-A | 49 | SER |
| 1 | 156-A | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 156-A | 64 | SER |
| 1 | 156-A | 65 | GLN |
| 1 | 156-A | 76 | LYS |
| 1 | 156-A | 104 | LEU |
| 1 | 156-A | 106 | LYS |
| 1 | 156-A | 122 | ASP |
| 1 | 156-A | 136 | VAL |
| 1 | 156-A | 148 | SER |
| 1 | 157-A | 1 | MET |
| 1 | 157-A | 4 | LEU |
| 1 | 157-A | 10 | VAL |
| 1 | 157-A | 13 | VAL |
| 1 | 157-A | 16 | MET |
| 1 | 157-A | 17 | GLU |
| 1 | 157-A | 18 | ASN |
| 1 | 157-A | 24 | LEU |
| 1 | 157-A | 27 | ASP |
| 1 | 157-A | 33 | ARG |
| 1 | 157-A | 59 | ASN |
| 1 | 157-A | 64 | SER |
| 1 | 157-A | 65 | GLN |
| 1 | 157-A | 68 | THR |
| 1 | 157-A | 76 | LYS |
| 1 | 157-A | 120 | GLU |
| 1 | 157-A | 122 | ASP |
| 1 | 157-A | 132 | ASP |
| 1 | 157-A | 148 | SER |
| 1 | 157-A | 156 | LEU |
| 1 | 158-A | 1 | MET |
| 1 | 158-A | 13 | VAL |
| 1 | 158-A | 16 | MET |
| 1 | 158-A | 18 | ASN |
| 1 | 158-A | 36 | LEU |
| 1 | 158-A | 52 | ARG |
| 1 | 158-A | 64 | SER |
| 1 | 158-A | 65 | GLN |
| 1 | 158-A | 68 | THR |
| 1 | 158-A | 76 | LYS |
| 1 | 158-A | 79 | ASP |
| 1 | 158-A | 87 | ASP |
| 1 | 158-A | 129 | GLU |
| 1 | 159-A | 36 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 159-A | 52 | ARG |
| 1 | 159-A | 64 | SER |
| 1 | 159-A | 65 | GLN |
| 1 | 159-A | 66 | PRO |
| 1 | 159-A | 76 | LYS |
| 1 | 159-A | 79 | ASP |
| 1 | 159-A | 87 | ASP |
| 1 | 159-A | 104 | LEU |
| 1 | 159-A | 118 | GLU |
| 1 | 159-A | 119 | VAL |
| 1 | 159-A | 120 | GLU |
| 1 | 159-A | 129 | GLU |
| 1 | 159-A | 131 | ASP |
| 1 | 159-A | 156 | LEU |
| 1 | 160-A | 16 | MET |
| 1 | 160-A | 20 | MET |
| 1 | 160-A | 36 | LEU |
| 1 | 160-A | 52 | ARG |
| 1 | 160-A | 65 | GLN |
| 1 | 160-A | 98 | ARG |
| 1 | 160-A | 104 | LEU |
| 1 | 160-A | 108 | GLN |
| 1 | 160-A | 118 | GLU |
| 1 | 160-A | 119 | VAL |
| 1 | 160-A | 120 | GLU |
| 1 | 160-A | 127 | ASP |
| 1 | 160-A | 128 | TYR |
| 1 | 160-A | 129 | GLU |
| 1 | 160-A | 130 | PRO |
| 1 | 160-A | 131 | ASP |
| 1 | 160-A | 148 | SER |
| 1 | 160-A | 156 | LEU |
| 1 | 161-A | 16 | MET |
| 1 | 161-A | 18 | ASN |
| 1 | 161-A | 44 | ARG |
| 1 | 161-A | 49 | SER |
| 1 | 161-A | 52 | ARG |
| 1 | 161-A | 65 | GLN |
| 1 | 161-A | 66 | PRO |
| 1 | 161-A | 98 | ARG |
| 1 | 161-A | 104 | LEU |
| 1 | 161-A | 108 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 161-A | 120 | GLU |
| 1 | 161-A | 128 | TYR |
| 1 | 161-A | 129 | GLU |
| 1 | 161-A | 130 | PRO |
| 1 | 161-A | 131 | ASP |
| 1 | 161-A | 135 | SER |
| 1 | 161-A | 137 | PHE |
| 1 | 161-A | 138 | SER |
| 1 | 161-A | 148 | SER |
| 1 | 161-A | 156 | LEU |
| 1 | 162-A | 1 | MET |
| 1 | 162-A | 13 | VAL |
| 1 | 162-A | 18 | ASN |
| 1 | 162-A | 20 | MET |
| 1 | 162-A | 33 | ARG |
| 1 | 162-A | 65 | GLN |
| 1 | 162-A | 87 | ASP |
| 1 | 162-A | 98 | ARG |
| 1 | 162-A | 104 | LEU |
| 1 | 162-A | 108 | GLN |
| 1 | 162-A | 128 | TYR |
| 1 | 162-A | 129 | GLU |
| 1 | 162-A | 130 | PRO |
| 1 | 162-A | 132 | ASP |
| 1 | 162-A | 158 | ARG |
| 1 | 163-A | 10 | VAL |
| 1 | 163-A | 13 | VAL |
| 1 | 163-A | 16 | MET |
| 1 | 163-A | 20 | MET |
| 1 | 163-A | 23 | ASN |
| 1 | 163-A | 59 | ASN |
| 1 | 163-A | 68 | THR |
| 1 | 163-A | 87 | ASP |
| 1 | 163-A | 98 | ARG |
| 1 | 163-A | 118 | GLU |
| 1 | 163-A | 119 | VAL |
| 1 | 163-A | 120 | GLU |
| 1 | 163-A | 128 | TYR |
| 1 | 163-A | 129 | GLU |
| 1 | 163-A | 130 | PRO |
| 1 | 163-A | 131 | ASP |
| 1 | 163-A | 132 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 163-A | 156 | LEU |
| 1 | 164-A | 16 | MET |
| 1 | 164-A | 18 | ASN |
| 1 | 164-A | 23 | ASN |
| 1 | 164-A | 33 | ARG |
| 1 | 164-A | 36 | LEU |
| 1 | 164-A | 65 | GLN |
| 1 | 164-A | 68 | THR |
| 1 | 164-A | 79 | ASP |
| 1 | 164-A | 106 | LYS |
| 1 | 164-A | 118 | GLU |
| 1 | 164-A | 127 | ASP |
| 1 | 164-A | 128 | TYR |
| 1 | 164-A | 129 | GLU |
| 1 | 164-A | 130 | PRO |
| 1 | 164-A | 135 | SER |
| 1 | 164-A | 139 | GLU |
| 1 | 164-A | 158 | ARG |
| 1 | 165-A | 4 | LEU |
| 1 | 165-A | 33 | ARG |
| 1 | 165-A | 36 | LEU |
| 1 | 165-A | 48 | GLU |
| 1 | 165-A | 59 | ASN |
| 1 | 165-A | 65 | GLN |
| 1 | 165-A | 68 | THR |
| 1 | 165-A | 79 | ASP |
| 1 | 165-A | 87 | ASP |
| 1 | 165-A | 131 | ASP |
| 1 | 165-A | 132 | ASP |
| 1 | 165-A | 135 | SER |
| 1 | 165-A | 158 | ARG |
| 1 | 166-A | 18 | ASN |
| 1 | 166-A | 33 | ARG |
| 1 | 166-A | 70 | ASP |
| 1 | 166-A | 87 | ASP |
| 1 | 166-A | 104 | LEU |
| 1 | 166-A | 108 | GLN |
| 1 | 166-A | 119 | VAL |
| 1 | 166-A | 128 | TYR |
| 1 | 166-A | 136 | VAL |
| 1 | 166-A | 139 | GLU |
| 1 | 166-A | 148 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 166-A | 159 | ARG |
| 1 | 167-A | 1 | MET |
| 1 | 167-A | 10 | VAL |
| 1 | 167-A | 13 | VAL |
| 1 | 167-A | 33 | ARG |
| 1 | 167-A | 49 | SER |
| 1 | 167-A | 52 | ARG |
| 1 | 167-A | 61 | ILE |
| 1 | 167-A | 68 | THR |
| 1 | 167-A | 79 | ASP |
| 1 | 167-A | 87 | ASP |
| 1 | 167-A | 98 | ARG |
| 1 | 167-A | 104 | LEU |
| 1 | 167-A | 120 | GLU |
| 1 | 167-A | 127 | ASP |
| 1 | 167-A | 128 | TYR |
| 1 | 167-A | 130 | PRO |
| 1 | 167-A | 131 | ASP |
| 1 | 167-A | 132 | ASP |
| 1 | 167-A | 134 | GLU |
| 1 | 167-A | 154 | GLU |
| 1 | 167-A | 158 | 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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 668 ligands modelled in this entry, 334 are monoatomic - leaving 334 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 | 1-A | 201 | - | 27,34,34 | 1.36 | 3 (11%) | 28,47,47 | 1.95 | 7 (25%) |
| 4 | NAP | 1-A | 204 | - | 45,52,52 | 1.70 | 9 (20%) | 55,80,80 | 1.41 | 12 (21%) |
| 2 | FOL | 10-A | 201 | - | 27,34,34 | 1.36 | 3 (11%) | 28,47,47 | 2.11 | 8 (28%) |
| 4 | NAP | 10-A | 204 | - | 45,52,52 | 1.74 | 9 (20%) | 55,80,80 | 1.25 | 8 (14%) |
| 2 | FOL | 100-A | 201 | - | 27,34,34 | 1.70 | 4 (14%) | 28,47,47 | 2.13 | 7 (25%) |
| 4 | NAP | 100-A | 204 | - | 45,52,52 | 1.77 | 10 (22%) | 55,80,80 | 1.36 | 11 (20%) |
| 2 | FOL | 101-A | 201 | - | 27,34,34 | 1.38 | 3 (11%) | 28,47,47 | 1.62 | 4 (14%) |
| 4 | NAP | 101-A | 204 | - | 45,52,52 | 1.72 | 10 (22%) | 55,80,80 | 1.32 | 10 (18%) |
| 2 | FOL | 102-A | 201 | - | 27,34,34 | 1.21 | 3 (11%) | 28,47,47 | 1.84 | 6 (21%) |
| 4 | NAP | 102-A | 204 | - | 45,52,52 | 1.77 | 10 (22%) | 55,80,80 | 1.34 | 11 (20%) |
| 2 | FOL | 103-A | 201 | - | 27,34,34 | 1.36 | 3 (11%) | 28,47,47 | 1.90 | 6 (21%) |
| 4 | NAP | 103-A | 204 | - | 45,52,52 | 1.82 | 11 (24%) | 55,80,80 | 1.36 | 10 (18%) |
| 2 | FOL | 104-A | 201 | - | 27,34,34 | 1.40 | 5 (18%) | 28,47,47 | 2.06 | 7 (25%) |
| 4 | NAP | 104-A | 204 | - | 45,52,52 | 1.80 | 11 (24%) | 55,80,80 | 1.54 | 13 (23%) |
| 2 | FOL | 105-A | 201 | - | 27,34,34 | 1.54 | 4 (14%) | 28,47,47 | 2.06 | 6 (21%) |
| 4 | NAP | 105-A | 204 | - | 45,52,52 | 1.78 | 9 (20%) | 55,80,80 | 1.28 | 9 (16%) |
| 2 | FOL | 106-A | 201 | - | 27,34,34 | 1.39 | 4 (14%) | 28,47,47 | 1.89 | 6 (21%) |
| 4 | NAP | 106-A | 204 | - | 45,52,52 | 1.81 | 11 (24%) | 55,80,80 | 1.26 | 10 (18%) |
| 2 | FOL | 107-A | 201 | - | 27,34,34 | 1.45 | 4 (14%) | 28,47,47 | 2.03 | 7 (25%) |
| 4 | NAP | 107-A | 204 | - | 45,52,52 | 1.76 | 11 (24%) | 55,80,80 | 1.34 | 12 (21%) |
| 2 | FOL | 108-A | 201 | - | 27,34,34 | 1.29 | 3 (11%) | 28,47,47 | 2.23 | 9 (32%) |
| 4 | NAP | 108-A | 204 | - | 45,52,52 | 1.71 | 12 (26%) | 55,80,80 | 1.38 | 7 (12%) |
| 2 | FOL | 109-A | 201 | - | 27,34,34 | 1.33 | 3 (11%) | 28,47,47 | 1.91 | 6 (21%) |
| 4 | NAP | 109-A | 204 | - | 45,52,52 | 1.66 | 11 (24%) | 55,80,80 | 1.27 | 9 (16%) |
| 2 | FOL | 11-A | 201 | - | 27,34,34 | 1.29 | 3 (11%) | 28,47,47 | 1.95 | 4 (14%) |
| 4 | NAP | 11-A | 204 | - | 45,52,52 | 1.74 | 11 (24%) | 55,80,80 | 1.36 | 12 (21%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 110-A | 201 | - | 27,34,34 | 1.41 | 3 (11%) | 28,47,47 | 2.62 | 7 (25%) |
| 4 | NAP | 110-A | 204 | - | 45,52,52 | 1.76 | 12 (26%) | 55,80,80 | 1.31 | 12 (21%) |
| 2 | FOL | 111-A | 201 | - | 27,34,34 | 1.48 | 3 (11%) | 28,47,47 | 2.05 | 4 (14%) |
| 4 | NAP | 111-A | 204 | - | 45,52,52 | 1.73 | 11 (24%) | 55,80,80 | 1.37 | 12 (21%) |
| 2 | FOL | 112-A | 201 | - | 27,34,34 | 1.28 | 3 (11%) | 28,47,47 | 2.38 | 7 (25%) |
| 4 | NAP | 112-A | 204 | - | 45,52,52 | 1.75 | 9 (20%) | 55,80,80 | 1.32 | 10 (18%) |
| 2 | FOL | 113-A | 201 | - | 27,34,34 | 1.45 | 3 (11%) | 28,47,47 | 1.94 | 5 (17%) |
| 4 | NAP | 113-A | 204 | - | 45,52,52 | 1.76 | 9 (20%) | 55,80,80 | 1.31 | 9 (16%) |
| 2 | FOL | 114-A | 201 | - | 27,34,34 | 1.39 | 3 (11%) | 28,47,47 | 2.23 | 5 (17%) |
| 4 | NAP | 114-A | 204 | - | 45,52,52 | 1.74 | 11 (24%) | 55,80,80 | 1.33 | 10 (18%) |
| 2 | FOL | 115-A | 201 | - | 27,34,34 | 1.41 | 3 (11%) | 28,47,47 | 2.54 | 8 (28%) |
| 4 | NAP | 115-A | 204 | - | 45,52,52 | 1.83 | 12 (26%) | 55,80,80 | 1.49 | 11 (20%) |
| 2 | FOL | 116-A | 201 | - | 27,34,34 | 1.38 | 4 (14%) | 28,47,47 | 1.81 | 7 (25%) |
| 4 | NAP | 116-A | 204 | - | 45,52,52 | 1.77 | 10 (22%) | 55,80,80 | 1.30 | 10 (18%) |
| 2 | FOL | 117-A | 201 | - | 27,34,34 | 1.52 | 4 (14%) | 28,47,47 | 1.60 | 4 (14%) |
| 4 | NAP | 117-A | 204 | - | 45,52,52 | 1.74 | 10 (22%) | 55,80,80 | 1.63 | 13 (23%) |
| 2 | FOL | 118-A | 201 | - | 27,34,34 | 1.53 | 3 (11%) | 28,47,47 | 2.35 | 12 (42%) |
| 4 | NAP | 118-A | 204 | - | 45,52,52 | 1.71 | 9 (20%) | 55,80,80 | 2.62 | 12 (21%) |
| 2 | FOL | 119-A | 201 | - | 27,34,34 | 1.45 | 3 (11%) | 28,47,47 | 1.94 | 6 (21%) |
| 4 | NAP | 119-A | 204 | - | 45,52,52 | 1.84 | 11 (24%) | 55,80,80 | 1.98 | 11 (20%) |
| 2 | FOL | 12-A | 201 | - | 27,34,34 | 1.55 | 3 (11%) | 28,47,47 | 1.83 | 5 (17%) |
| 4 | NAP | 12-A | 204 | - | 45,52,52 | 1.69 | 9 (20%) | 55,80,80 | 1.37 | 13 (23%) |
| 2 | FOL | 120-A | 201 | - | 27,34,34 | 1.50 | 5 (18%) | 28,47,47 | 1.91 | 6 (21%) |
| 4 | NAP | 120-A | 204 | - | 45,52,52 | 1.71 | 10 (22%) | 55,80,80 | 1.20 | 6 (10%) |
| 2 | FOL | 121-A | 201 | - | 27,34,34 | 1.55 | 3 (11%) | 28,47,47 | 1.88 | 5 (17%) |
| 4 | NAP | 121-A | 204 | - | 45,52,52 | 1.66 | 10 (22%) | 55,80,80 | 1.27 | 10 (18%) |
| 2 | FOL | 122-A | 201 | - | 27,34,34 | 1.48 | 4 (14%) | 28,47,47 | 1.82 | 5 (17%) |
| 4 | NAP | 122-A | 204 | - | 45,52,52 | 1.73 | 9 (20%) | 55,80,80 | 1.36 | 11 (20%) |
| 2 | FOL | 123-A | 201 | - | 27,34,34 | 1.52 | 5 (18%) | 28,47,47 | 1.75 | 4 (14%) |
| 4 | NAP | 123-A | 204 | - | 45,52,52 | 1.68 | 10 (22%) | 55,80,80 | 1.39 | 11 (20%) |
| 2 | FOL | 124-A | 201 | - | 27,34,34 | 1.41 | 3 (11%) | 28,47,47 | 2.05 | 8 (28%) |
| 4 | NAP | 124-A | 204 | - | 45,52,52 | 1.65 | 8 (17%) | 55,80,80 | 1.33 | 11 (20%) |
| 2 | FOL | 125-A | 201 | - | 27,34,34 | 1.41 | 4 (14%) | 28,47,47 | 1.97 | 5 (17%) |
| 4 | NAP | 125-A | 204 | - | 45,52,52 | 1.64 | 7 (15%) | 55,80,80 | 1.30 | 9 (16%) |
| 2 | FOL | 126-A | 201 | - | 27,34,34 | 1.69 | 5 (18%) | 28,47,47 | 2.59 | 10 (35%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | NAP | 126-A | 204 | - | 45,52,52 | 1.65 | 9 (20%) | 55,80,80 | 1.23 | 10 (18%) |
| 2 | FOL | 127-A | 201 | - | 27,34,34 | 1.37 | 3 (11%) | 28,47,47 | 2.11 | 8 (28%) |
| 4 | NAP | 127-A | 204 | - | 45,52,52 | 1.69 | 9 (20%) | 55,80,80 | 1.36 | 11 (20%) |
| 2 | FOL | 128-A | 201 | - | 27,34,34 | 1.37 | 4 (14%) | 28,47,47 | 2.14 | 7 (25%) |
| 4 | NAP | 128-A | 204 | - | 45,52,52 | 1.70 | 9 (20%) | 55,80,80 | 1.43 | 10 (18%) |
| 2 | FOL | 129-A | 201 | - | 27,34,34 | 1.55 | 3 (11%) | 28,47,47 | 2.20 | 10 (35%) |
| 4 | NAP | 129-A | 204 | - | 45,52,52 | 1.72 | 9 (20%) | 55,80,80 | 1.45 | 11 (20%) |
| 2 | FOL | 13-A | 201 | - | 27,34,34 | 1.52 | 4 (14%) | 28,47,47 | 2.76 | 9 (32%) |
| 4 | NAP | 13-A | 204 | - | 45,52,52 | 1.72 | 10 (22%) | 55,80,80 | 1.23 | 8 (14%) |
| 2 | FOL | 130-A | 201 | - | 27,34,34 | 1.43 | 3 (11%) | 28,47,47 | 1.94 | 7 (25%) |
| 4 | NAP | 130-A | 204 | - | 45,52,52 | 1.71 | 9 (20%) | 55,80,80 | 1.42 | 13 (23%) |
| 2 | FOL | 131-A | 201 | - | 27,34,34 | 1.39 | 4 (14%) | 28,47,47 | 1.96 | 6 (21%) |
| 4 | NAP | 131-A | 204 | - | 45,52,52 | 1.63 | 9 (20%) | 55,80,80 | 1.24 | 6 (10%) |
| 2 | FOL | 132-A | 201 | - | 27,34,34 | 1.55 | 5 (18%) | 28,47,47 | 1.76 | 5 (17%) |
| 4 | NAP | 132-A | 204 | - | 45,52,52 | 1.53 | 7 (15%) | 55,80,80 | 1.19 | 5 (9%) |
| 2 | FOL | 133-A | 201 | - | 27,34,34 | 1.41 | 3 (11%) | 28,47,47 | 2.14 | 3 (10%) |
| 4 | NAP | 133-A | 204 | - | 45,52,52 | 1.61 | 10 (22%) | 55,80,80 | 1.09 | 2 (3%) |
| 2 | FOL | 134-A | 201 | - | 27,34,34 | 1.52 | 4 (14%) | 28,47,47 | 2.27 | 8 (28%) |
| 4 | NAP | 134-A | 204 | - | 45,52,52 | 1.58 | 8 (17%) | 55,80,80 | 1.14 | 5 (9%) |
| 2 | FOL | 135-A | 201 | - | 27,34,34 | 1.46 | 4 (14%) | 28,47,47 | 1.83 | 5 (17%) |
| 4 | NAP | 135-A | 204 | - | 45,52,52 | 1.72 | 9 (20%) | 55,80,80 | 1.33 | 9 (16%) |
| 2 | FOL | 136-A | 201 | - | 27,34,34 | 1.34 | 3 (11%) | 28,47,47 | 2.13 | 9 (32%) |
| 4 | NAP | 136-A | 204 | - | 45,52,52 | 1.71 | 9 (20%) | 55,80,80 | 1.30 | 9 (16%) |
| 2 | FOL | 137-A | 201 | - | 27,34,34 | 1.46 | 3 (11%) | 28,47,47 | 1.74 | 5 (17%) |
| 4 | NAP | 137-A | 204 | - | 45,52,52 | 1.71 | 8 (17%) | 55,80,80 | 1.29 | 8 (14%) |
| 2 | FOL | 138-A | 201 | - | 27,34,34 | 1.29 | 3 (11%) | 28,47,47 | 2.31 | 9 (32%) |
| 4 | NAP | 138-A | 204 | - | 45,52,52 | 1.67 | 9 (20%) | 55,80,80 | 1.32 | 11 (20%) |
| 2 | FOL | 139-A | 201 | - | 27,34,34 | 1.45 | 4 (14%) | 28,47,47 | 2.23 | 8 (28%) |
| 4 | NAP | 139-A | 204 | - | 45,52,52 | 1.69 | 9 (20%) | 55,80,80 | 1.39 | 10 (18%) |
| 2 | FOL | 14-A | 201 | - | 27,34,34 | 1.42 | 4 (14%) | 28,47,47 | 2.45 | 6 (21%) |
| 4 | NAP | 14-A | 204 | - | 45,52,52 | 1.74 | 11 (24%) | 55,80,80 | 1.26 | 10 (18%) |
| 2 | FOL | 140-A | 201 | - | 27,34,34 | 1.26 | 3 (11%) | 28,47,47 | 1.82 | 6 (21%) |
| 4 | NAP | 140-A | 204 | - | 45,52,52 | 1.73 | 9 (20%) | 55,80,80 | 1.33 | 10 (18%) |
| 2 | FOL | 141-A | 201 | - | 27,34,34 | 1.36 | 3 (11%) | 28,47,47 | 1.84 | 6 (21%) |
| 4 | NAP | 141-A | 204 | - | 45,52,52 | 1.70 | 9 (20%) | 55,80,80 | 1.25 | 9 (16%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 142-A | 201 | - | 27,34,34 | 1.29 | 3 (11%) | 28,47,47 | 2.00 | 6 (21%) |
| 4 | NAP | 142-A | 204 | - | 45,52,52 | 1.66 | 8 (17%) | 55,80,80 | 1.32 | 12 (21%) |
| 2 | FOL | 143-A | 201 | - | 27,34,34 | 1.52 | 4 (14%) | 28,47,47 | 2.00 | 7 (25%) |
| 4 | NAP | 143-A | 204 | - | 45,52,52 | 1.72 | 9 (20%) | 55,80,80 | 1.24 | 10 (18%) |
| 2 | FOL | 144-A | 201 | - | 27,34,34 | 1.41 | 4 (14%) | 28,47,47 | 2.13 | 9 (32%) |
| 4 | NAP | 144-A | 204 | - | 45,52,52 | 1.71 | 9 (20%) | 55,80,80 | 1.25 | 10 (18%) |
| 2 | FOL | 145-A | 201 | - | 27,34,34 | 1.37 | 3 (11%) | 28,47,47 | 1.89 | 5 (17%) |
| 4 | NAP | 145-A | 204 | - | 45,52,52 | 1.75 | 10 (22%) | 55,80,80 | 1.22 | 10 (18%) |
| 2 | FOL | 146-A | 201 | - | 27,34,34 | 1.42 | 3 (11%) | 28,47,47 | 1.80 | 5 (17%) |
| 4 | NAP | 146-A | 204 | - | 45,52,52 | 1.73 | 10 (22%) | 55,80,80 | 1.25 | 9 (16%) |
| 2 | FOL | 147-A | 201 | - | 27,34,34 | 1.47 | 3 (11%) | 28,47,47 | 1.90 | 8 (28%) |
| 4 | NAP | 147-A | 204 | - | 45,52,52 | 1.77 | 12 (26%) | 55,80,80 | 1.31 | 10 (18%) |
| 2 | FOL | 148-A | 201 | - | 27,34,34 | 1.53 | 4 (14%) | 28,47,47 | 1.84 | 5 (17%) |
| 4 | NAP | 148-A | 204 | - | 45,52,52 | 1.72 | 10 (22%) | 55,80,80 | 1.33 | 11 (20%) |
| 2 | FOL | 149-A | 201 | - | 27,34,34 | 1.42 | 3 (11%) | 28,47,47 | 1.86 | 6 (21%) |
| 4 | NAP | 149-A | 204 | - | 45,52,52 | 1.73 | 9 (20%) | 55,80,80 | 1.34 | 9 (16%) |
| 2 | FOL | 15-A | 201 | - | 27,34,34 | 1.64 | 4 (14%) | 28,47,47 | 1.90 | 5 (17%) |
| 4 | NAP | 15-A | 204 | - | 45,52,52 | 1.71 | 10 (22%) | 55,80,80 | 1.37 | 12 (21%) |
| 2 | FOL | 150-A | 201 | - | 27,34,34 | 1.40 | 4 (14%) | 28,47,47 | 1.73 | 4 (14%) |
| 4 | NAP | 150-A | 204 | - | 45,52,52 | 1.66 | 9 (20%) | 55,80,80 | 1.34 | 11 (20%) |
| 2 | FOL | 151-A | 201 | - | 27,34,34 | 1.52 | 3 (11%) | 28,47,47 | 2.05 | 5 (17%) |
| 4 | NAP | 151-A | 204 | - | 45,52,52 | 1.66 | 10 (22%) | 55,80,80 | 1.40 | 12 (21%) |
| 2 | FOL | 152-A | 201 | - | 27,34,34 | 1.66 | 4 (14%) | 28,47,47 | 1.77 | 4 (14%) |
| 4 | NAP | 152-A | 204 | - | 45,52,52 | 1.63 | 7 (15%) | 55,80,80 | 1.20 | 8 (14%) |
| 2 | FOL | 153-A | 201 | - | 27,34,34 | 1.39 | 4 (14%) | 28,47,47 | 1.96 | 9 (32%) |
| 4 | NAP | 153-A | 204 | - | 45,52,52 | 1.68 | 10 (22%) | 55,80,80 | 1.21 | 7 (12%) |
| 2 | FOL | 154-A | 201 | - | 27,34,34 | 1.49 | 3 (11%) | 28,47,47 | 1.95 | 5 (17%) |
| 4 | NAP | 154-A | 204 | - | 45,52,52 | 1.66 | 10 (22%) | 55,80,80 | 1.36 | 10 (18%) |
| 2 | FOL | 155-A | 201 | - | 27,34,34 | 1.44 | 3 (11%) | 28,47,47 | 2.07 | 8 (28%) |
| 4 | NAP | 155-A | 204 | - | 45,52,52 | 1.67 | 9 (20%) | 55,80,80 | 1.31 | 8 (14%) |
| 2 | FOL | 156-A | 201 | - | 27,34,34 | 1.57 | 6 (22%) | 28,47,47 | 2.22 | 4 (14%) |
| 4 | NAP | 156-A | 204 | - | 45,52,52 | 1.70 | 9 (20%) | 55,80,80 | 1.45 | 12 (21%) |
| 2 | FOL | 157-A | 201 | - | 27,34,34 | 1.44 | 3 (11%) | 28,47,47 | 1.80 | 7 (25%) |
| 4 | NAP | 157-A | 204 | - | 45,52,52 | 1.59 | 8 (17%) | 55,80,80 | 1.11 | 4 (7%) |
| 2 | FOL | 158-A | 201 | - | 27,34,34 | 1.47 | 3 (11%) | 28,47,47 | 1.95 | 8 (28%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | NAP | 158-A | 204 | - | 45,52,52 | 1.56 | 9 (20%) | 55,80,80 | 1.20 | 5 (9%) |
| 2 | FOL | 159-A | 201 | - | 27,34,34 | 1.40 | 5 (18%) | 28,47,47 | 1.71 | 4 (14%) |
| 4 | NAP | 159-A | 204 | - | 45,52,52 | 1.53 | 6 (13%) | 55,80,80 | 1.27 | 10 (18%) |
| 2 | FOL | 16-A | 201 | - | 27,34,34 | 1.48 | 5 (18%) | 28,47,47 | 1.95 | 5 (17%) |
| 4 | NAP | 16-A | 204 | - | 45,52,52 | 1.74 | 10 (22%) | 55,80,80 | 1.31 | 12 (21%) |
| 2 | FOL | 160-A | 201 | - | 27,34,34 | 1.50 | 4 (14%) | 28,47,47 | 2.11 | 5 (17%) |
| 4 | NAP | 160-A | 204 | - | 45,52,52 | 1.70 | 10 (22%) | 55,80,80 | 1.25 | 9 (16%) |
| 2 | FOL | 161-A | 201 | - | 27,34,34 | 1.29 | 5 (18%) | 28,47,47 | 1.92 | 5 (17%) |
| 4 | NAP | 161-A | 204 | - | 45,52,52 | 1.69 | 9 (20%) | 55,80,80 | 1.31 | 10 (18%) |
| 2 | FOL | 162-A | 201 | - | 27,34,34 | 1.49 | 4 (14%) | 28,47,47 | 1.73 | 6 (21%) |
| 4 | NAP | 162-A | 204 | - | 45,52,52 | 1.69 | 10 (22%) | 55,80,80 | 1.27 | 10 (18%) |
| 2 | FOL | 163-A | 201 | - | 27,34,34 | 1.32 | 5 (18%) | 28,47,47 | 1.93 | 5 (17%) |
| 4 | NAP | 163-A | 204 | - | 45,52,52 | 1.70 | 10 (22%) | 55,80,80 | 1.27 | 9 (16%) |
| 2 | FOL | 164-A | 201 | - | 27,34,34 | 1.44 | 4 (14%) | 28,47,47 | 1.96 | 3 (10%) |
| 4 | NAP | 164-A | 204 | - | 45,52,52 | 1.66 | 9 (20%) | 55,80,80 | 1.37 | 11 (20%) |
| 2 | FOL | 165-A | 201 | - | 27,34,34 | 1.47 | 5 (18%) | 28,47,47 | 2.19 | 6 (21%) |
| 4 | NAP | 165-A | 204 | - | 45,52,52 | 1.77 | 10 (22%) | 55,80,80 | 1.31 | 9 (16%) |
| 2 | FOL | 166-A | 201 | - | 27,34,34 | 1.51 | 4 (14%) | 28,47,47 | 1.61 | 5 (17%) |
| 4 | NAP | 166-A | 204 | - | 45,52,52 | 1.63 | 9 (20%) | 55,80,80 | 1.37 | 10 (18%) |
| 2 | FOL | 167-A | 201 | - | 27,34,34 | 1.50 | 3 (11%) | 28,47,47 | 2.28 | 6 (21%) |
| 4 | NAP | 167-A | 204 | - | 45,52,52 | 1.73 | 10 (22%) | 55,80,80 | 1.34 | 10 (18%) |
| 2 | FOL | 17-A | 201 | - | 27,34,34 | 1.47 | 3 (11%) | 28,47,47 | 1.55 | 4 (14%) |
| 4 | NAP | 17-A | 204 | - | 45,52,52 | 1.75 | 10 (22%) | 55,80,80 | 1.35 | 12 (21%) |
| 2 | FOL | 18-A | 201 | - | 27,34,34 | 1.45 | 4 (14%) | 28,47,47 | 1.85 | 5 (17%) |
| 4 | NAP | 18-A | 204 | - | 45,52,52 | 1.78 | 11 (24%) | 55,80,80 | 1.44 | 12 (21%) |
| 2 | FOL | 19-A | 201 | - | 27,34,34 | 1.53 | 3 (11%) | 28,47,47 | 1.85 | 5 (17%) |
| 4 | NAP | 19-A | 204 | - | 45,52,52 | 1.75 | 9 (20%) | 55,80,80 | 1.30 | 9 (16%) |
| 2 | FOL | 2-A | 201 | - | 27,34,34 | 1.47 | 3 (11%) | 28,47,47 | 1.64 | 5 (17%) |
| 4 | NAP | 2-A | 204 | - | 45,52,52 | 1.68 | 8 (17%) | 55,80,80 | 1.30 | 11 (20%) |
| 2 | FOL | 20-A | 201 | - | 27,34,34 | 1.43 | 3 (11%) | 28,47,47 | 1.78 | 6 (21%) |
| 4 | NAP | 20-A | 204 | - | 45,52,52 | 1.75 | 10 (22%) | 55,80,80 | 1.25 | 7 (12%) |
| 2 | FOL | 21-A | 201 | - | 27,34,34 | 1.67 | 3 (11%) | 28,47,47 | 2.11 | 9 (32%) |
| 4 | NAP | 21-A | 204 | - | 45,52,52 | 1.71 | 9 (20%) | 55,80,80 | 1.33 | 11 (20%) |
| 2 | FOL | 22-A | 201 | - | 27,34,34 | 1.44 | 3 (11%) | 28,47,47 | 1.82 | 4 (14%) |
| 4 | NAP | 22-A | 204 | - | 45,52,52 | 1.80 | 12 (26%) | 55,80,80 | 1.21 | 7 (12%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 23-A | 201 | - | 27,34,34 | 1.34 | 3 (11%) | 28,47,47 | 1.92 | 7 (25%) |
| 4 | NAP | 23-A | 204 | - | 45,52,52 | 1.77 | 10 (22%) | 55,80,80 | 1.39 | 13 (23%) |
| 2 | FOL | 24-A | 201 | - | 27,34,34 | 1.36 | 4 (14%) | 28,47,47 | 2.04 | 9 (32%) |
| 4 | NAP | 24-A | 204 | - | 45,52,52 | 1.75 | 10 (22%) | 55,80,80 | 1.27 | 9 (16%) |
| 2 | FOL | 25-A | 201 | - | 27,34,34 | 1.54 | 4 (14%) | 28,47,47 | 2.33 | 7 (25%) |
| 4 | NAP | 25-A | 204 | - | 45,52,52 | 1.79 | 11 (24%) | 55,80,80 | 1.40 | 11 (20%) |
| 2 | FOL | 26-A | 201 | - | 27,34,34 | 1.56 | 4 (14%) | 28,47,47 | 2.25 | 9 (32%) |
| 4 | NAP | 26-A | 204 | - | 45,52,52 | 1.74 | 10 (22%) | 55,80,80 | 1.32 | 10 (18%) |
| 2 | FOL | 27-A | 201 | - | 27,34,34 | 1.53 | 3 (11%) | 28,47,47 | 1.97 | 4 (14%) |
| 4 | NAP | 27-A | 204 | - | 45,52,52 | 1.77 | 10 (22%) | 55,80,80 | 1.32 | 10 (18%) |
| 2 | FOL | 28-A | 201 | - | 27,34,34 | 1.54 | 3 (11%) | 28,47,47 | 1.83 | 3 (10%) |
| 4 | NAP | 28-A | 204 | - | 45,52,52 | 1.76 | 12 (26%) | 55,80,80 | 1.34 | 9 (16%) |
| 2 | FOL | 29-A | 201 | - | 27,34,34 | 1.37 | 4 (14%) | 28,47,47 | 2.01 | 7 (25%) |
| 4 | NAP | 29-A | 204 | - | 45,52,52 | 1.74 | 11 (24%) | 55,80,80 | 1.32 | 9 (16%) |
| 2 | FOL | 3-A | 201 | - | 27,34,34 | 1.33 | 3 (11%) | 28,47,47 | 1.63 | 4 (14%) |
| 4 | NAP | 3-A | 204 | - | 45,52,52 | 1.73 | 9 (20%) | 55,80,80 | 1.34 | 11 (20%) |
| 2 | FOL | 30-A | 201 | - | 27,34,34 | 1.59 | 3 (11%) | 28,47,47 | 1.79 | 6 (21%) |
| 4 | NAP | 30-A | 204 | - | 45,52,52 | 1.82 | 10 (22%) | 55,80,80 | 1.35 | 9 (16%) |
| 2 | FOL | 31-A | 201 | - | 27,34,34 | 1.36 | 3 (11%) | 28,47,47 | 1.93 | 7 (25%) |
| 4 | NAP | 31-A | 204 | - | 45,52,52 | 1.67 | 11 (24%) | 55,80,80 | 1.34 | 5 (9%) |
| 2 | FOL | 32-A | 201 | - | 27,34,34 | 1.42 | 3 (11%) | 28,47,47 | 1.80 | 6 (21%) |
| 4 | NAP | 32-A | 204 | - | 45,52,52 | 1.64 | 11 (24%) | 55,80,80 | 1.23 | 6 (10%) |
| 2 | FOL | 33-A | 201 | - | 27,34,34 | 1.45 | 3 (11%) | 28,47,47 | 1.84 | 6 (21%) |
| 4 | NAP | 33-A | 204 | - | 45,52,52 | 1.78 | 10 (22%) | 55,80,80 | 1.41 | 10 (18%) |
| 2 | FOL | 34-A | 201 | - | 27,34,34 | 1.44 | 3 (11%) | 28,47,47 | 2.29 | 13 (46%) |
| 4 | NAP | 34-A | 204 | - | 45,52,52 | 1.56 | 8 (17%) | 55,80,80 | 1.21 | 6 (10%) |
| 2 | FOL | 35-A | 201 | - | 27,34,34 | 1.39 | 4 (14%) | 28,47,47 | 1.70 | 5 (17%) |
| 4 | NAP | 35-A | 204 | - | 45,52,52 | 1.75 | 12 (26%) | 55,80,80 | 1.42 | 10 (18%) |
| 2 | FOL | 36-A | 201 | - | 27,34,34 | 1.42 | 4 (14%) | 28,47,47 | 1.88 | 6 (21%) |
| 4 | NAP | 36-A | 204 | - | 45,52,52 | 1.70 | 11 (24%) | 55,80,80 | 1.28 | 10 (18%) |
| 2 | FOL | 37-A | 201 | - | 27,34,34 | 1.41 | 3 (11%) | 28,47,47 | 2.02 | 8 (28%) |
| 4 | NAP | 37-A | 204 | - | 45,52,52 | 1.71 | 11 (24%) | 55,80,80 | 1.25 | 9 (16%) |
| 2 | FOL | 38-A | 201 | - | 27,34,34 | 1.21 | 3 (11%) | 28,47,47 | 1.98 | 5 (17%) |
| 4 | NAP | 38-A | 204 | - | 45,52,52 | 1.77 | 10 (22%) | 55,80,80 | 1.33 | 12 (21%) |
| 2 | FOL | 39-A | 201 | - | 27,34,34 | 1.45 | 4 (14%) | 28,47,47 | 2.46 | 6 (21%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | NAP | 39-A | 204 | - | 45,52,52 | 1.82 | 11 (24%) | 55,80,80 | 1.31 | 11 (20%) |
| 2 | FOL | 4-A | 201 | - | 27,34,34 | 1.54 | 3 (11%) | 28,47,47 | 2.08 | 7 (25%) |
| 4 | NAP | 4-A | 204 | - | 45,52,52 | 1.74 | 8 (17%) | 55,80,80 | 1.42 | 12 (21%) |
| 2 | FOL | 40-A | 201 | - | 27,34,34 | 1.46 | 3 (11%) | 28,47,47 | 2.00 | 7 (25%) |
| 4 | NAP | 40-A | 204 | - | 45,52,52 | 1.76 | 9 (20%) | 55,80,80 | 1.37 | 12 (21%) |
| 2 | FOL | 41-A | 201 | - | 27,34,34 | 1.52 | 3 (11%) | 28,47,47 | 2.02 | 7 (25%) |
| 4 | NAP | 41-A | 204 | - | 45,52,52 | 1.76 | 11 (24%) | 55,80,80 | 1.37 | 11 (20%) |
| 2 | FOL | 42-A | 201 | - | 27,34,34 | 1.63 | 3 (11%) | 28,47,47 | 2.01 | 8 (28%) |
| 4 | NAP | 42-A | 204 | - | 45,52,52 | 1.78 | 11 (24%) | 55,80,80 | 1.52 | 11 (20%) |
| 2 | FOL | 43-A | 201 | - | 27,34,34 | 1.38 | 3 (11%) | 28,47,47 | 2.19 | 5 (17%) |
| 4 | NAP | 43-A | 204 | - | 45,52,52 | 1.71 | 8 (17%) | 55,80,80 | 1.35 | 10 (18%) |
| 2 | FOL | 44-A | 201 | - | 27,34,34 | 1.49 | 3 (11%) | 28,47,47 | 2.06 | 5 (17%) |
| 4 | NAP | 44-A | 204 | - | 45,52,52 | 1.74 | 10 (22%) | 55,80,80 | 1.23 | 8 (14%) |
| 2 | FOL | 45-A | 201 | - | 27,34,34 | 1.43 | 3 (11%) | 28,47,47 | 1.69 | 4 (14%) |
| 4 | NAP | 45-A | 204 | - | 45,52,52 | 1.72 | 10 (22%) | 55,80,80 | 1.21 | 9 (16%) |
| 2 | FOL | 46-A | 201 | - | 27,34,34 | 1.51 | 5 (18%) | 28,47,47 | 2.03 | 6 (21%) |
| 4 | NAP | 46-A | 204 | - | 45,52,52 | 1.68 | 9 (20%) | 55,80,80 | 1.20 | 8 (14%) |
| 2 | FOL | 47-A | 201 | - | 27,34,34 | 1.54 | 3 (11%) | 28,47,47 | 1.95 | 5 (17%) |
| 4 | NAP | 47-A | 204 | - | 45,52,52 | 1.76 | 9 (20%) | 55,80,80 | 1.26 | 8 (14%) |
| 2 | FOL | 48-A | 201 | - | 27,34,34 | 1.45 | 3 (11%) | 28,47,47 | 2.16 | 9 (32%) |
| 4 | NAP | 48-A | 204 | - | 45,52,52 | 1.75 | 9 (20%) | 55,80,80 | 1.38 | 10 (18%) |
| 2 | FOL | 49-A | 201 | - | 27,34,34 | 1.32 | 3 (11%) | 28,47,47 | 1.92 | 5 (17%) |
| 4 | NAP | 49-A | 204 | - | 45,52,52 | 1.76 | 10 (22%) | 55,80,80 | 1.55 | 14 (25%) |
| 2 | FOL | 5-A | 201 | - | 27,34,34 | 1.48 | 4 (14%) | 28,47,47 | 2.02 | 8 (28%) |
| 4 | NAP | 5-A | 204 | - | 45,52,52 | 1.70 | 8 (17%) | 55,80,80 | 1.47 | 12 (21%) |
| 2 | FOL | 50-A | 201 | - | 27,34,34 | 1.50 | 3 (11%) | 28,47,47 | 1.84 | 4 (14%) |
| 4 | NAP | 50-A | 204 | - | 45,52,52 | 1.76 | 9 (20%) | 55,80,80 | 1.32 | 11 (20%) |
| 2 | FOL | 51-A | 201 | - | 27,34,34 | 1.49 | 3 (11%) | 28,47,47 | 1.95 | 5 (17%) |
| 4 | NAP | 51-A | 204 | - | 45,52,52 | 1.76 | 10 (22%) | 55,80,80 | 1.31 | 10 (18%) |
| 2 | FOL | 52-A | 201 | - | 27,34,34 | 1.69 | 5 (18%) | 28,47,47 | 2.19 | 9 (32%) |
| 4 | NAP | 52-A | 204 | - | 45,52,52 | 1.78 | 9 (20%) | 55,80,80 | 1.39 | 9 (16%) |
| 2 | FOL | 53-A | 201 | - | 27,34,34 | 1.52 | 3 (11%) | 28,47,47 | 2.10 | 4 (14%) |
| 4 | NAP | 53-A | 204 | - | 45,52,52 | 1.75 | 9 (20%) | 55,80,80 | 1.25 | 8 (14%) |
| 2 | FOL | 54-A | 201 | - | 27,34,34 | 1.37 | 4 (14%) | 28,47,47 | 2.01 | 6 (21%) |
| 4 | NAP | 54-A | 204 | - | 45,52,52 | 1.72 | 10 (22%) | 55,80,80 | 1.40 | 10 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 55-A | 201 | - | 27,34,34 | 1.37 | 4 (14%) | 28,47,47 | 1.92 | 7 (25%) |
| 4 | NAP | 55-A | 204 | - | 45,52,52 | 1.75 | 10 (22%) | 55,80,80 | 1.25 | 10 (18%) |
| 2 | FOL | 56-A | 201 | - | 27,34,34 | 1.51 | 4 (14%) | 28,47,47 | 2.20 | 5 (17%) |
| 4 | NAP | 56-A | 204 | - | 45,52,52 | 1.64 | 7 (15%) | 55,80,80 | 2.30 | 12 (21%) |
| 2 | FOL | 57-A | 201 | - | 27,34,34 | 1.61 | 4 (14%) | 28,47,47 | 2.28 | 11 (39%) |
| 4 | NAP | 57-A | 204 | - | 45,52,52 | 1.59 | 8 (17%) | 55,80,80 | 2.51 | 6 (10%) |
| 2 | FOL | 58-A | 201 | - | 27,34,34 | 1.46 | 3 (11%) | 28,47,47 | 2.13 | 9 (32%) |
| 4 | NAP | 58-A | 204 | - | 45,52,52 | 1.67 | 8 (17%) | 55,80,80 | 1.07 | 2 (3%) |
| 2 | FOL | 59-A | 201 | - | 27,34,34 | 1.60 | 3 (11%) | 28,47,47 | 1.80 | 6 (21%) |
| 4 | NAP | 59-A | 204 | - | 45,52,52 | 1.64 | 8 (17%) | 55,80,80 | 1.34 | 8 (14%) |
| 2 | FOL | 6-A | 201 | - | 27,34,34 | 1.75 | 4 (14%) | 28,47,47 | 1.93 | 5 (17%) |
| 4 | NAP | 6-A | 204 | - | 45,52,52 | 1.63 | 8 (17%) | 55,80,80 | 1.22 | 6 (10%) |
| 2 | FOL | 60-A | 201 | - | 27,34,34 | 1.45 | 3 (11%) | 28,47,47 | 2.07 | 6 (21%) |
| 4 | NAP | 60-A | 204 | - | 45,52,52 | 1.80 | 10 (22%) | 55,80,80 | 1.31 | 7 (12%) |
| 2 | FOL | 61-A | 201 | - | 27,34,34 | 1.38 | 3 (11%) | 28,47,47 | 1.95 | 5 (17%) |
| 4 | NAP | 61-A | 204 | - | 45,52,52 | 1.73 | 9 (20%) | 55,80,80 | 1.26 | 8 (14%) |
| 2 | FOL | 62-A | 201 | - | 27,34,34 | 1.43 | 3 (11%) | 28,47,47 | 2.20 | 7 (25%) |
| 4 | NAP | 62-A | 204 | - | 45,52,52 | 1.74 | 7 (15%) | 55,80,80 | 1.34 | 10 (18%) |
| 2 | FOL | 63-A | 201 | - | 27,34,34 | 1.35 | 3 (11%) | 28,47,47 | 2.29 | 8 (28%) |
| 4 | NAP | 63-A | 204 | - | 45,52,52 | 1.69 | 8 (17%) | 55,80,80 | 1.39 | 9 (16%) |
| 2 | FOL | 64-A | 201 | - | 27,34,34 | 1.37 | 3 (11%) | 28,47,47 | 2.05 | 9 (32%) |
| 4 | NAP | 64-A | 204 | - | 45,52,52 | 1.75 | 8 (17%) | 55,80,80 | 1.22 | 7 (12%) |
| 2 | FOL | 65-A | 201 | - | 27,34,34 | 1.71 | 4 (14%) | 28,47,47 | 1.90 | 7 (25%) |
| 4 | NAP | 65-A | 204 | - | 45,52,52 | 1.78 | 10 (22%) | 55,80,80 | 1.24 | 7 (12%) |
| 2 | FOL | 66-A | 201 | - | 27,34,34 | 1.39 | 3 (11%) | 28,47,47 | 2.12 | 8 (28%) |
| 4 | NAP | 66-A | 204 | - | 45,52,52 | 1.74 | 11 (24%) | 55,80,80 | 1.29 | 10 (18%) |
| 2 | FOL | 67-A | 201 | - | 27,34,34 | 1.38 | 3 (11%) | 28,47,47 | 1.92 | 5 (17%) |
| 4 | NAP | 67-A | 204 | - | 45,52,52 | 1.74 | 11 (24%) | 55,80,80 | 1.25 | 8 (14%) |
| 2 | FOL | 68-A | 201 | - | 27,34,34 | 1.50 | 3 (11%) | 28,47,47 | 1.85 | 4 (14%) |
| 4 | NAP | 68-A | 204 | - | 45,52,52 | 1.74 | 11 (24%) | 55,80,80 | 1.15 | 6 (10%) |
| 2 | FOL | 69-A | 201 | - | 27,34,34 | 1.48 | 4 (14%) | 28,47,47 | 2.15 | 6 (21%) |
| 4 | NAP | 69-A | 204 | - | 45,52,52 | 1.80 | 10 (22%) | 55,80,80 | 1.32 | 9 (16%) |
| 2 | FOL | 7-A | 201 | - | 27,34,34 | 1.57 | 3 (11%) | 28,47,47 | 1.97 | 5 (17%) |
| 4 | NAP | 7-A | 204 | - | 45,52,52 | 1.59 | 10 (22%) | 55,80,80 | 1.01 | 2 (3%) |
| 2 | FOL | 70-A | 201 | - | 27,34,34 | 1.55 | 4 (14%) | 28,47,47 | 2.17 | 8 (28%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 4 | NAP | 70-A | 204 | - | 45,52,52 | 1.79 | 10 (22%) | 55,80,80 | 1.39 | 11 (20%) |
| 2 | FOL | 71-A | 201 | - | 27,34,34 | 1.41 | 3 (11%) | 28,47,47 | 1.86 | 5 (17%) |
| 4 | NAP | 71-A | 204 | - | 45,52,52 | 1.74 | 11 (24%) | 55,80,80 | 1.35 | 10 (18%) |
| 2 | FOL | 72-A | 201 | - | 27,34,34 | 1.38 | 3 (11%) | 28,47,47 | 2.11 | 5 (17%) |
| 4 | NAP | 72-A | 204 | - | 45,52,52 | 1.74 | 12 (26%) | 55,80,80 | 1.28 | 10 (18%) |
| 2 | FOL | 73-A | 201 | - | 27,34,34 | 1.58 | 3 (11%) | 28,47,47 | 1.76 | 6 (21%) |
| 4 | NAP | 73-A | 204 | - | 45,52,52 | 1.71 | 11 (24%) | 55,80,80 | 1.29 | 9 (16%) |
| 2 | FOL | 74-A | 201 | - | 27,34,34 | 1.62 | 3 (11%) | 28,47,47 | 1.94 | 6 (21%) |
| 4 | NAP | 74-A | 204 | - | 45,52,52 | 1.75 | 12 (26%) | 55,80,80 | 1.35 | 10 (18%) |
| 2 | FOL | 75-A | 201 | - | 27,34,34 | 1.40 | 4 (14%) | 28,47,47 | 1.96 | 5 (17%) |
| 4 | NAP | 75-A | 204 | - | 45,52,52 | 1.75 | 10 (22%) | 55,80,80 | 1.36 | 10 (18%) |
| 2 | FOL | 76-A | 201 | - | 27,34,34 | 1.62 | 3 (11%) | 28,47,47 | 2.31 | 6 (21%) |
| 4 | NAP | 76-A | 204 | - | 45,52,52 | 1.75 | 10 (22%) | 55,80,80 | 1.30 | 10 (18%) |
| 2 | FOL | 77-A | 201 | - | 27,34,34 | 1.54 | 5 (18%) | 28,47,47 | 2.22 | 5 (17%) |
| 4 | NAP | 77-A | 204 | - | 45,52,52 | 1.71 | 10 (22%) | 55,80,80 | 1.35 | 9 (16%) |
| 2 | FOL | 78-A | 201 | - | 27,34,34 | 1.35 | 3 (11%) | 28,47,47 | 2.06 | 7 (25%) |
| 4 | NAP | 78-A | 204 | - | 45,52,52 | 1.71 | 9 (20%) | 55,80,80 | 1.33 | 8 (14%) |
| 2 | FOL | 79-A | 201 | - | 27,34,34 | 1.32 | 3 (11%) | 28,47,47 | 1.86 | 7 (25%) |
| 4 | NAP | 79-A | 204 | - | 45,52,52 | 1.75 | 10 (22%) | 55,80,80 | 1.52 | 12 (21%) |
| 2 | FOL | 8-A | 201 | - | 27,34,34 | 1.50 | 3 (11%) | 28,47,47 | 2.04 | 4 (14%) |
| 4 | NAP | 8-A | 204 | - | 45,52,52 | 1.60 | 9 (20%) | 55,80,80 | 1.11 | 4 (7%) |
| 2 | FOL | 80-A | 201 | - | 27,34,34 | 1.56 | 4 (14%) | 28,47,47 | 2.30 | 9 (32%) |
| 4 | NAP | 80-A | 204 | - | 45,52,52 | 1.76 | 10 (22%) | 55,80,80 | 1.40 | 11 (20%) |
| 2 | FOL | 81-A | 201 | - | 27,34,34 | 1.47 | 4 (14%) | 28,47,47 | 2.03 | 6 (21%) |
| 4 | NAP | 81-A | 204 | - | 45,52,52 | 1.67 | 9 (20%) | 55,80,80 | 1.24 | 7 (12%) |
| 2 | FOL | 82-A | 201 | - | 27,34,34 | 1.53 | 5 (18%) | 28,47,47 | 2.16 | 7 (25%) |
| 4 | NAP | 82-A | 204 | - | 45,52,52 | 1.65 | 9 (20%) | 55,80,80 | 1.17 | 5 (9%) |
| 2 | FOL | 83-A | 201 | - | 27,34,34 | 1.67 | 4 (14%) | 28,47,47 | 2.32 | 8 (28%) |
| 4 | NAP | 83-A | 204 | - | 45,52,52 | 1.62 | 9 (20%) | 55,80,80 | 1.29 | 6 (10%) |
| 2 | FOL | 84-A | 201 | - | 27,34,34 | 1.40 | 3 (11%) | 28,47,47 | 2.13 | 7 (25%) |
| 4 | NAP | 84-A | 204 | - | 45,52,52 | 1.62 | 8 (17%) | 55,80,80 | 1.19 | 5 (9%) |
| 2 | FOL | 85-A | 201 | - | 27,34,34 | 1.44 | 4 (14%) | 28,47,47 | 1.97 | 5 (17%) |
| 4 | NAP | 85-A | 204 | - | 45,52,52 | 1.71 | 10 (22%) | 55,80,80 | 1.35 | 10 (18%) |
| 2 | FOL | 86-A | 201 | - | 27,34,34 | 1.34 | 3 (11%) | 28,47,47 | 1.77 | 6 (21%) |
| 4 | NAP | 86-A | 204 | - | 45,52,52 | 1.68 | 10 (22%) | 55,80,80 | 1.25 | 10 (18%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 87-A | 201 | - | 27,34,34 | 1.41 | 4 (14%) | 28,47,47 | 1.92 | 7 (25%) |
| 4 | NAP | 87-A | 204 | - | 45,52,52 | 1.70 | 9 (20%) | 55,80,80 | 1.24 | 6 (10%) |
| 2 | FOL | 88-A | 201 | - | 27,34,34 | 1.31 | 3 (11%) | 28,47,47 | 1.79 | 5 (17%) |
| 4 | NAP | 88-A | 204 | - | 45,52,52 | 1.69 | 10 (22%) | 55,80,80 | 1.31 | 9 (16%) |
| 2 | FOL | 89-A | 201 | - | 27,34,34 | 1.51 | 3 (11%) | 28,47,47 | 1.83 | 5 (17%) |
| 4 | NAP | 89-A | 204 | - | 45,52,52 | 1.70 | 10 (22%) | 55,80,80 | 1.36 | 9 (16%) |
| 2 | FOL | 9-A | 201 | - | 27,34,34 | 1.54 | 3 (11%) | 28,47,47 | 1.86 | 8 (28%) |
| 4 | NAP | 9-A | 204 | - | 45,52,52 | 1.63 | 8 (17%) | 55,80,80 | 1.14 | 6 (10%) |
| 2 | FOL | 90-A | 201 | - | 27,34,34 | 1.36 | 3 (11%) | 28,47,47 | 1.78 | 6 (21%) |
| 4 | NAP | 90-A | 204 | - | 45,52,52 | 1.66 | 8 (17%) | 55,80,80 | 1.44 | 12 (21%) |
| 2 | FOL | 91-A | 201 | - | 27,34,34 | 1.31 | 2 (7%) | 28,47,47 | 1.90 | 6 (21%) |
| 4 | NAP | 91-A | 204 | - | 45,52,52 | 1.69 | 11 (24%) | 55,80,80 | 1.19 | 9 (16%) |
| 2 | FOL | 92-A | 201 | - | 27,34,34 | 1.47 | 3 (11%) | 28,47,47 | 2.02 | 7 (25%) |
| 4 | NAP | 92-A | 204 | - | 45,52,52 | 1.70 | 10 (22%) | 55,80,80 | 1.27 | 9 (16%) |
| 2 | FOL | 93-A | 201 | - | 27,34,34 | 1.43 | 4 (14%) | 28,47,47 | 2.11 | 6 (21%) |
| 4 | NAP | 93-A | 204 | - | 45,52,52 | 1.69 | 11 (24%) | 55,80,80 | 1.34 | 10 (18%) |
| 2 | FOL | 94-A | 201 | - | 27,34,34 | 1.45 | 3 (11%) | 28,47,47 | 1.93 | 9 (32%) |
| 4 | NAP | 94-A | 204 | - | 45,52,52 | 1.70 | 9 (20%) | 55,80,80 | 1.26 | 7 (12%) |
| 2 | FOL | 95-A | 201 | - | 27,34,34 | 1.33 | 3 (11%) | 28,47,47 | 1.73 | 6 (21%) |
| 4 | NAP | 95-A | 204 | - | 45,52,52 | 1.65 | 9 (20%) | 55,80,80 | 1.31 | 8 (14%) |
| 2 | FOL | 96-A | 201 | - | 27,34,34 | 1.42 | 3 (11%) | 28,47,47 | 1.66 | 6 (21%) |
| 4 | NAP | 96-A | 204 | - | 45,52,52 | 1.74 | 10 (22%) | 55,80,80 | 1.23 | 7 (12%) |
| 2 | FOL | 97-A | 201 | - | 27,34,34 | 1.38 | 4 (14%) | 28,47,47 | 1.88 | 5 (17%) |
| 4 | NAP | 97-A | 204 | - | 45,52,52 | 1.76 | 11 (24%) | 55,80,80 | 1.20 | 7 (12%) |
| 2 | FOL | 98-A | 201 | - | 27,34,34 | 1.45 | 3 (11%) | 28,47,47 | 2.07 | 4 (14%) |
| 4 | NAP | 98-A | 204 | - | 45,52,52 | 1.75 | 10 (22%) | 55,80,80 | 1.32 | 10 (18%) |
| 2 | FOL | 99-A | 201 | - | 27,34,34 | 1.45 | 3 (11%) | 28,47,47 | 2.02 | 7 (25%) |
| 4 | NAP | 99-A | 204 | - | 45,52,52 | 1.79 | 11 (24%) | 55,80,80 | 1.42 | 9 (16%) |

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 | 1-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 4 | NAP | 1-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 10-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 10-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 100-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 100-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 101-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 101-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 102-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 102-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 103-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 103-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 104-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 104-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 105-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 105-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 106-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 106-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 107-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 107-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 108-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 108-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 109-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 109-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 11-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 11-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 110-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 110-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 111-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 111-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 112-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 112-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 113-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 113-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 114-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 114-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 115-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 115-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 116-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 116-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 117-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 117-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 118-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 4 | NAP | 118-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 119-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 119-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 12-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 12-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 120-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 120-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 121-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 121-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 122-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 122-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 123-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 123-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 124-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 124-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 125-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 125-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 126-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 126-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 127-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 127-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 128-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 128-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 129-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 129-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 13-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 13-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 130-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 130-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 131-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 131-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 132-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 132-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 133-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 133-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 134-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 134-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 135-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 135-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 136-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 136-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 137-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 4 | NAP | 137-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 138-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 138-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 139-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 139-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 14-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 14-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 140-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 140-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 141-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 141-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 142-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 142-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 143-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 143-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 144-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 144-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 145-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 145-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 146-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 146-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 147-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 147-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 148-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 148-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 149-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 149-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 15-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 15-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 150-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 150-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 151-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 151-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 152-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 152-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 153-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 153-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 154-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 154-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 155-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 155-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 156-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 4 | NAP | 156-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 157-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 157-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 158-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 158-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 159-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 159-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 16-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 16-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 160-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 160-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 161-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 161-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 162-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 162-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 163-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 163-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 164-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 164-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 165-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 165-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 166-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 166-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 167-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 167-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 17-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 17-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 18-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 18-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 19-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 19-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 2-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 2-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 20-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 20-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 21-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 21-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 22-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 22-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 23-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 23-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 24-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 4 | NAP | 24-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 25-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 25-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 26-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 26-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 27-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 27-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 28-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 28-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 29-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 29-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 3-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 3-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 30-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 30-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 31-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 31-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 32-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 32-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 33-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 33-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 34-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 34-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 35-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 35-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 36-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 36-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 37-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 37-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 38-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 38-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 39-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 39-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 4-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 4-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 40-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 40-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 41-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 41-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 42-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 42-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 43-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 4 | NAP | 43-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 44-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 44-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 45-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 45-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 46-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 46-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 47-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 47-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 48-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 48-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 49-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 49-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 5-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 5-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 50-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 50-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 51-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 51-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 52-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 52-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 53-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 53-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 54-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 54-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 55-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 55-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 56-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 56-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 57-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 57-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 58-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 58-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 59-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 59-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 6-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 6-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 60-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 60-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 61-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 61-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 62-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 4 | NAP | 62-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 63-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 63-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 64-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 64-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 65-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 65-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 66-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 66-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 67-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 67-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 68-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 68-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 69-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 69-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 7-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 7-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 70-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 70-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 71-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 71-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 72-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 72-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 73-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 73-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 74-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 74-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 75-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 75-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 76-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 76-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 77-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 77-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 78-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 78-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 79-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 79-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 8-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 8-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 80-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 80-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 81-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 4 | NAP | 81-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 82-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 82-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 83-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 83-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 84-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 84-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 85-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 85-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 86-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 86-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 87-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 87-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 88-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 88-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 89-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 89-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 9-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 9-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 90-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 90-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 91-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 91-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 92-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 92-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 93-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 93-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 94-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 94-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 95-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 95-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 96-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 96-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 97-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 97-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 98-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 98-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |
| 2 | FOL | 99-A | 201 | - | - | 0/16/22/22 | 0/3/3/3 |
| 4 | NAP | 99-A | 204 | - | - | 0/27/67/67 | 0/5/5/5 |

All (2193) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | 6-A | 201 | FOL | C8A-N1 | -6.65 | 1.30 | 1.37 |
| 2 | 152-A | 201 | FOL | C8A-N1 | -6.44 | 1.30 | 1.37 |
| 2 | 12-A | 201 | FOL | C8A-N1 | -6.43 | 1.30 | 1.37 |
| 4 | 69-A | 204 | NAP | O3B-C3B | -6.42 | 1.27 | 1.43 |
| 4 | 25-A | 204 | NAP | O3B-C3B | -6.41 | 1.27 | 1.43 |
| 4 | 75-A | 204 | NAP | O3B-C3B | -6.37 | 1.28 | 1.43 |
| 4 | 22-A | 204 | NAP | O3B-C3B | -6.36 | 1.28 | 1.43 |
| 2 | 15-A | 201 | FOL | C8A-N1 | -6.32 | 1.30 | 1.37 |
| 2 | 7-A | 201 | FOL | C8A-N1 | -6.31 | 1.30 | 1.37 |
| 4 | 116-A | 204 | NAP | O3B-C3B | -6.31 | 1.28 | 1.43 |
| 4 | 26-A | 204 | NAP | O3B-C3B | -6.30 | 1.28 | 1.43 |
| 4 | 70-A | 204 | NAP | O3B-C3B | -6.27 | 1.28 | 1.43 |
| 4 | 23-A | 204 | NAP | O3B-C3B | -6.26 | 1.28 | 1.43 |
| 4 | 33-A | 204 | NAP | O3B-C3B | -6.24 | 1.28 | 1.43 |
| 4 | 52-A | 204 | NAP | O3B-C3B | -6.24 | 1.28 | 1.43 |
| 2 | 9-A | 201 | FOL | C8A-N1 | -6.23 | 1.30 | 1.37 |
| 4 | 30-A | 204 | NAP | O3B-C3B | -6.22 | 1.28 | 1.43 |
| 2 | 76-A | 201 | FOL | C8A-N1 | -6.22 | 1.30 | 1.37 |
| 4 | 74-A | 204 | NAP | O3B-C3B | -6.22 | 1.28 | 1.43 |
| 4 | 71-A | 204 | NAP | O3B-C3B | -6.21 | 1.28 | 1.43 |
| 4 | 19-A | 204 | NAP | O3B-C3B | -6.19 | 1.28 | 1.43 |
| 2 | 21-A | 201 | FOL | C8A-N1 | -6.19 | 1.30 | 1.37 |
| 4 | 68-A | 204 | NAP | O3B-C3B | -6.19 | 1.28 | 1.43 |
| 4 | 11-A | 204 | NAP | O3B-C3B | -6.17 | 1.28 | 1.43 |
| 4 | 64-A | 204 | NAP | O3B-C3B | -6.17 | 1.28 | 1.43 |
| 4 | 99-A | 204 | NAP | O3B-C3B | -6.16 | 1.28 | 1.43 |
| 2 | 59-A | 201 | FOL | C8A-N1 | -6.15 | 1.30 | 1.37 |
| 2 | 42-A | 201 | FOL | C8A-N1 | -6.14 | 1.30 | 1.37 |
| 4 | 147-A | 204 | NAP | O3B-C3B | -6.13 | 1.28 | 1.43 |
| 4 | 17-A | 204 | NAP | O3B-C3B | -6.13 | 1.28 | 1.43 |
| 4 | 76-A | 204 | NAP | O3B-C3B | -6.13 | 1.28 | 1.43 |
| 4 | 67-A | 204 | NAP | O3B-C3B | -6.12 | 1.28 | 1.43 |
| 2 | 19-A | 201 | FOL | C8A-N1 | -6.12 | 1.30 | 1.37 |
| 4 | 51-A | 204 | NAP | O3B-C3B | -6.11 | 1.28 | 1.43 |
| 4 | 24-A | 204 | NAP | O3B-C3B | -6.11 | 1.28 | 1.43 |
| 4 | 27-A | 204 | NAP | O3B-C3B | -6.10 | 1.28 | 1.43 |
| 4 | 20-A | 204 | NAP | O3B-C3B | -6.09 | 1.28 | 1.43 |
| 4 | 60-A | 204 | NAP | O3B-C3B | -6.08 | 1.28 | 1.43 |
| 4 | 10-A | 204 | NAP | O3B-C3B | -6.08 | 1.28 | 1.43 |
| 2 | 73-A | 201 | FOL | C8A-N1 | -6.07 | 1.30 | 1.37 |
| 4 | 122-A | 204 | NAP | O3B-C3B | -6.07 | 1.28 | 1.43 |
| 2 | 50-A | 201 | FOL | C8A-N1 | -6.07 | 1.30 | 1.37 |
| 4 | 18-A | 204 | NAP | O3B-C3B | -6.07 | 1.28 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 106-A | 204 | NAP | O3B-C3B | -6.07 | 1.28 | 1.43 |
| 4 | 4-A | 204 | NAP | O3B-C3B | -6.06 | 1.28 | 1.43 |
| 4 | 65-A | 204 | NAP | O3B-C3B | -6.05 | 1.28 | 1.43 |
| 4 | 145-A | 204 | NAP | O3B-C3B | -6.05 | 1.28 | 1.43 |
| 4 | 140-A | 204 | NAP | O3B-C3B | -6.05 | 1.28 | 1.43 |
| 4 | 39-A | 204 | NAP | O3B-C3B | -6.04 | 1.28 | 1.43 |
| 2 | 4-A | 201 | FOL | C8A-N1 | -6.04 | 1.30 | 1.37 |
| 4 | 103-A | 204 | NAP | O3B-C3B | -6.03 | 1.28 | 1.43 |
| 4 | 62-A | 204 | NAP | O3B-C3B | -6.02 | 1.28 | 1.43 |
| 4 | 40-A | 204 | NAP | O3B-C3B | -6.02 | 1.28 | 1.43 |
| 4 | 117-A | 204 | NAP | O3B-C3B | -6.01 | 1.28 | 1.43 |
| 4 | 165-A | 204 | NAP | O3B-C3B | -6.00 | 1.28 | 1.43 |
| 4 | 115-A | 204 | NAP | O3B-C3B | -5.99 | 1.28 | 1.43 |
| 4 | 149-A | 204 | NAP | O3B-C3B | -5.98 | 1.28 | 1.43 |
| 4 | 53-A | 204 | NAP | O3B-C3B | -5.98 | 1.28 | 1.43 |
| 4 | 129-A | 204 | NAP | O3B-C3B | -5.98 | 1.28 | 1.43 |
| 4 | 16-A | 204 | NAP | O3B-C3B | -5.98 | 1.28 | 1.43 |
| 4 | 80-A | 204 | NAP | O3B-C3B | -5.98 | 1.28 | 1.43 |
| 4 | 77-A | 204 | NAP | O3B-C3B | -5.98 | 1.28 | 1.43 |
| 4 | 38-A | 204 | NAP | O3B-C3B | -5.97 | 1.28 | 1.43 |
| 4 | 3-A | 204 | NAP | O3B-C3B | -5.97 | 1.28 | 1.43 |
| 4 | 28-A | 204 | NAP | O3B-C3B | -5.97 | 1.28 | 1.43 |
| 2 | 117-A | 201 | FOL | C8A-N1 | -5.96 | 1.30 | 1.37 |
| 4 | 50-A | 204 | NAP | O3B-C3B | -5.96 | 1.28 | 1.43 |
| 4 | 49-A | 204 | NAP | O3B-C3B | -5.95 | 1.28 | 1.43 |
| 4 | 128-A | 204 | NAP | O3B-C3B | -5.95 | 1.28 | 1.43 |
| 4 | 127-A | 204 | NAP | O3B-C3B | -5.95 | 1.28 | 1.43 |
| 4 | 151-A | 204 | NAP | O3B-C3B | -5.95 | 1.28 | 1.43 |
| 4 | 42-A | 204 | NAP | O3B-C3B | -5.94 | 1.29 | 1.43 |
| 4 | 78-A | 204 | NAP | O3B-C3B | -5.93 | 1.29 | 1.43 |
| 4 | 98-A | 204 | NAP | O3B-C3B | -5.93 | 1.29 | 1.43 |
| 4 | 163-A | 204 | NAP | O3B-C3B | -5.93 | 1.29 | 1.43 |
| 4 | 161-A | 204 | NAP | O3B-C3B | -5.92 | 1.29 | 1.43 |
| 4 | 63-A | 204 | NAP | O3B-C3B | -5.92 | 1.29 | 1.43 |
| 2 | 47-A | 201 | FOL | C8A-N1 | -5.92 | 1.30 | 1.37 |
| 4 | 124-A | 204 | NAP | O3B-C3B | -5.92 | 1.29 | 1.43 |
| 2 | 74-A | 201 | FOL | C8A-N1 | -5.92 | 1.30 | 1.37 |
| 4 | 104-A | 204 | NAP | O3B-C3B | -5.91 | 1.29 | 1.43 |
| 4 | 55-A | 204 | NAP | O3B-C3B | -5.91 | 1.29 | 1.43 |
| 4 | 126-A | 204 | NAP | O3B-C3B | -5.91 | 1.29 | 1.43 |
| 4 | 100-A | 204 | NAP | O3B-C3B | -5.91 | 1.29 | 1.43 |
| 4 | 85-A | 204 | NAP | O3B-C3B | -5.91 | 1.29 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 119-A | 204 | NAP | O3B-C3B | -5.90 | 1.29 | 1.43 |
| 4 | 79-A | 204 | NAP | O3B-C3B | -5.89 | 1.29 | 1.43 |
| 4 | 72-A | 204 | NAP | O3B-C3B | -5.89 | 1.29 | 1.43 |
| 4 | 162-A | 204 | NAP | O3B-C3B | -5.89 | 1.29 | 1.43 |
| 4 | 47-A | 204 | NAP | O3B-C3B | -5.88 | 1.29 | 1.43 |
| 4 | 114-A | 204 | NAP | O3B-C3B | -5.88 | 1.29 | 1.43 |
| 4 | 141-A | 204 | NAP | O3B-C3B | -5.88 | 1.29 | 1.43 |
| 2 | 83-A | 201 | FOL | C8A-N1 | -5.88 | 1.31 | 1.37 |
| 4 | 66-A | 204 | NAP | O3B-C3B | -5.87 | 1.29 | 1.43 |
| 2 | 8-A | 201 | FOL | C8A-N1 | -5.87 | 1.31 | 1.37 |
| 4 | 123-A | 204 | NAP | O3B-C3B | -5.87 | 1.29 | 1.43 |
| 4 | 146-A | 204 | NAP | O3B-C3B | -5.86 | 1.29 | 1.43 |
| 4 | 143-A | 204 | NAP | O3B-C3B | -5.86 | 1.29 | 1.43 |
| 4 | 5-A | 204 | NAP | O3B-C3B | -5.85 | 1.29 | 1.43 |
| 4 | 97-A | 204 | NAP | O3B-C3B | -5.85 | 1.29 | 1.43 |
| 4 | 153-A | 204 | NAP | O3B-C3B | -5.85 | 1.29 | 1.43 |
| 4 | 148-A | 204 | NAP | O3B-C3B | -5.85 | 1.29 | 1.43 |
| 4 | 35-A | 204 | NAP | O3B-C3B | -5.84 | 1.29 | 1.43 |
| 4 | 73-A | 204 | NAP | O3B-C3B | -5.84 | 1.29 | 1.43 |
| 4 | 15-A | 204 | NAP | O3B-C3B | -5.83 | 1.29 | 1.43 |
| 4 | 105-A | 204 | NAP | O3B-C3B | -5.83 | 1.29 | 1.43 |
| 4 | 86-A | 204 | NAP | O3B-C3B | -5.83 | 1.29 | 1.43 |
| 4 | 21-A | 204 | NAP | O3B-C3B | -5.81 | 1.29 | 1.43 |
| 4 | 110-A | 204 | NAP | O3B-C3B | -5.81 | 1.29 | 1.43 |
| 4 | 156-A | 204 | NAP | O3B-C3B | -5.81 | 1.29 | 1.43 |
| 4 | 139-A | 204 | NAP | O3B-C3B | -5.80 | 1.29 | 1.43 |
| 4 | 102-A | 204 | NAP | O3B-C3B | -5.80 | 1.29 | 1.43 |
| 4 | 1-A | 204 | NAP | O3B-C3B | -5.80 | 1.29 | 1.43 |
| 4 | 107-A | 204 | NAP | O3B-C3B | -5.79 | 1.29 | 1.43 |
| 4 | 13-A | 204 | NAP | O3B-C3B | -5.79 | 1.29 | 1.43 |
| 4 | 48-A | 204 | NAP | O3B-C3B | -5.78 | 1.29 | 1.43 |
| 4 | 144-A | 204 | NAP | O3B-C3B | -5.78 | 1.29 | 1.43 |
| 4 | 37-A | 204 | NAP | O3B-C3B | -5.77 | 1.29 | 1.43 |
| 4 | 130-A | 204 | NAP | O3B-C3B | -5.76 | 1.29 | 1.43 |
| 4 | 167-A | 204 | NAP | O3B-C3B | -5.76 | 1.29 | 1.43 |
| 4 | 120-A | 204 | NAP | O3B-C3B | -5.75 | 1.29 | 1.43 |
| 4 | 135-A | 204 | NAP | O3B-C3B | -5.75 | 1.29 | 1.43 |
| 4 | 164-A | 204 | NAP | O3B-C3B | -5.75 | 1.29 | 1.43 |
| 4 | 61-A | 204 | NAP | O3B-C3B | -5.74 | 1.29 | 1.43 |
| 4 | 101-A | 204 | NAP | O3B-C3B | -5.74 | 1.29 | 1.43 |
| 4 | 91-A | 204 | NAP | O3B-C3B | -5.74 | 1.29 | 1.43 |
| 4 | 166-A | 204 | NAP | O3B-C3B | -5.72 | 1.29 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 14-A | 204 | NAP | O3B-C3B | -5.71 | 1.29 | 1.43 |
| 4 | 142-A | 204 | NAP | O3B-C3B | -5.71 | 1.29 | 1.43 |
| 4 | 45-A | 204 | NAP | O3B-C3B | -5.71 | 1.29 | 1.43 |
| 4 | 87-A | 204 | NAP | O3B-C3B | -5.69 | 1.29 | 1.43 |
| 4 | 2-A | 204 | NAP | O3B-C3B | -5.68 | 1.29 | 1.43 |
| 4 | 160-A | 204 | NAP | O3B-C3B | -5.68 | 1.29 | 1.43 |
| 4 | 36-A | 204 | NAP | O3B-C3B | -5.68 | 1.29 | 1.43 |
| 4 | 113-A | 204 | NAP | O3B-C3B | -5.68 | 1.29 | 1.43 |
| 2 | 89-A | 201 | FOL | C8A-N1 | -5.67 | 1.31 | 1.37 |
| 4 | 12-A | 204 | NAP | O3B-C3B | -5.67 | 1.29 | 1.43 |
| 4 | 41-A | 204 | NAP | O3B-C3B | -5.67 | 1.29 | 1.43 |
| 4 | 118-A | 204 | NAP | O3B-C3B | -5.66 | 1.29 | 1.43 |
| 2 | 45-A | 201 | FOL | C8A-N1 | -5.66 | 1.31 | 1.37 |
| 4 | 150-A | 204 | NAP | O3B-C3B | -5.66 | 1.29 | 1.43 |
| 2 | 2-A | 201 | FOL | C8A-N1 | -5.66 | 1.31 | 1.37 |
| 4 | 136-A | 204 | NAP | O3B-C3B | -5.65 | 1.29 | 1.43 |
| 4 | 96-A | 204 | NAP | O3B-C3B | -5.65 | 1.29 | 1.43 |
| 4 | 88-A | 204 | NAP | O3B-C3B | -5.65 | 1.29 | 1.43 |
| 4 | 29-A | 204 | NAP | O3B-C3B | -5.65 | 1.29 | 1.43 |
| 4 | 92-A | 204 | NAP | O3B-C3B | -5.65 | 1.29 | 1.43 |
| 4 | 59-A | 204 | NAP | O3B-C3B | -5.65 | 1.29 | 1.43 |
| 4 | 44-A | 204 | NAP | O3B-C3B | -5.64 | 1.29 | 1.43 |
| 4 | 125-A | 204 | NAP | O3B-C3B | -5.62 | 1.29 | 1.43 |
| 2 | 57-A | 201 | FOL | C8A-N1 | -5.62 | 1.31 | 1.37 |
| 4 | 43-A | 204 | NAP | O3B-C3B | -5.62 | 1.29 | 1.43 |
| 2 | 70-A | 201 | FOL | C8A-N1 | -5.61 | 1.31 | 1.37 |
| 4 | 90-A | 204 | NAP | O3B-C3B | -5.61 | 1.29 | 1.43 |
| 4 | 121-A | 204 | NAP | O3B-C3B | -5.60 | 1.29 | 1.43 |
| 4 | 152-A | 204 | NAP | O3B-C3B | -5.60 | 1.29 | 1.43 |
| 2 | 56-A | 201 | FOL | C8A-N1 | -5.60 | 1.31 | 1.37 |
| 4 | 154-A | 204 | NAP | O3B-C3B | -5.60 | 1.29 | 1.43 |
| 2 | 110-A | 201 | FOL | C8A-N1 | -5.60 | 1.31 | 1.37 |
| 4 | 138-A | 204 | NAP | O3B-C3B | -5.59 | 1.29 | 1.43 |
| 4 | 54-A | 204 | NAP | O3B-C3B | -5.58 | 1.29 | 1.43 |
| 2 | 118-A | 201 | FOL | C8A-N1 | -5.58 | 1.31 | 1.37 |
| 4 | 112-A | 204 | NAP | O3B-C3B | -5.58 | 1.29 | 1.43 |
| 2 | 71-A | 201 | FOL | C8A-N1 | -5.58 | 1.31 | 1.37 |
| 2 | 51-A | 201 | FOL | C8A-N1 | -5.57 | 1.31 | 1.37 |
| 2 | 20-A | 201 | FOL | C8A-N1 | -5.57 | 1.31 | 1.37 |
| 4 | 111-A | 204 | NAP | O3B-C3B | -5.56 | 1.29 | 1.43 |
| 2 | 134-A | 201 | FOL | C8A-N1 | -5.56 | 1.31 | 1.37 |
| 2 | 167-A | 201 | FOL | C8A-N1 | -5.56 | 1.31 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 89-A | 204 | NAP | O3B-C3B | -5.53 | 1.29 | 1.43 |
| 4 | 137-A | 204 | NAP | O3B-C3B | -5.53 | 1.29 | 1.43 |
| 2 | 151-A | 201 | FOL | C8A-N1 | -5.53 | 1.31 | 1.37 |
| 2 | 32-A | 201 | FOL | C8A-N1 | -5.51 | 1.31 | 1.37 |
| 4 | 93-A | 204 | NAP | O3B-C3B | -5.51 | 1.30 | 1.43 |
| 2 | 92-A | 201 | FOL | C8A-N1 | -5.49 | 1.31 | 1.37 |
| 4 | 155-A | 204 | NAP | O3B-C3B | -5.48 | 1.30 | 1.43 |
| 4 | 46-A | 204 | NAP | O3B-C3B | -5.46 | 1.30 | 1.43 |
| 4 | 81-A | 204 | NAP | O3B-C3B | -5.45 | 1.30 | 1.43 |
| 2 | 160-A | 201 | FOL | C8A-N1 | -5.43 | 1.31 | 1.37 |
| 2 | 129-A | 201 | FOL | C8A-N1 | -5.43 | 1.31 | 1.37 |
| 2 | 158-A | 201 | FOL | C8A-N1 | -5.43 | 1.31 | 1.37 |
| 2 | 68-A | 201 | FOL | C8A-N1 | -5.42 | 1.31 | 1.37 |
| 2 | 143-A | 201 | FOL | C8A-N1 | -5.41 | 1.31 | 1.37 |
| 2 | 137-A | 201 | FOL | C8A-N1 | -5.40 | 1.31 | 1.37 |
| 2 | 162-A | 201 | FOL | C8A-N1 | -5.39 | 1.31 | 1.37 |
| 2 | 146-A | 201 | FOL | C8A-N1 | -5.38 | 1.31 | 1.37 |
| 2 | 119-A | 201 | FOL | C8A-N1 | -5.37 | 1.31 | 1.37 |
| 2 | 30-A | 201 | FOL | C8A-N1 | -5.37 | 1.31 | 1.37 |
| 4 | 94-A | 204 | NAP | O3B-C3B | -5.37 | 1.30 | 1.43 |
| 2 | 28-A | 201 | FOL | C8A-N1 | -5.36 | 1.31 | 1.37 |
| 2 | 1-A | 201 | FOL | C8A-N1 | -5.35 | 1.31 | 1.37 |
| 2 | 22-A | 201 | FOL | C8A-N1 | -5.35 | 1.31 | 1.37 |
| 2 | 132-A | 201 | FOL | C8A-N1 | -5.34 | 1.31 | 1.37 |
| 2 | 34-A | 201 | FOL | C8A-N1 | -5.34 | 1.31 | 1.37 |
| 4 | 131-A | 204 | NAP | O3B-C3B | -5.34 | 1.30 | 1.43 |
| 2 | 126-A | 201 | FOL | C8A-N1 | -5.34 | 1.31 | 1.37 |
| 2 | 23-A | 201 | FOL | C8A-N1 | -5.34 | 1.31 | 1.37 |
| 4 | 58-A | 204 | NAP | O3B-C3B | -5.34 | 1.30 | 1.43 |
| 2 | 27-A | 201 | FOL | C8A-N1 | -5.32 | 1.31 | 1.37 |
| 2 | 154-A | 201 | FOL | C8A-N1 | -5.30 | 1.31 | 1.37 |
| 2 | 157-A | 201 | FOL | C8A-N1 | -5.30 | 1.31 | 1.37 |
| 2 | 111-A | 201 | FOL | C8A-N1 | -5.29 | 1.31 | 1.37 |
| 2 | 94-A | 201 | FOL | C8A-N1 | -5.28 | 1.31 | 1.37 |
| 2 | 98-A | 201 | FOL | C8A-N1 | -5.28 | 1.31 | 1.37 |
| 2 | 65-A | 201 | FOL | C8A-N1 | -5.28 | 1.31 | 1.37 |
| 2 | 40-A | 201 | FOL | C8A-N1 | -5.27 | 1.31 | 1.37 |
| 2 | 44-A | 201 | FOL | C8A-N1 | -5.26 | 1.31 | 1.37 |
| 2 | 17-A | 201 | FOL | C8A-N1 | -5.24 | 1.31 | 1.37 |
| 2 | 66-A | 201 | FOL | C8A-N1 | -5.22 | 1.31 | 1.37 |
| 4 | 95-A | 204 | NAP | O3B-C3B | -5.22 | 1.30 | 1.43 |
| 2 | 39-A | 201 | FOL | C8A-N1 | -5.21 | 1.31 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 34-A | 204 | NAP | O3B-C3B | -5.21 | 1.30 | 1.43 |
| 2 | 69-A | 201 | FOL | C8A-N1 | -5.19 | 1.31 | 1.37 |
| 2 | 36-A | 201 | FOL | C8A-N1 | -5.18 | 1.31 | 1.37 |
| 2 | 62-A | 201 | FOL | C8A-N1 | -5.18 | 1.31 | 1.37 |
| 2 | 133-A | 201 | FOL | C8A-N1 | -5.17 | 1.31 | 1.37 |
| 4 | 32-A | 204 | NAP | O3B-C3B | -5.16 | 1.30 | 1.43 |
| 4 | 31-A | 204 | NAP | O3B-C3B | -5.16 | 1.30 | 1.43 |
| 2 | 53-A | 201 | FOL | C8A-N1 | -5.15 | 1.31 | 1.37 |
| 2 | 77-A | 201 | FOL | C8A-N1 | -5.15 | 1.31 | 1.37 |
| 2 | 121-A | 201 | FOL | C8A-N1 | -5.15 | 1.31 | 1.37 |
| 4 | 82-A | 204 | NAP | O3B-C3B | -5.14 | 1.30 | 1.43 |
| 2 | 18-A | 201 | FOL | C8A-N1 | -5.14 | 1.31 | 1.37 |
| 2 | 147-A | 201 | FOL | C8A-N1 | -5.13 | 1.31 | 1.37 |
| 2 | 85-A | 201 | FOL | C8A-N1 | -5.11 | 1.31 | 1.37 |
| 2 | 105-A | 201 | FOL | C8A-N1 | -5.11 | 1.31 | 1.37 |
| 4 | 84-A | 204 | NAP | O3B-C3B | -5.11 | 1.30 | 1.43 |
| 2 | 100-A | 201 | FOL | C8A-N1 | -5.08 | 1.31 | 1.37 |
| 4 | 108-A | 204 | NAP | O3B-C3B | -5.08 | 1.31 | 1.43 |
| 2 | 16-A | 201 | FOL | C8A-N1 | -5.08 | 1.31 | 1.37 |
| 2 | 25-A | 201 | FOL | C8A-N1 | -5.07 | 1.31 | 1.37 |
| 2 | 41-A | 201 | FOL | C8A-N1 | -5.06 | 1.31 | 1.37 |
| 2 | 26-A | 201 | FOL | C8A-N1 | -5.06 | 1.31 | 1.37 |
| 2 | 33-A | 201 | FOL | C8A-N1 | -5.05 | 1.31 | 1.37 |
| 2 | 72-A | 201 | FOL | C8A-N1 | -5.04 | 1.31 | 1.37 |
| 2 | 58-A | 201 | FOL | C8A-N1 | -5.04 | 1.31 | 1.37 |
| 2 | 113-A | 201 | FOL | C8A-N1 | -5.02 | 1.31 | 1.37 |
| 2 | 52-A | 201 | FOL | C8A-N1 | -5.01 | 1.31 | 1.37 |
| 2 | 148-A | 201 | FOL | C8A-N1 | -5.00 | 1.31 | 1.37 |
| 2 | 136-A | 201 | FOL | C8A-N1 | -4.99 | 1.31 | 1.37 |
| 2 | 123-A | 201 | FOL | C8A-N1 | -4.98 | 1.31 | 1.37 |
| 4 | 157-A | 204 | NAP | O3B-C3B | -4.98 | 1.31 | 1.43 |
| 2 | 37-A | 201 | FOL | C8A-N1 | -4.97 | 1.32 | 1.37 |
| 4 | 83-A | 204 | NAP | O3B-C3B | -4.96 | 1.31 | 1.43 |
| 2 | 96-A | 201 | FOL | C8A-N1 | -4.95 | 1.32 | 1.37 |
| 2 | 139-A | 201 | FOL | C8A-N1 | -4.95 | 1.32 | 1.37 |
| 4 | 158-A | 204 | NAP | O3B-C3B | -4.95 | 1.31 | 1.43 |
| 2 | 144-A | 201 | FOL | C8A-N1 | -4.95 | 1.32 | 1.37 |
| 4 | 57-A | 204 | NAP | O3B-C3B | -4.94 | 1.31 | 1.43 |
| 4 | 56-A | 204 | NAP | O3B-C3B | -4.94 | 1.31 | 1.43 |
| 2 | 124-A | 201 | FOL | C8A-N1 | -4.94 | 1.32 | 1.37 |
| 2 | 13-A | 201 | FOL | C8A-N1 | -4.91 | 1.32 | 1.37 |
| 2 | 145-A | 201 | FOL | C8A-N1 | -4.90 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 133-A | 204 | NAP | O3B-C3B | -4.89 | 1.31 | 1.43 |
| 2 | 55-A | 201 | FOL | C8A-N1 | -4.89 | 1.32 | 1.37 |
| 2 | 149-A | 201 | FOL | C8A-N1 | -4.88 | 1.32 | 1.37 |
| 4 | 9-A | 204 | NAP | O3B-C3B | -4.88 | 1.31 | 1.43 |
| 2 | 82-A | 201 | FOL | C8A-N1 | -4.87 | 1.32 | 1.37 |
| 2 | 99-A | 201 | FOL | C8A-N1 | -4.86 | 1.32 | 1.37 |
| 2 | 153-A | 201 | FOL | C8A-N1 | -4.85 | 1.32 | 1.37 |
| 2 | 109-A | 201 | FOL | C8A-N1 | -4.85 | 1.32 | 1.37 |
| 2 | 164-A | 201 | FOL | C8A-N1 | -4.85 | 1.32 | 1.37 |
| 4 | 6-A | 204 | NAP | O3B-C3B | -4.84 | 1.31 | 1.43 |
| 4 | 8-A | 204 | NAP | O3B-C3B | -4.84 | 1.31 | 1.43 |
| 2 | 155-A | 201 | FOL | C8A-N1 | -4.83 | 1.32 | 1.37 |
| 2 | 46-A | 201 | FOL | C8A-N1 | -4.83 | 1.32 | 1.37 |
| 2 | 43-A | 201 | FOL | C8A-N1 | -4.82 | 1.32 | 1.37 |
| 4 | 132-A | 204 | NAP | O3B-C3B | -4.82 | 1.31 | 1.43 |
| 2 | 48-A | 201 | FOL | C8A-N1 | -4.80 | 1.32 | 1.37 |
| 4 | 159-A | 204 | NAP | O3B-C3B | -4.78 | 1.31 | 1.43 |
| 2 | 67-A | 201 | FOL | C8A-N1 | -4.78 | 1.32 | 1.37 |
| 4 | 109-A | 204 | NAP | O3B-C3B | -4.78 | 1.31 | 1.43 |
| 2 | 166-A | 201 | FOL | C8A-N1 | -4.77 | 1.32 | 1.37 |
| 2 | 60-A | 201 | FOL | C8A-N1 | -4.77 | 1.32 | 1.37 |
| 2 | 35-A | 201 | FOL | C8A-N1 | -4.76 | 1.32 | 1.37 |
| 2 | 115-A | 201 | FOL | C8A-N1 | -4.76 | 1.32 | 1.37 |
| 4 | 134-A | 204 | NAP | O3B-C3B | -4.75 | 1.31 | 1.43 |
| 2 | 108-A | 201 | FOL | C8A-N1 | -4.75 | 1.32 | 1.37 |
| 2 | 141-A | 201 | FOL | C8A-N1 | -4.74 | 1.32 | 1.37 |
| 2 | 91-A | 201 | FOL | C8A-N1 | -4.74 | 1.32 | 1.37 |
| 2 | 78-A | 201 | FOL | C8A-N1 | -4.71 | 1.32 | 1.37 |
| 2 | 103-A | 201 | FOL | C8A-N1 | -4.70 | 1.32 | 1.37 |
| 2 | 14-A | 201 | FOL | C8A-N1 | -4.69 | 1.32 | 1.37 |
| 2 | 114-A | 201 | FOL | C8A-N1 | -4.68 | 1.32 | 1.37 |
| 2 | 107-A | 201 | FOL | C8A-N1 | -4.67 | 1.32 | 1.37 |
| 2 | 11-A | 201 | FOL | C8A-N1 | -4.66 | 1.32 | 1.37 |
| 2 | 5-A | 201 | FOL | C8A-N1 | -4.65 | 1.32 | 1.37 |
| 2 | 80-A | 201 | FOL | C8A-N1 | -4.65 | 1.32 | 1.37 |
| 2 | 130-A | 201 | FOL | C8A-N1 | -4.65 | 1.32 | 1.37 |
| 2 | 54-A | 201 | FOL | C8A-N1 | -4.63 | 1.32 | 1.37 |
| 2 | 116-A | 201 | FOL | C8A-N1 | -4.61 | 1.32 | 1.37 |
| 2 | 3-A | 201 | FOL | C8A-N1 | -4.60 | 1.32 | 1.37 |
| 2 | 75-A | 201 | FOL | C8A-N1 | -4.59 | 1.32 | 1.37 |
| 4 | 7-A | 204 | NAP | O3B-C3B | -4.59 | 1.32 | 1.43 |
| 2 | 150-A | 201 | FOL | C8A-N1 | -4.55 | 1.32 | 1.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | 135-A | 201 | FOL | C8A-N1 | -4.55 | 1.32 | 1.37 |
| 2 | 101-A | 201 | FOL | C8A-N1 | -4.54 | 1.32 | 1.37 |
| 2 | 84-A | 201 | FOL | C8A-N1 | -4.52 | 1.32 | 1.37 |
| 2 | 112-A | 201 | FOL | C8A-N1 | -4.52 | 1.32 | 1.37 |
| 2 | 24-A | 201 | FOL | C8A-N1 | -4.51 | 1.32 | 1.37 |
| 2 | 122-A | 201 | FOL | C8A-N1 | -4.49 | 1.32 | 1.37 |
| 2 | 140-A | 201 | FOL | C8A-N1 | -4.48 | 1.32 | 1.37 |
| 2 | 81-A | 201 | FOL | C8A-N1 | -4.45 | 1.32 | 1.37 |
| 2 | 93-A | 201 | FOL | C8A-N1 | -4.41 | 1.32 | 1.37 |
| 2 | 61-A | 201 | FOL | C8A-N1 | -4.41 | 1.32 | 1.37 |
| 2 | 87-A | 201 | FOL | C8A-N1 | -4.41 | 1.32 | 1.37 |
| 2 | 86-A | 201 | FOL | C8A-N1 | -4.40 | 1.32 | 1.37 |
| 2 | 90-A | 201 | FOL | C8A-N1 | -4.40 | 1.32 | 1.37 |
| 2 | 31-A | 201 | FOL | C8A-N1 | -4.39 | 1.32 | 1.37 |
| 2 | 95-A | 201 | FOL | C8A-N1 | -4.39 | 1.32 | 1.37 |
| 2 | 165-A | 201 | FOL | C8A-N1 | -4.38 | 1.32 | 1.37 |
| 2 | 79-A | 201 | FOL | C8A-N1 | -4.38 | 1.32 | 1.37 |
| 2 | 120-A | 201 | FOL | C8A-N1 | -4.37 | 1.32 | 1.37 |
| 2 | 64-A | 201 | FOL | C8A-N1 | -4.33 | 1.32 | 1.37 |
| 2 | 63-A | 201 | FOL | C8A-N1 | -4.31 | 1.32 | 1.37 |
| 2 | 125-A | 201 | FOL | C8A-N1 | -4.31 | 1.32 | 1.37 |
| 4 | 119-A | 204 | NAP | O4B-C4B | -4.30 | 1.35 | 1.45 |
| 2 | 142-A | 201 | FOL | C8A-N1 | -4.28 | 1.32 | 1.37 |
| 2 | 10-A | 201 | FOL | C8A-N1 | -4.21 | 1.32 | 1.37 |
| 2 | 156-A | 201 | FOL | C8A-N1 | -4.10 | 1.32 | 1.37 |
| 2 | 131-A | 201 | FOL | C8A-N1 | -4.10 | 1.32 | 1.37 |
| 2 | 49-A | 201 | FOL | C8A-N1 | -4.07 | 1.32 | 1.37 |
| 2 | 100-A | 201 | FOL | CA-N | -4.07 | 1.40 | 1.46 |
| 2 | 65-A | 201 | FOL | CA-N | -4.04 | 1.40 | 1.46 |
| 2 | 159-A | 201 | FOL | C8A-N1 | -4.01 | 1.33 | 1.37 |
| 2 | 88-A | 201 | FOL | C8A-N1 | -3.96 | 1.33 | 1.37 |
| 2 | 102-A | 201 | FOL | C8A-N1 | -3.95 | 1.33 | 1.37 |
| 2 | 97-A | 201 | FOL | C8A-N1 | -3.92 | 1.33 | 1.37 |
| 4 | 39-A | 204 | NAP | C2D-C1D | -3.90 | 1.47 | 1.53 |
| 2 | 52-A | 201 | FOL | CA-N | -3.89 | 1.41 | 1.46 |
| 2 | 156-A | 201 | FOL | CA-N | -3.87 | 1.41 | 1.46 |
| 4 | 112-A | 204 | NAP | C2D-C1D | -3.76 | 1.47 | 1.53 |
| 2 | 138-A | 201 | FOL | C8A-N1 | -3.75 | 1.33 | 1.37 |
| 4 | 33-A | 204 | NAP | O4B-C4B | -3.75 | 1.36 | 1.45 |
| 2 | 29-A | 201 | FOL | C8A-N1 | -3.75 | 1.33 | 1.37 |
| 4 | 113-A | 204 | NAP | C2D-C1D | -3.74 | 1.47 | 1.53 |
| 4 | 107-A | 204 | NAP | C2D-C1D | -3.73 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | 38-A | 201 | FOL | C8A-N1 | -3.71 | 1.33 | 1.37 |
| 2 | 127-A | 201 | FOL | C8A-N1 | -3.61 | 1.33 | 1.37 |
| 4 | 165-A | 204 | NAP | C2D-C1D | -3.59 | 1.47 | 1.53 |
| 4 | 118-A | 204 | NAP | C2D-C1D | -3.56 | 1.48 | 1.53 |
| 4 | 111-A | 204 | NAP | C2D-C1D | -3.56 | 1.48 | 1.53 |
| 4 | 104-A | 204 | NAP | C2D-C1D | -3.56 | 1.48 | 1.53 |
| 2 | 106-A | 201 | FOL | C8A-N1 | -3.55 | 1.33 | 1.37 |
| 4 | 100-A | 204 | NAP | C2D-C1D | -3.55 | 1.48 | 1.53 |
| 4 | 106-A | 204 | NAP | C2D-C1D | -3.52 | 1.48 | 1.53 |
| 4 | 115-A | 204 | NAP | C2D-C1D | -3.50 | 1.48 | 1.53 |
| 2 | 161-A | 201 | FOL | C8A-N1 | -3.49 | 1.33 | 1.37 |
| 4 | 157-A | 204 | NAP | C2D-C1D | -3.45 | 1.48 | 1.53 |
| 4 | 22-A | 204 | NAP | C2D-C1D | -3.44 | 1.48 | 1.53 |
| 4 | 85-A | 204 | NAP | C2D-C1D | -3.41 | 1.48 | 1.53 |
| 4 | 18-A | 204 | NAP | C2D-C1D | -3.41 | 1.48 | 1.53 |
| 4 | 14-A | 204 | NAP | C2D-C1D | -3.38 | 1.48 | 1.53 |
| 4 | 101-A | 204 | NAP | C2D-C1D | -3.37 | 1.48 | 1.53 |
| 2 | 163-A | 201 | FOL | C8A-N1 | -3.37 | 1.33 | 1.37 |
| 4 | 95-A | 204 | NAP | C2D-C1D | -3.37 | 1.48 | 1.53 |
| 4 | 2-A | 204 | NAP | C2D-C1D | -3.36 | 1.48 | 1.53 |
| 4 | 17-A | 204 | NAP | C2D-C1D | -3.34 | 1.48 | 1.53 |
| 4 | 12-A | 204 | NAP | C2D-C1D | -3.33 | 1.48 | 1.53 |
| 4 | 105-A | 204 | NAP | C2D-C1D | -3.32 | 1.48 | 1.53 |
| 4 | 23-A | 204 | NAP | C2D-C1D | -3.31 | 1.48 | 1.53 |
| 4 | 99-A | 204 | NAP | C2D-C1D | -3.31 | 1.48 | 1.53 |
| 4 | 83-A | 204 | NAP | C2D-C1D | -3.31 | 1.48 | 1.53 |
| 4 | 63-A | 204 | NAP | C2D-C1D | -3.30 | 1.48 | 1.53 |
| 4 | 110-A | 204 | NAP | C2D-C1D | -3.30 | 1.48 | 1.53 |
| 4 | 108-A | 204 | NAP | C2D-C1D | -3.30 | 1.48 | 1.53 |
| 4 | 147-A | 204 | NAP | C2D-C1D | -3.29 | 1.48 | 1.53 |
| 4 | 65-A | 204 | NAP | C2D-C1D | -3.28 | 1.48 | 1.53 |
| 4 | 94-A | 204 | NAP | C2D-C1D | -3.26 | 1.48 | 1.53 |
| 4 | 116-A | 204 | NAP | C2D-C1D | -3.25 | 1.48 | 1.53 |
| 4 | 117-A | 204 | NAP | C2D-C1D | -3.25 | 1.48 | 1.53 |
| 4 | 15-A | 204 | NAP | C2D-C1D | -3.25 | 1.48 | 1.53 |
| 4 | 97-A | 204 | NAP | C2D-C1D | -3.24 | 1.48 | 1.53 |
| 4 | 155-A | 204 | NAP | C2D-C1D | -3.22 | 1.48 | 1.53 |
| 4 | 89-A | 204 | NAP | C2D-C1D | -3.21 | 1.48 | 1.53 |
| 4 | 86-A | 204 | NAP | C2D-C1D | -3.21 | 1.48 | 1.53 |
| 4 | 148-A | 204 | NAP | C2D-C1D | -3.21 | 1.48 | 1.53 |
| 4 | 166-A | 204 | NAP | C2D-C1D | -3.20 | 1.48 | 1.53 |
| 4 | 16-A | 204 | NAP | C2D-C1D | -3.20 | 1.48 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 98-A | 204 | NAP | C2D-C1D | -3.20 | 1.48 | 1.53 |
| 4 | 119-A | 204 | NAP | C2D-C1D | -3.20 | 1.48 | 1.53 |
| 4 | 96-A | 204 | NAP | C2D-C1D | -3.20 | 1.48 | 1.53 |
| 4 | 109-A | 204 | NAP | C2D-C1D | -3.19 | 1.48 | 1.53 |
| 2 | 104-A | 201 | FOL | C8A-N1 | -3.19 | 1.33 | 1.37 |
| 4 | 81-A | 204 | NAP | C2D-C1D | -3.18 | 1.48 | 1.53 |
| 4 | 9-A | 204 | NAP | C2D-C1D | -3.17 | 1.48 | 1.53 |
| 4 | 82-A | 204 | NAP | C2D-C1D | -3.17 | 1.48 | 1.53 |
| 4 | 61-A | 204 | NAP | C2D-C1D | -3.16 | 1.48 | 1.53 |
| 4 | 13-A | 204 | NAP | C2D-C1D | -3.16 | 1.48 | 1.53 |
| 4 | 102-A | 204 | NAP | O4B-C4B | -3.16 | 1.37 | 1.45 |
| 4 | 42-A | 204 | NAP | O4B-C4B | -3.15 | 1.37 | 1.45 |
| 4 | 10-A | 204 | NAP | C2D-C1D | -3.15 | 1.48 | 1.53 |
| 4 | 50-A | 204 | NAP | O4B-C4B | -3.14 | 1.37 | 1.45 |
| 4 | 88-A | 204 | NAP | C2D-C1D | -3.14 | 1.48 | 1.53 |
| 4 | 132-A | 204 | NAP | C2D-C1D | -3.13 | 1.48 | 1.53 |
| 4 | 87-A | 204 | NAP | C2D-C1D | -3.12 | 1.48 | 1.53 |
| 4 | 7-A | 204 | NAP | C2D-C1D | -3.12 | 1.48 | 1.53 |
| 4 | 64-A | 204 | NAP | C2D-C1D | -3.12 | 1.48 | 1.53 |
| 4 | 5-A | 204 | NAP | C2D-C1D | -3.12 | 1.48 | 1.53 |
| 4 | 72-A | 204 | NAP | C2D-C1D | -3.11 | 1.48 | 1.53 |
| 4 | 103-A | 204 | NAP | C2D-C1D | -3.11 | 1.48 | 1.53 |
| 4 | 146-A | 204 | NAP | C2D-C1D | -3.10 | 1.48 | 1.53 |
| 4 | 66-A | 204 | NAP | C2D-C1D | -3.10 | 1.48 | 1.53 |
| 4 | 114-A | 204 | NAP | C2D-C1D | -3.09 | 1.48 | 1.53 |
| 4 | 92-A | 204 | NAP | C2D-C1D | -3.09 | 1.48 | 1.53 |
| 4 | 11-A | 204 | NAP | C2D-C1D | -3.09 | 1.48 | 1.53 |
| 4 | 62-A | 204 | NAP | C2D-C1D | -3.09 | 1.48 | 1.53 |
| 4 | 29-A | 204 | NAP | C2D-C1D | -3.08 | 1.48 | 1.53 |
| 4 | 70-A | 204 | NAP | C2D-C1D | -3.08 | 1.48 | 1.53 |
| 4 | 20-A | 204 | NAP | C2D-C1D | -3.07 | 1.48 | 1.53 |
| 4 | 161-A | 204 | NAP | C2D-C1D | -3.07 | 1.48 | 1.53 |
| 4 | 150-A | 204 | NAP | C2D-C1D | -3.07 | 1.48 | 1.53 |
| 4 | 143-A | 204 | NAP | C2D-C1D | -3.07 | 1.48 | 1.53 |
| 4 | 6-A | 204 | NAP | C2D-C1D | -3.06 | 1.48 | 1.53 |
| 4 | 19-A | 204 | NAP | C2D-C1D | -3.06 | 1.48 | 1.53 |
| 4 | 60-A | 204 | NAP | C2D-C1D | -3.06 | 1.48 | 1.53 |
| 4 | 133-A | 204 | NAP | C2D-C1D | -3.06 | 1.48 | 1.53 |
| 4 | 80-A | 204 | NAP | C2D-C1D | -3.05 | 1.48 | 1.53 |
| 4 | 24-A | 204 | NAP | O4B-C4B | -3.04 | 1.38 | 1.45 |
| 4 | 131-A | 204 | NAP | C2D-C1D | -3.04 | 1.48 | 1.53 |
| 4 | 152-A | 204 | NAP | C2D-C1D | -3.03 | 1.48 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 135-A | 204 | NAP | C2D-C1D | -3.03 | 1.48 | 1.53 |
| 4 | 137-A | 204 | NAP | C2D-C1D | -3.03 | 1.48 | 1.53 |
| 4 | 71-A | 204 | NAP | C2D-C1D | -3.02 | 1.48 | 1.53 |
| 4 | 154-A | 204 | NAP | C2D-C1D | -3.02 | 1.48 | 1.53 |
| 4 | 151-A | 204 | NAP | C2D-C1D | -3.02 | 1.48 | 1.53 |
| 4 | 56-A | 204 | NAP | C2D-C1D | -3.02 | 1.48 | 1.53 |
| 4 | 74-A | 204 | NAP | C2D-C1D | -3.02 | 1.48 | 1.53 |
| 4 | 118-A | 204 | NAP | O4B-C4B | -3.02 | 1.38 | 1.45 |
| 2 | 128-A | 201 | FOL | C8A-N1 | -3.02 | 1.34 | 1.37 |
| 4 | 144-A | 204 | NAP | C2D-C1D | -3.01 | 1.48 | 1.53 |
| 4 | 156-A | 204 | NAP | C2D-C1D | -3.01 | 1.48 | 1.53 |
| 4 | 1-A | 204 | NAP | C2D-C1D | -3.01 | 1.48 | 1.53 |
| 4 | 136-A | 204 | NAP | C2D-C1D | -2.99 | 1.48 | 1.53 |
| 4 | 167-A | 204 | NAP | C2D-C1D | -2.99 | 1.48 | 1.53 |
| 4 | 142-A | 204 | NAP | C2D-C1D | -2.99 | 1.48 | 1.53 |
| 4 | 84-A | 204 | NAP | C2D-C1D | -2.99 | 1.48 | 1.53 |
| 4 | 53-A | 204 | NAP | C2D-C1D | -2.99 | 1.48 | 1.53 |
| 4 | 145-A | 204 | NAP | C2D-C1D | -2.98 | 1.48 | 1.53 |
| 4 | 24-A | 204 | NAP | C2D-C1D | -2.98 | 1.48 | 1.53 |
| 4 | 30-A | 204 | NAP | C2D-C1D | -2.98 | 1.48 | 1.53 |
| 4 | 21-A | 204 | NAP | C2D-C1D | -2.98 | 1.48 | 1.53 |
| 4 | 102-A | 204 | NAP | C2D-C1D | -2.98 | 1.48 | 1.53 |
| 4 | 79-A | 204 | NAP | C2D-C1D | -2.97 | 1.48 | 1.53 |
| 4 | 43-A | 204 | NAP | C2D-C1D | -2.97 | 1.48 | 1.53 |
| 4 | 75-A | 204 | NAP | C2D-C1D | -2.97 | 1.48 | 1.53 |
| 4 | 55-A | 204 | NAP | C2D-C1D | -2.97 | 1.48 | 1.53 |
| 4 | 160-A | 204 | NAP | C2D-C1D | -2.96 | 1.48 | 1.53 |
| 4 | 159-A | 204 | NAP | C2D-C1D | -2.95 | 1.48 | 1.53 |
| 4 | 128-A | 204 | NAP | C2D-C1D | -2.95 | 1.49 | 1.53 |
| 4 | 28-A | 204 | NAP | C2D-C1D | -2.94 | 1.49 | 1.53 |
| 4 | 115-A | 204 | NAP | O7N-C7N | -2.94 | 1.18 | 1.24 |
| 4 | 123-A | 204 | NAP | C2D-C1D | -2.94 | 1.49 | 1.53 |
| 4 | 51-A | 204 | NAP | O4B-C4B | -2.93 | 1.38 | 1.45 |
| 4 | 120-A | 204 | NAP | C2D-C1D | -2.93 | 1.49 | 1.53 |
| 4 | 94-A | 204 | NAP | O4B-C4B | -2.93 | 1.38 | 1.45 |
| 4 | 47-A | 204 | NAP | C2D-C1D | -2.92 | 1.49 | 1.53 |
| 4 | 73-A | 204 | NAP | C2D-C1D | -2.92 | 1.49 | 1.53 |
| 4 | 44-A | 204 | NAP | C2D-C1D | -2.92 | 1.49 | 1.53 |
| 4 | 67-A | 204 | NAP | C2D-C1D | -2.92 | 1.49 | 1.53 |
| 4 | 91-A | 204 | NAP | C2D-C1D | -2.92 | 1.49 | 1.53 |
| 4 | 140-A | 204 | NAP | C2D-C1D | -2.91 | 1.49 | 1.53 |
| 4 | 134-A | 204 | NAP | C2D-C1D | -2.91 | 1.49 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 80-A | 204 | NAP | O4B-C4B | -2.91 | 1.38 | 1.45 |
| 4 | 20-A | 204 | NAP | O4B-C4B | -2.91 | 1.38 | 1.45 |
| 4 | 25-A | 204 | NAP | C2D-C1D | -2.91 | 1.49 | 1.53 |
| 4 | 34-A | 204 | NAP | O4B-C4B | -2.90 | 1.38 | 1.45 |
| 4 | 38-A | 204 | NAP | O4B-C4B | -2.90 | 1.38 | 1.45 |
| 4 | 82-A | 204 | NAP | O4B-C4B | -2.90 | 1.38 | 1.45 |
| 4 | 21-A | 204 | NAP | O4B-C4B | -2.90 | 1.38 | 1.45 |
| 4 | 76-A | 204 | NAP | C2D-C1D | -2.89 | 1.49 | 1.53 |
| 4 | 38-A | 204 | NAP | C2D-C1D | -2.89 | 1.49 | 1.53 |
| 4 | 53-A | 204 | NAP | O4B-C4B | -2.87 | 1.38 | 1.45 |
| 4 | 93-A | 204 | NAP | C2D-C1D | -2.87 | 1.49 | 1.53 |
| 4 | 162-A | 204 | NAP | C2D-C1D | -2.86 | 1.49 | 1.53 |
| 4 | 97-A | 204 | NAP | O4B-C4B | -2.85 | 1.38 | 1.45 |
| 4 | 129-A | 204 | NAP | C2D-C1D | -2.85 | 1.49 | 1.53 |
| 4 | 69-A | 204 | NAP | C2D-C1D | -2.85 | 1.49 | 1.53 |
| 4 | 25-A | 204 | NAP | O4B-C4B | -2.85 | 1.38 | 1.45 |
| 4 | 23-A | 204 | NAP | O4B-C4B | -2.85 | 1.38 | 1.45 |
| 4 | 31-A | 204 | NAP | C2D-C1D | -2.84 | 1.49 | 1.53 |
| 4 | 54-A | 204 | NAP | C2D-C1D | -2.84 | 1.49 | 1.53 |
| 4 | 77-A | 204 | NAP | C2D-C1D | -2.84 | 1.49 | 1.53 |
| 4 | 121-A | 204 | NAP | C2D-C1D | -2.83 | 1.49 | 1.53 |
| 4 | 49-A | 204 | NAP | O4B-C4B | -2.83 | 1.38 | 1.45 |
| 4 | 149-A | 204 | NAP | C2D-C1D | -2.83 | 1.49 | 1.53 |
| 4 | 18-A | 204 | NAP | O4B-C4B | -2.83 | 1.38 | 1.45 |
| 4 | 95-A | 204 | NAP | O4B-C4B | -2.83 | 1.38 | 1.45 |
| 4 | 41-A | 204 | NAP | O4B-C4B | -2.82 | 1.38 | 1.45 |
| 4 | 163-A | 204 | NAP | C2D-C1D | -2.82 | 1.49 | 1.53 |
| 4 | 55-A | 204 | NAP | O4B-C4B | -2.81 | 1.38 | 1.45 |
| 4 | 153-A | 204 | NAP | C2D-C1D | -2.81 | 1.49 | 1.53 |
| 4 | 39-A | 204 | NAP | O4B-C4B | -2.81 | 1.38 | 1.45 |
| 4 | 40-A | 204 | NAP | C2D-C1D | -2.81 | 1.49 | 1.53 |
| 4 | 98-A | 204 | NAP | O4B-C4B | -2.80 | 1.38 | 1.45 |
| 4 | 138-A | 204 | NAP | C2D-C1D | -2.80 | 1.49 | 1.53 |
| 4 | 19-A | 204 | NAP | O4B-C4B | -2.80 | 1.38 | 1.45 |
| 4 | 107-A | 204 | NAP | O4B-C4B | -2.79 | 1.38 | 1.45 |
| 4 | 99-A | 204 | NAP | O4B-C4B | -2.79 | 1.38 | 1.45 |
| 4 | 52-A | 204 | NAP | O4B-C4B | -2.79 | 1.38 | 1.45 |
| 4 | 48-A | 204 | NAP | C2D-C1D | -2.79 | 1.49 | 1.53 |
| 4 | 96-A | 204 | NAP | O4B-C4B | -2.78 | 1.38 | 1.45 |
| 4 | 38-A | 204 | NAP | C2D-C3D | -2.78 | 1.45 | 1.53 |
| 4 | 164-A | 204 | NAP | C2D-C1D | -2.78 | 1.49 | 1.53 |
| 4 | 52-A | 204 | NAP | C2D-C1D | -2.78 | 1.49 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 122-A | 204 | NAP | C2D-C1D | -2.78 | 1.49 | 1.53 |
| 4 | 130-A | 204 | NAP | C2D-C1D | -2.78 | 1.49 | 1.53 |
| 4 | 8-A | 204 | NAP | C2D-C1D | -2.77 | 1.49 | 1.53 |
| 4 | 93-A | 204 | NAP | O4B-C4B | -2.77 | 1.38 | 1.45 |
| 4 | 60-A | 204 | NAP | O4B-C4B | -2.77 | 1.38 | 1.45 |
| 4 | 39-A | 204 | NAP | C2D-C3D | -2.77 | 1.46 | 1.53 |
| 4 | 33-A | 204 | NAP | O7N-C7N | -2.77 | 1.18 | 1.24 |
| 2 | 143-A | 201 | FOL | CA-N | -2.77 | 1.42 | 1.46 |
| 4 | 90-A | 204 | NAP | C2D-C1D | -2.77 | 1.49 | 1.53 |
| 4 | 58-A | 204 | NAP | C2D-C1D | -2.76 | 1.49 | 1.53 |
| 4 | 3-A | 204 | NAP | C2D-C1D | -2.76 | 1.49 | 1.53 |
| 4 | 69-A | 204 | NAP | O4B-C4B | -2.76 | 1.38 | 1.45 |
| 4 | 36-A | 204 | NAP | O4B-C4B | -2.75 | 1.38 | 1.45 |
| 4 | 54-A | 204 | NAP | O4B-C4B | -2.75 | 1.38 | 1.45 |
| 4 | 158-A | 204 | NAP | C2D-C1D | -2.75 | 1.49 | 1.53 |
| 4 | 139-A | 204 | NAP | C2D-C1D | -2.75 | 1.49 | 1.53 |
| 4 | 78-A | 204 | NAP | C2D-C1D | -2.75 | 1.49 | 1.53 |
| 4 | 127-A | 204 | NAP | C2D-C1D | -2.75 | 1.49 | 1.53 |
| 2 | 77-A | 201 | FOL | CA-N | -2.74 | 1.42 | 1.46 |
| 4 | 67-A | 204 | NAP | O4B-C4B | -2.74 | 1.38 | 1.45 |
| 4 | 117-A | 204 | NAP | O4B-C4B | -2.74 | 1.38 | 1.45 |
| 4 | 26-A | 204 | NAP | O4B-C4B | -2.74 | 1.38 | 1.45 |
| 4 | 35-A | 204 | NAP | O4B-C4B | -2.74 | 1.38 | 1.45 |
| 4 | 11-A | 204 | NAP | O4B-C4B | -2.74 | 1.38 | 1.45 |
| 4 | 22-A | 204 | NAP | O4B-C4B | -2.73 | 1.38 | 1.45 |
| 4 | 81-A | 204 | NAP | O4B-C4B | -2.73 | 1.38 | 1.45 |
| 4 | 27-A | 204 | NAP | C2D-C1D | -2.72 | 1.49 | 1.53 |
| 4 | 126-A | 204 | NAP | C2D-C1D | -2.72 | 1.49 | 1.53 |
| 4 | 37-A | 204 | NAP | C2D-C1D | -2.72 | 1.49 | 1.53 |
| 4 | 68-A | 204 | NAP | C2D-C1D | -2.72 | 1.49 | 1.53 |
| 4 | 62-A | 204 | NAP | O4B-C4B | -2.72 | 1.38 | 1.45 |
| 4 | 41-A | 204 | NAP | C2D-C1D | -2.72 | 1.49 | 1.53 |
| 4 | 124-A | 204 | NAP | C2D-C1D | -2.71 | 1.49 | 1.53 |
| 4 | 4-A | 204 | NAP | C2D-C1D | -2.71 | 1.49 | 1.53 |
| 4 | 137-A | 204 | NAP | O4B-C4B | -2.71 | 1.38 | 1.45 |
| 4 | 100-A | 204 | NAP | O4B-C4B | -2.71 | 1.38 | 1.45 |
| 4 | 68-A | 204 | NAP | O4B-C4B | -2.71 | 1.38 | 1.45 |
| 4 | 77-A | 204 | NAP | O4B-C4B | -2.71 | 1.38 | 1.45 |
| 4 | 138-A | 204 | NAP | O4B-C4B | -2.71 | 1.38 | 1.45 |
| 4 | 108-A | 204 | NAP | O7N-C7N | -2.71 | 1.18 | 1.24 |
| 4 | 17-A | 204 | NAP | O4B-C4B | -2.71 | 1.38 | 1.45 |
| 2 | 106-A | 201 | FOL | CA-N | -2.70 | 1.42 | 1.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 103-A | 204 | NAP | O4B-C4B | -2.70 | 1.38 | 1.45 |
| 4 | 165-A | 204 | NAP | C3D-C4D | -2.70 | 1.45 | 1.53 |
| 4 | 32-A | 204 | NAP | C2D-C1D | -2.70 | 1.49 | 1.53 |
| 4 | 12-A | 204 | NAP | O4B-C4B | -2.70 | 1.38 | 1.45 |
| 4 | 16-A | 204 | NAP | O4B-C4B | -2.69 | 1.38 | 1.45 |
| 4 | 136-A | 204 | NAP | O4B-C4B | -2.69 | 1.38 | 1.45 |
| 4 | 115-A | 204 | NAP | O4B-C4B | -2.69 | 1.38 | 1.45 |
| 4 | 116-A | 204 | NAP | O4B-C4B | -2.69 | 1.38 | 1.45 |
| 4 | 149-A | 204 | NAP | O4B-C4B | -2.69 | 1.38 | 1.45 |
| 4 | 141-A | 204 | NAP | C2D-C1D | -2.68 | 1.49 | 1.53 |
| 4 | 120-A | 204 | NAP | O4B-C4B | -2.67 | 1.38 | 1.45 |
| 4 | 45-A | 204 | NAP | C2D-C1D | -2.67 | 1.49 | 1.53 |
| 4 | 70-A | 204 | NAP | O4B-C4B | -2.67 | 1.38 | 1.45 |
| 4 | 101-A | 204 | NAP | O4B-C4B | -2.67 | 1.38 | 1.45 |
| 4 | 37-A | 204 | NAP | O4B-C4B | -2.67 | 1.38 | 1.45 |
| 4 | 46-A | 204 | NAP | C2D-C1D | -2.67 | 1.49 | 1.53 |
| 4 | 124-A | 204 | NAP | O4B-C4B | -2.67 | 1.38 | 1.45 |
| 4 | 13-A | 204 | NAP | O4B-C4B | -2.66 | 1.38 | 1.45 |
| 4 | 92-A | 204 | NAP | O4B-C4B | -2.66 | 1.38 | 1.45 |
| 4 | 6-A | 204 | NAP | O7N-C7N | -2.65 | 1.18 | 1.24 |
| 4 | 42-A | 204 | NAP | C2D-C1D | -2.65 | 1.49 | 1.53 |
| 4 | 14-A | 204 | NAP | O4B-C4B | -2.64 | 1.39 | 1.45 |
| 4 | 78-A | 204 | NAP | O4B-C4B | -2.64 | 1.39 | 1.45 |
| 4 | 59-A | 204 | NAP | C2D-C1D | -2.64 | 1.49 | 1.53 |
| 4 | 34-A | 204 | NAP | C2D-C1D | -2.63 | 1.49 | 1.53 |
| 4 | 51-A | 204 | NAP | C2D-C1D | -2.63 | 1.49 | 1.53 |
| 4 | 110-A | 204 | NAP | O4B-C4B | -2.62 | 1.39 | 1.45 |
| 4 | 90-A | 204 | NAP | O4B-C4B | -2.62 | 1.39 | 1.45 |
| 4 | 65-A | 204 | NAP | O4B-C4B | -2.62 | 1.39 | 1.45 |
| 4 | 91-A | 204 | NAP | O4B-C4B | -2.62 | 1.39 | 1.45 |
| 4 | 44-A | 204 | NAP | O4B-C4B | -2.62 | 1.39 | 1.45 |
| 4 | 32-A | 204 | NAP | O4B-C4B | -2.62 | 1.39 | 1.45 |
| 4 | 130-A | 204 | NAP | O4B-C4B | -2.61 | 1.39 | 1.45 |
| 4 | 131-A | 204 | NAP | O4B-C4B | -2.61 | 1.39 | 1.45 |
| 4 | 135-A | 204 | NAP | O4B-C4B | -2.61 | 1.39 | 1.45 |
| 4 | 26-A | 204 | NAP | C2D-C1D | -2.60 | 1.49 | 1.53 |
| 4 | 104-A | 204 | NAP | O4B-C4B | -2.60 | 1.39 | 1.45 |
| 4 | 40-A | 204 | NAP | O4B-C4B | -2.60 | 1.39 | 1.45 |
| 4 | 79-A | 204 | NAP | O4B-C4B | -2.60 | 1.39 | 1.45 |
| 4 | 31-A | 204 | NAP | O7N-C7N | -2.60 | 1.18 | 1.24 |
| 4 | 134-A | 204 | NAP | C2B-C1B | -2.60 | 1.46 | 1.53 |
| 4 | 35-A | 204 | NAP | C2D-C1D | -2.60 | 1.49 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 89-A | 204 | NAP | O4B-C4B | -2.60 | 1.39 | 1.45 |
| 4 | 105-A | 204 | NAP | O4B-C4B | -2.60 | 1.39 | 1.45 |
| 4 | 27-A | 204 | NAP | O4B-C4B | -2.60 | 1.39 | 1.45 |
| 4 | 36-A | 204 | NAP | C2D-C1D | -2.59 | 1.49 | 1.53 |
| 4 | 66-A | 204 | NAP | O4B-C4B | -2.59 | 1.39 | 1.45 |
| 4 | 46-A | 204 | NAP | O4B-C4B | -2.59 | 1.39 | 1.45 |
| 4 | 106-A | 204 | NAP | O4B-C4B | -2.59 | 1.39 | 1.45 |
| 4 | 48-A | 204 | NAP | O4B-C4B | -2.59 | 1.39 | 1.45 |
| 4 | 4-A | 204 | NAP | O4B-C4B | -2.58 | 1.39 | 1.45 |
| 4 | 57-A | 204 | NAP | C2D-C1D | -2.58 | 1.49 | 1.53 |
| 4 | 134-A | 204 | NAP | O4B-C4B | -2.57 | 1.39 | 1.45 |
| 4 | 41-A | 204 | NAP | O7N-C7N | -2.56 | 1.18 | 1.24 |
| 4 | 145-A | 204 | NAP | O4B-C4B | -2.56 | 1.39 | 1.45 |
| 4 | 114-A | 204 | NAP | O4B-C4B | -2.56 | 1.39 | 1.45 |
| 4 | 111-A | 204 | NAP | O4B-C4B | -2.56 | 1.39 | 1.45 |
| 4 | 150-A | 204 | NAP | O4B-C4B | -2.55 | 1.39 | 1.45 |
| 4 | 43-A | 204 | NAP | O4B-C4B | -2.54 | 1.39 | 1.45 |
| 4 | 125-A | 204 | NAP | O4B-C4B | -2.54 | 1.39 | 1.45 |
| 4 | 49-A | 204 | NAP | O7N-C7N | -2.53 | 1.18 | 1.24 |
| 4 | 132-A | 204 | NAP | O4B-C4B | -2.53 | 1.39 | 1.45 |
| 4 | 64-A | 204 | NAP | O4B-C4B | -2.53 | 1.39 | 1.45 |
| 4 | 5-A | 204 | NAP | O4B-C4B | -2.53 | 1.39 | 1.45 |
| 4 | 75-A | 204 | NAP | O4B-C4B | -2.53 | 1.39 | 1.45 |
| 4 | 139-A | 204 | NAP | O4B-C4B | -2.53 | 1.39 | 1.45 |
| 4 | 59-A | 204 | NAP | O4B-C4B | -2.52 | 1.39 | 1.45 |
| 4 | 45-A | 204 | NAP | O4B-C4B | -2.51 | 1.39 | 1.45 |
| 4 | 73-A | 204 | NAP | O4B-C4B | -2.51 | 1.39 | 1.45 |
| 4 | 35-A | 204 | NAP | O7N-C7N | -2.51 | 1.18 | 1.24 |
| 4 | 112-A | 204 | NAP | O4B-C4B | -2.51 | 1.39 | 1.45 |
| 4 | 74-A | 204 | NAP | O4B-C4B | -2.50 | 1.39 | 1.45 |
| 4 | 148-A | 204 | NAP | O4B-C4B | -2.50 | 1.39 | 1.45 |
| 4 | 47-A | 204 | NAP | O4B-C4B | -2.50 | 1.39 | 1.45 |
| 4 | 15-A | 204 | NAP | O4B-C4B | -2.50 | 1.39 | 1.45 |
| 4 | 49-A | 204 | NAP | C2D-C1D | -2.50 | 1.49 | 1.53 |
| 4 | 151-A | 204 | NAP | O4B-C4B | -2.49 | 1.39 | 1.45 |
| 4 | 122-A | 204 | NAP | O4B-C4B | -2.49 | 1.39 | 1.45 |
| 4 | 10-A | 204 | NAP | O4B-C4B | -2.49 | 1.39 | 1.45 |
| 4 | 29-A | 204 | NAP | C2B-C1B | -2.49 | 1.46 | 1.53 |
| 4 | 3-A | 204 | NAP | O4B-C4B | -2.49 | 1.39 | 1.45 |
| 4 | 83-A | 204 | NAP | O7N-C7N | -2.49 | 1.18 | 1.24 |
| 4 | 63-A | 204 | NAP | O4B-C4B | -2.48 | 1.39 | 1.45 |
| 4 | 9-A | 204 | NAP | O7N-C7N | -2.48 | 1.18 | 1.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 109-A | 204 | NAP | O4B-C4B | -2.48 | 1.39 | 1.45 |
| 4 | 30-A | 204 | NAP | O4B-C4B | -2.47 | 1.39 | 1.45 |
| 4 | 76-A | 204 | NAP | O4B-C4B | -2.47 | 1.39 | 1.45 |
| 4 | 56-A | 204 | NAP | O4B-C4B | -2.47 | 1.39 | 1.45 |
| 4 | 121-A | 204 | NAP | O4B-C4B | -2.47 | 1.39 | 1.45 |
| 4 | 147-A | 204 | NAP | O4B-C4B | -2.46 | 1.39 | 1.45 |
| 4 | 140-A | 204 | NAP | O4B-C4B | -2.46 | 1.39 | 1.45 |
| 4 | 166-A | 204 | NAP | O4B-C4B | -2.46 | 1.39 | 1.45 |
| 4 | 156-A | 204 | NAP | O4B-C4B | -2.45 | 1.39 | 1.45 |
| 4 | 123-A | 204 | NAP | O4B-C4B | -2.45 | 1.39 | 1.45 |
| 4 | 154-A | 204 | NAP | C2B-C1B | -2.45 | 1.46 | 1.53 |
| 4 | 32-A | 204 | NAP | O7N-C7N | -2.45 | 1.19 | 1.24 |
| 4 | 144-A | 204 | NAP | O4B-C4B | -2.45 | 1.39 | 1.45 |
| 4 | 71-A | 204 | NAP | O4B-C4B | -2.44 | 1.39 | 1.45 |
| 4 | 131-A | 204 | NAP | O7N-C7N | -2.44 | 1.19 | 1.24 |
| 4 | 28-A | 204 | NAP | C2B-C1B | -2.44 | 1.46 | 1.53 |
| 4 | 28-A | 204 | NAP | O4B-C4B | -2.44 | 1.39 | 1.45 |
| 4 | 113-A | 204 | NAP | O4B-C4B | -2.43 | 1.39 | 1.45 |
| 4 | 133-A | 204 | NAP | O4B-C4B | -2.43 | 1.39 | 1.45 |
| 4 | 153-A | 204 | NAP | O4B-C4B | -2.43 | 1.39 | 1.45 |
| 4 | 8-A | 204 | NAP | O7N-C7N | -2.43 | 1.19 | 1.24 |
| 4 | 61-A | 204 | NAP | O4B-C4B | -2.43 | 1.39 | 1.45 |
| 4 | 125-A | 204 | NAP | C2D-C1D | -2.43 | 1.49 | 1.53 |
| 4 | 82-A | 204 | NAP | O7N-C7N | -2.43 | 1.19 | 1.24 |
| 4 | 57-A | 204 | NAP | O4B-C4B | -2.42 | 1.39 | 1.45 |
| 4 | 150-A | 204 | NAP | O7N-C7N | -2.42 | 1.19 | 1.24 |
| 4 | 67-A | 204 | NAP | C2B-C1B | -2.42 | 1.46 | 1.53 |
| 4 | 9-A | 204 | NAP | O4B-C4B | -2.42 | 1.39 | 1.45 |
| 2 | 126-A | 201 | FOL | CB-CA | -2.42 | 1.50 | 1.53 |
| 4 | 159-A | 204 | NAP | O4B-C4B | -2.41 | 1.39 | 1.45 |
| 4 | 146-A | 204 | NAP | O4B-C4B | -2.41 | 1.39 | 1.45 |
| 4 | 35-A | 204 | NAP | C2B-C1B | -2.41 | 1.46 | 1.53 |
| 4 | 4-A | 204 | NAP | C2B-C1B | -2.41 | 1.46 | 1.53 |
| 4 | 160-A | 204 | NAP | O4B-C4B | -2.41 | 1.39 | 1.45 |
| 4 | 89-A | 204 | NAP | O7N-C7N | -2.41 | 1.19 | 1.24 |
| 4 | 89-A | 204 | NAP | C2B-C1B | -2.41 | 1.46 | 1.53 |
| 4 | 50-A | 204 | NAP | C2D-C1D | -2.40 | 1.49 | 1.53 |
| 4 | 152-A | 204 | NAP | O4B-C4B | -2.40 | 1.39 | 1.45 |
| 4 | 31-A | 204 | NAP | O4B-C4B | -2.40 | 1.39 | 1.45 |
| 4 | 129-A | 204 | NAP | C2B-C1B | -2.40 | 1.46 | 1.53 |
| 4 | 157-A | 204 | NAP | O7N-C7N | -2.39 | 1.19 | 1.24 |
| 4 | 165-A | 204 | NAP | C2B-C1B | -2.39 | 1.46 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 129-A | 204 | NAP | O4B-C4B | -2.39 | 1.39 | 1.45 |
| 4 | 88-A | 204 | NAP | O4B-C4B | -2.39 | 1.39 | 1.45 |
| 4 | 141-A | 204 | NAP | O4B-C4B | -2.39 | 1.39 | 1.45 |
| 4 | 119-A | 204 | NAP | C2B-C1B | -2.38 | 1.46 | 1.53 |
| 4 | 167-A | 204 | NAP | O4B-C4B | -2.38 | 1.39 | 1.45 |
| 4 | 151-A | 204 | NAP | C2B-C1B | -2.38 | 1.46 | 1.53 |
| 4 | 58-A | 204 | NAP | O4B-C4B | -2.37 | 1.39 | 1.45 |
| 4 | 96-A | 204 | NAP | O7N-C7N | -2.37 | 1.19 | 1.24 |
| 4 | 86-A | 204 | NAP | O4B-C4B | -2.37 | 1.39 | 1.45 |
| 4 | 25-A | 204 | NAP | O7N-C7N | -2.37 | 1.19 | 1.24 |
| 4 | 124-A | 204 | NAP | C2B-C1B | -2.37 | 1.46 | 1.53 |
| 4 | 143-A | 204 | NAP | O4B-C4B | -2.37 | 1.39 | 1.45 |
| 2 | 123-A | 201 | FOL | CA-N | -2.36 | 1.43 | 1.46 |
| 4 | 155-A | 204 | NAP | O4B-C4B | -2.36 | 1.39 | 1.45 |
| 4 | 2-A | 204 | NAP | O4B-C4B | -2.36 | 1.39 | 1.45 |
| 4 | 72-A | 204 | NAP | O4B-C4B | -2.35 | 1.39 | 1.45 |
| 4 | 36-A | 204 | NAP | O7N-C7N | -2.35 | 1.19 | 1.24 |
| 4 | 122-A | 204 | NAP | C2B-C1B | -2.35 | 1.46 | 1.53 |
| 4 | 145-A | 204 | NAP | C2B-C1B | -2.34 | 1.46 | 1.53 |
| 4 | 161-A | 204 | NAP | O4B-C4B | -2.34 | 1.39 | 1.45 |
| 4 | 74-A | 204 | NAP | C2B-C1B | -2.34 | 1.46 | 1.53 |
| 4 | 72-A | 204 | NAP | O7N-C7N | -2.34 | 1.19 | 1.24 |
| 4 | 110-A | 204 | NAP | O7N-C7N | -2.34 | 1.19 | 1.24 |
| 4 | 154-A | 204 | NAP | O4B-C4B | -2.34 | 1.39 | 1.45 |
| 4 | 33-A | 204 | NAP | C2D-C1D | -2.34 | 1.49 | 1.53 |
| 4 | 128-A | 204 | NAP | C2B-C1B | -2.33 | 1.46 | 1.53 |
| 4 | 92-A | 204 | NAP | C2B-C1B | -2.33 | 1.46 | 1.53 |
| 4 | 86-A | 204 | NAP | C2B-C1B | -2.33 | 1.46 | 1.53 |
| 4 | 158-A | 204 | NAP | O7N-C7N | -2.33 | 1.19 | 1.24 |
| 4 | 103-A | 204 | NAP | C2B-C1B | -2.33 | 1.46 | 1.53 |
| 4 | 162-A | 204 | NAP | O4B-C4B | -2.32 | 1.39 | 1.45 |
| 4 | 22-A | 204 | NAP | C2B-C1B | -2.32 | 1.46 | 1.53 |
| 4 | 108-A | 204 | NAP | O4B-C4B | -2.32 | 1.39 | 1.45 |
| 4 | 163-A | 204 | NAP | O4B-C4B | -2.32 | 1.39 | 1.45 |
| 4 | 109-A | 204 | NAP | O7N-C7N | -2.32 | 1.19 | 1.24 |
| 4 | 127-A | 204 | NAP | O4B-C4B | -2.32 | 1.39 | 1.45 |
| 4 | 131-A | 204 | NAP | C2B-C1B | -2.32 | 1.46 | 1.53 |
| 4 | 157-A | 204 | NAP | O4B-C4B | -2.31 | 1.39 | 1.45 |
| 4 | 29-A | 204 | NAP | O4B-C4B | -2.31 | 1.39 | 1.45 |
| 4 | 42-A | 204 | NAP | O7N-C7N | -2.31 | 1.19 | 1.24 |
| 4 | 155-A | 204 | NAP | C2B-C1B | -2.30 | 1.46 | 1.53 |
| 4 | 87-A | 204 | NAP | O4B-C4B | -2.30 | 1.39 | 1.45 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 85-A | 204 | NAP | C2B-C1B | -2.30 | 1.46 | 1.53 |
| 4 | 17-A | 204 | NAP | C2B-C1B | -2.29 | 1.46 | 1.53 |
| 4 | 27-A | 204 | NAP | C2B-C1B | -2.29 | 1.46 | 1.53 |
| 4 | 33-A | 204 | NAP | C2B-C1B | -2.29 | 1.46 | 1.53 |
| 4 | 160-A | 204 | NAP | O7N-C7N | -2.29 | 1.19 | 1.24 |
| 4 | 147-A | 204 | NAP | O7N-C7N | -2.29 | 1.19 | 1.24 |
| 4 | 78-A | 204 | NAP | C2B-C1B | -2.29 | 1.46 | 1.53 |
| 4 | 14-A | 204 | NAP | C2B-C1B | -2.29 | 1.46 | 1.53 |
| 4 | 148-A | 204 | NAP | O7N-C7N | -2.29 | 1.19 | 1.24 |
| 4 | 137-A | 204 | NAP | C2B-C1B | -2.29 | 1.46 | 1.53 |
| 4 | 90-A | 204 | NAP | O7N-C7N | -2.28 | 1.19 | 1.24 |
| 4 | 79-A | 204 | NAP | O7N-C7N | -2.28 | 1.19 | 1.24 |
| 4 | 25-A | 204 | NAP | C2B-C1B | -2.28 | 1.46 | 1.53 |
| 4 | 42-A | 204 | NAP | C2B-C1B | -2.28 | 1.46 | 1.53 |
| 4 | 148-A | 204 | NAP | C2B-C1B | -2.28 | 1.46 | 1.53 |
| 4 | 54-A | 204 | NAP | C2B-C1B | -2.27 | 1.46 | 1.53 |
| 4 | 93-A | 204 | NAP | C2B-C1B | -2.27 | 1.46 | 1.53 |
| 4 | 165-A | 204 | NAP | O4B-C4B | -2.27 | 1.39 | 1.45 |
| 4 | 146-A | 204 | NAP | O7N-C7N | -2.27 | 1.19 | 1.24 |
| 4 | 85-A | 204 | NAP | O4B-C4B | -2.27 | 1.39 | 1.45 |
| 4 | 153-A | 204 | NAP | C2B-C1B | -2.27 | 1.46 | 1.53 |
| 4 | 68-A | 204 | NAP | C2B-C1B | -2.27 | 1.46 | 1.53 |
| 2 | 132-A | 201 | FOL | CA-N | -2.26 | 1.43 | 1.46 |
| 4 | 94-A | 204 | NAP | C2B-C1B | -2.26 | 1.46 | 1.53 |
| 4 | 13-A | 204 | NAP | C2B-C1B | -2.26 | 1.46 | 1.53 |
| 4 | 91-A | 204 | NAP | C2B-C1B | -2.26 | 1.46 | 1.53 |
| 4 | 161-A | 204 | NAP | C2B-C1B | -2.26 | 1.46 | 1.53 |
| 4 | 126-A | 204 | NAP | O4B-C4B | -2.26 | 1.39 | 1.45 |
| 4 | 59-A | 204 | NAP | C2B-C1B | -2.26 | 1.46 | 1.53 |
| 4 | 106-A | 204 | NAP | C2B-C1B | -2.26 | 1.46 | 1.53 |
| 4 | 51-A | 204 | NAP | O7N-C7N | -2.26 | 1.19 | 1.24 |
| 4 | 128-A | 204 | NAP | O4B-C4B | -2.25 | 1.39 | 1.45 |
| 4 | 3-A | 204 | NAP | C2B-C1B | -2.25 | 1.46 | 1.53 |
| 4 | 77-A | 204 | NAP | C2B-C1B | -2.25 | 1.46 | 1.53 |
| 4 | 1-A | 204 | NAP | O4B-C4B | -2.25 | 1.39 | 1.45 |
| 4 | 53-A | 204 | NAP | C2B-C1B | -2.24 | 1.46 | 1.53 |
| 4 | 11-A | 204 | NAP | C2B-C1B | -2.24 | 1.46 | 1.53 |
| 4 | 38-A | 204 | NAP | O7N-C7N | -2.24 | 1.19 | 1.24 |
| 4 | 84-A | 204 | NAP | O4B-C4B | -2.24 | 1.39 | 1.45 |
| 4 | 146-A | 204 | NAP | C2B-C1B | -2.24 | 1.46 | 1.53 |
| 4 | 108-A | 204 | NAP | C2B-C1B | -2.23 | 1.47 | 1.53 |
| 4 | 30-A | 204 | NAP | C2B-C1B | -2.23 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 97-A | 204 | NAP | O7N-C7N | -2.23 | 1.19 | 1.24 |
| 4 | 32-A | 204 | NAP | C2D-C3D | -2.23 | 1.47 | 1.53 |
| 4 | 16-A | 204 | NAP | C2B-C1B | -2.23 | 1.47 | 1.53 |
| 4 | 24-A | 204 | NAP | C2B-C1B | -2.22 | 1.47 | 1.53 |
| 4 | 153-A | 204 | NAP | O7N-C7N | -2.22 | 1.19 | 1.24 |
| 4 | 120-A | 204 | NAP | C2B-C1B | -2.22 | 1.47 | 1.53 |
| 4 | 58-A | 204 | NAP | C2B-C1B | -2.22 | 1.47 | 1.53 |
| 4 | 74-A | 204 | NAP | O7N-C7N | -2.22 | 1.19 | 1.24 |
| 4 | 18-A | 204 | NAP | C2B-C1B | -2.22 | 1.47 | 1.53 |
| 4 | 7-A | 204 | NAP | O7N-C7N | -2.22 | 1.19 | 1.24 |
| 4 | 15-A | 204 | NAP | C2B-C1B | -2.22 | 1.47 | 1.53 |
| 2 | 16-A | 201 | FOL | CA-N | -2.22 | 1.43 | 1.46 |
| 4 | 7-A | 204 | NAP | C2B-C1B | -2.22 | 1.47 | 1.53 |
| 4 | 72-A | 204 | NAP | C2B-C1B | -2.22 | 1.47 | 1.53 |
| 4 | 142-A | 204 | NAP | O4B-C4B | -2.21 | 1.40 | 1.45 |
| 4 | 52-A | 204 | NAP | C2B-C1B | -2.21 | 1.47 | 1.53 |
| 4 | 108-A | 204 | NAP | C2D-C3D | -2.21 | 1.47 | 1.53 |
| 4 | 49-A | 204 | NAP | C2B-C1B | -2.21 | 1.47 | 1.53 |
| 4 | 10-A | 204 | NAP | C2B-C1B | -2.21 | 1.47 | 1.53 |
| 4 | 8-A | 204 | NAP | O4B-C4B | -2.20 | 1.40 | 1.45 |
| 4 | 65-A | 204 | NAP | C2B-C1B | -2.20 | 1.47 | 1.53 |
| 4 | 144-A | 204 | NAP | C2B-C1B | -2.20 | 1.47 | 1.53 |
| 4 | 99-A | 204 | NAP | O7N-C7N | -2.20 | 1.19 | 1.24 |
| 2 | 156-A | 201 | FOL | CB-CA | -2.20 | 1.50 | 1.53 |
| 4 | 156-A | 204 | NAP | O7N-C7N | -2.20 | 1.19 | 1.24 |
| 4 | 6-A | 204 | NAP | O4B-C4B | -2.20 | 1.40 | 1.45 |
| 4 | 93-A | 204 | NAP | O7N-C7N | -2.20 | 1.19 | 1.24 |
| 4 | 103-A | 204 | NAP | O7N-C7N | -2.20 | 1.19 | 1.24 |
| 2 | 77-A | 201 | FOL | CB-CA | -2.20 | 1.50 | 1.53 |
| 4 | 123-A | 204 | NAP | C2B-C1B | -2.20 | 1.47 | 1.53 |
| 4 | 105-A | 204 | NAP | C2B-C1B | -2.19 | 1.47 | 1.53 |
| 4 | 2-A | 204 | NAP | C2B-C1B | -2.19 | 1.47 | 1.53 |
| 4 | 22-A | 204 | NAP | C2D-C3D | -2.19 | 1.47 | 1.53 |
| 4 | 164-A | 204 | NAP | O4B-C4B | -2.19 | 1.40 | 1.45 |
| 4 | 95-A | 204 | NAP | C2B-C1B | -2.19 | 1.47 | 1.53 |
| 4 | 133-A | 204 | NAP | C2B-C1B | -2.19 | 1.47 | 1.53 |
| 4 | 80-A | 204 | NAP | C2B-C1B | -2.19 | 1.47 | 1.53 |
| 4 | 50-A | 204 | NAP | O7N-C7N | -2.18 | 1.19 | 1.24 |
| 4 | 51-A | 204 | NAP | C2B-C1B | -2.18 | 1.47 | 1.53 |
| 4 | 121-A | 204 | NAP | C2B-C1B | -2.18 | 1.47 | 1.53 |
| 4 | 163-A | 204 | NAP | C2B-C1B | -2.18 | 1.47 | 1.53 |
| 4 | 141-A | 204 | NAP | C2B-C1B | -2.18 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 26-A | 204 | NAP | C2B-C1B | -2.17 | 1.47 | 1.53 |
| 4 | 87-A | 204 | NAP | C2B-C1B | -2.17 | 1.47 | 1.53 |
| 4 | 36-A | 204 | NAP | C2B-C1B | -2.17 | 1.47 | 1.53 |
| 2 | 35-A | 201 | FOL | CA-N | -2.17 | 1.43 | 1.46 |
| 4 | 63-A | 204 | NAP | C2B-C1B | -2.17 | 1.47 | 1.53 |
| 4 | 96-A | 204 | NAP | C2B-C1B | -2.17 | 1.47 | 1.53 |
| 4 | 104-A | 204 | NAP | C2B-C1B | -2.17 | 1.47 | 1.53 |
| 4 | 47-A | 204 | NAP | O7N-C7N | -2.16 | 1.19 | 1.24 |
| 4 | 139-A | 204 | NAP | C2B-C1B | -2.16 | 1.47 | 1.53 |
| 4 | 149-A | 204 | NAP | C2B-C1B | -2.16 | 1.47 | 1.53 |
| 4 | 143-A | 204 | NAP | C2B-C1B | -2.16 | 1.47 | 1.53 |
| 4 | 156-A | 204 | NAP | C2B-C1B | -2.16 | 1.47 | 1.53 |
| 4 | 14-A | 204 | NAP | C2D-C3D | -2.16 | 1.47 | 1.53 |
| 4 | 23-A | 204 | NAP | C2B-C1B | -2.16 | 1.47 | 1.53 |
| 4 | 34-A | 204 | NAP | C2B-C1B | -2.16 | 1.47 | 1.53 |
| 4 | 127-A | 204 | NAP | C2B-C1B | -2.16 | 1.47 | 1.53 |
| 4 | 76-A | 204 | NAP | C2B-C1B | -2.16 | 1.47 | 1.53 |
| 4 | 44-A | 204 | NAP | O7N-C7N | -2.15 | 1.19 | 1.24 |
| 4 | 63-A | 204 | NAP | C2N-C3N | -2.15 | 1.35 | 1.39 |
| 4 | 109-A | 204 | NAP | C2B-C1B | -2.15 | 1.47 | 1.53 |
| 4 | 41-A | 204 | NAP | C2B-C1B | -2.15 | 1.47 | 1.53 |
| 4 | 83-A | 204 | NAP | O4B-C4B | -2.15 | 1.40 | 1.45 |
| 4 | 116-A | 204 | NAP | C2B-C1B | -2.15 | 1.47 | 1.53 |
| 4 | 91-A | 204 | NAP | O7N-C7N | -2.15 | 1.19 | 1.24 |
| 4 | 22-A | 204 | NAP | O7N-C7N | -2.15 | 1.19 | 1.24 |
| 4 | 29-A | 204 | NAP | C2D-C3D | -2.15 | 1.47 | 1.53 |
| 4 | 147-A | 204 | NAP | C2B-C1B | -2.15 | 1.47 | 1.53 |
| 4 | 45-A | 204 | NAP | C2B-C1B | -2.15 | 1.47 | 1.53 |
| 4 | 45-A | 204 | NAP | O7N-C7N | -2.14 | 1.19 | 1.24 |
| 4 | 117-A | 204 | NAP | C2B-C1B | -2.14 | 1.47 | 1.53 |
| 4 | 69-A | 204 | NAP | C2B-C1B | -2.14 | 1.47 | 1.53 |
| 4 | 162-A | 204 | NAP | O7N-C7N | -2.14 | 1.19 | 1.24 |
| 4 | 37-A | 204 | NAP | O7N-C7N | -2.14 | 1.19 | 1.24 |
| 4 | 79-A | 204 | NAP | C2B-C1B | -2.14 | 1.47 | 1.53 |
| 4 | 20-A | 204 | NAP | C2B-C1B | -2.13 | 1.47 | 1.53 |
| 4 | 158-A | 204 | NAP | O4B-C4B | -2.13 | 1.40 | 1.45 |
| 4 | 39-A | 204 | NAP | C2B-C1B | -2.13 | 1.47 | 1.53 |
| 4 | 97-A | 204 | NAP | C2B-C1B | -2.13 | 1.47 | 1.53 |
| 4 | 86-A | 204 | NAP | C2D-C3D | -2.13 | 1.47 | 1.53 |
| 4 | 12-A | 204 | NAP | C2B-C1B | -2.12 | 1.47 | 1.53 |
| 4 | 167-A | 204 | NAP | O7N-C7N | -2.12 | 1.19 | 1.24 |
| 4 | 68-A | 204 | NAP | C2D-C3D | -2.12 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 2 | 6-A | 201 | FOL | CA-N | -2.12 | 1.43 | 1.46 |
| 4 | 118-A | 204 | NAP | C2B-C1B | -2.12 | 1.47 | 1.53 |
| 4 | 164-A | 204 | NAP | C2B-C1B | -2.12 | 1.47 | 1.53 |
| 4 | 84-A | 204 | NAP | C2B-C1B | -2.12 | 1.47 | 1.53 |
| 4 | 56-A | 204 | NAP | C2B-C1B | -2.12 | 1.47 | 1.53 |
| 4 | 114-A | 204 | NAP | C2B-C1B | -2.11 | 1.47 | 1.53 |
| 4 | 55-A | 204 | NAP | C2B-C1B | -2.11 | 1.47 | 1.53 |
| 4 | 158-A | 204 | NAP | C2B-C1B | -2.11 | 1.47 | 1.53 |
| 4 | 111-A | 204 | NAP | C2D-C3D | -2.11 | 1.47 | 1.53 |
| 4 | 73-A | 204 | NAP | C2D-C3D | -2.11 | 1.47 | 1.53 |
| 4 | 66-A | 204 | NAP | C2B-C1B | -2.11 | 1.47 | 1.53 |
| 4 | 61-A | 204 | NAP | C2B-C1B | -2.11 | 1.47 | 1.53 |
| 4 | 18-A | 204 | NAP | O7N-C7N | -2.10 | 1.19 | 1.24 |
| 4 | 110-A | 204 | NAP | C2B-C1B | -2.10 | 1.47 | 1.53 |
| 4 | 147-A | 204 | NAP | C2D-C3D | -2.10 | 1.47 | 1.53 |
| 4 | 32-A | 204 | NAP | C2B-C1B | -2.10 | 1.47 | 1.53 |
| 4 | 166-A | 204 | NAP | C2B-C1B | -2.10 | 1.47 | 1.53 |
| 4 | 75-A | 204 | NAP | C2B-C1B | -2.10 | 1.47 | 1.53 |
| 4 | 57-A | 204 | NAP | C2D-C3D | -2.09 | 1.47 | 1.53 |
| 4 | 136-A | 204 | NAP | C2B-C1B | -2.09 | 1.47 | 1.53 |
| 4 | 108-A | 204 | NAP | C2N-C3N | -2.09 | 1.35 | 1.39 |
| 4 | 44-A | 204 | NAP | C2B-C1B | -2.09 | 1.47 | 1.53 |
| 4 | 130-A | 204 | NAP | C2B-C1B | -2.09 | 1.47 | 1.53 |
| 4 | 90-A | 204 | NAP | C2B-C1B | -2.08 | 1.47 | 1.53 |
| 4 | 162-A | 204 | NAP | C2B-C1B | -2.08 | 1.47 | 1.53 |
| 4 | 153-A | 204 | NAP | C2D-C3D | -2.08 | 1.47 | 1.53 |
| 4 | 123-A | 204 | NAP | O7N-C7N | -2.08 | 1.19 | 1.24 |
| 4 | 111-A | 204 | NAP | C2B-C1B | -2.08 | 1.47 | 1.53 |
| 4 | 163-A | 204 | NAP | O7N-C7N | -2.08 | 1.19 | 1.24 |
| 4 | 102-A | 204 | NAP | C2B-C1B | -2.08 | 1.47 | 1.53 |
| 4 | 7-A | 204 | NAP | O4B-C4B | -2.07 | 1.40 | 1.45 |
| 4 | 31-A | 204 | NAP | C2B-C1B | -2.07 | 1.47 | 1.53 |
| 4 | 152-A | 204 | NAP | C2B-C1B | -2.07 | 1.47 | 1.53 |
| 4 | 104-A | 204 | NAP | O7N-C7N | -2.07 | 1.19 | 1.24 |
| 4 | 98-A | 204 | NAP | C2B-C1B | -2.07 | 1.47 | 1.53 |
| 4 | 107-A | 204 | NAP | C2B-C1B | -2.06 | 1.47 | 1.53 |
| 4 | 65-A | 204 | NAP | C2D-C3D | -2.06 | 1.47 | 1.53 |
| 4 | 66-A | 204 | NAP | O7N-C7N | -2.06 | 1.19 | 1.24 |
| 4 | 37-A | 204 | NAP | C2B-C1B | -2.06 | 1.47 | 1.53 |
| 4 | 73-A | 204 | NAP | C2B-C1B | -2.06 | 1.47 | 1.53 |
| 4 | 28-A | 204 | NAP | C2D-C3D | -2.06 | 1.47 | 1.53 |
| 4 | 71-A | 204 | NAP | C2B-C1B | -2.05 | 1.47 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 4 | 60-A | 204 | NAP | C2B-C1B | -2.05 | 1.47 | 1.53 |
| 4 | 107-A | 204 | NAP | C2D-C3D | -2.05 | 1.47 | 1.53 |
| 4 | 54-A | 204 | NAP | O7N-C7N | -2.05 | 1.19 | 1.24 |
| 4 | 72-A | 204 | NAP | C2D-C3D | -2.04 | 1.47 | 1.53 |
| 2 | 135-A | 201 | FOL | CA-N | -2.04 | 1.43 | 1.46 |
| 4 | 88-A | 204 | NAP | C2B-C1B | -2.04 | 1.47 | 1.53 |
| 4 | 70-A | 204 | NAP | C2B-C1B | -2.04 | 1.47 | 1.53 |
| 4 | 126-A | 204 | NAP | C2B-C1B | -2.04 | 1.47 | 1.53 |
| 4 | 140-A | 204 | NAP | O7N-C7N | -2.04 | 1.19 | 1.24 |
| 4 | 71-A | 204 | NAP | O7N-C7N | -2.04 | 1.19 | 1.24 |
| 4 | 48-A | 204 | NAP | C2B-C1B | -2.03 | 1.47 | 1.53 |
| 4 | 167-A | 204 | NAP | C2B-C1B | -2.03 | 1.47 | 1.53 |
| 4 | 99-A | 204 | NAP | C2B-C1B | -2.03 | 1.47 | 1.53 |
| 4 | 46-A | 204 | NAP | C2B-C1B | -2.03 | 1.47 | 1.53 |
| 4 | 64-A | 204 | NAP | C2B-C1B | -2.03 | 1.47 | 1.53 |
| 2 | 159-A | 201 | FOL | CA-N | -2.03 | 1.43 | 1.46 |
| 2 | 36-A | 201 | FOL | CA-N | -2.03 | 1.43 | 1.46 |
| 4 | 135-A | 204 | NAP | C2B-C1B | -2.03 | 1.47 | 1.53 |
| 4 | 133-A | 204 | NAP | O7N-C7N | -2.02 | 1.19 | 1.24 |
| 4 | 115-A | 204 | NAP | C2B-C1B | -2.02 | 1.47 | 1.53 |
| 4 | 110-A | 204 | NAP | C2D-C3D | -2.02 | 1.48 | 1.53 |
| 4 | 88-A | 204 | NAP | C2D-C3D | -2.02 | 1.48 | 1.53 |
| 4 | 60-A | 204 | NAP | C2D-C3D | -2.01 | 1.48 | 1.53 |
| 4 | 104-A | 204 | NAP | C2D-C3D | -2.01 | 1.48 | 1.53 |
| 4 | 85-A | 204 | NAP | O7N-C7N | -2.01 | 1.19 | 1.24 |
| 4 | 151-A | 204 | NAP | O7N-C7N | -2.01 | 1.19 | 1.24 |
| 4 | 11-A | 204 | NAP | O7N-C7N | -2.01 | 1.19 | 1.24 |
| 2 | 97-A | 201 | FOL | CA-N | -2.00 | 1.43 | 1.46 |
| 4 | 138-A | 204 | NAP | C2B-C1B | -2.00 | 1.47 | 1.53 |
| 4 | 160-A | 204 | NAP | C2B-C1B | -2.00 | 1.47 | 1.53 |
| 4 | 81-A | 204 | NAP | C2B-C1B | -2.00 | 1.47 | 1.53 |
| 4 | 2-A | 204 | NAP | C2D-C3D | -2.00 | 1.48 | 1.53 |
| 4 | 147-A | 204 | NAP | C6A-N6A | 2.00 | 1.42 | 1.34 |
| 4 | 80-A | 204 | NAP | C5A-N7A | 2.00 | 1.46 | 1.39 |
| 4 | 55-A | 204 | NAP | C5A-N7A | 2.00 | 1.46 | 1.39 |
| 4 | 78-A | 204 | NAP | O4D-C1D | 2.00 | 1.44 | 1.41 |
| 2 | 107-A | 201 | FOL | C2-N3 | 2.00 | 1.36 | 1.33 |
| 4 | 154-A | 204 | NAP | C5A-N7A | 2.00 | 1.46 | 1.39 |
| 4 | 21-A | 204 | NAP | C6N-N1N | 2.00 | 1.41 | 1.35 |
| 4 | 132-A | 204 | NAP | O4D-C1D | 2.00 | 1.44 | 1.41 |
| 4 | 15-A | 204 | NAP | C5A-N7A | 2.00 | 1.46 | 1.39 |
| 2 | 123-A | 201 | FOL | C2-N3 | 2.01 | 1.36 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 151-A | 204 | NAP | C5A-N7A | 2.01 | 1.46 | 1.39 |
| 2 | 140-A | 201 | FOL | C4A-C8A | 2.01 | 1.44 | 1.40 |
| 2 | 153-A | 201 | FOL | C2-N3 | 2.01 | 1.36 | 1.33 |
| 4 | 1-A | 204 | NAP | C6N-N1N | 2.01 | 1.41 | 1.35 |
| 4 | 13-A | 204 | NAP | C6N-N1N | 2.01 | 1.41 | 1.35 |
| 4 | 11-A | 204 | NAP | C6N-N1N | 2.01 | 1.41 | 1.35 |
| 2 | 142-A | 201 | FOL | C8A-N8 | 2.01 | 1.36 | 1.34 |
| 4 | 121-A | 204 | NAP | C6N-N1N | 2.02 | 1.41 | 1.35 |
| 4 | 35-A | 204 | NAP | C8A-N7A | 2.02 | 1.38 | 1.34 |
| 4 | 68-A | 204 | NAP | O4D-C1D | 2.02 | 1.44 | 1.41 |
| 4 | 114-A | 204 | NAP | C5A-N7A | 2.02 | 1.46 | 1.39 |
| 4 | 158-A | 204 | NAP | O4D-C1D | 2.02 | 1.44 | 1.41 |
| 4 | 97-A | 204 | NAP | C6N-N1N | 2.02 | 1.41 | 1.35 |
| 4 | 78-A | 204 | NAP | C6N-N1N | 2.02 | 1.41 | 1.35 |
| 4 | 66-A | 204 | NAP | C6N-N1N | 2.02 | 1.41 | 1.35 |
| 4 | 100-A | 204 | NAP | C5A-N7A | 2.02 | 1.46 | 1.39 |
| 2 | 80-A | 201 | FOL | C8A-N8 | 2.02 | 1.36 | 1.34 |
| 4 | 103-A | 204 | NAP | C6N-N1N | 2.03 | 1.41 | 1.35 |
| 2 | 104-A | 201 | FOL | C2-N3 | 2.03 | 1.36 | 1.33 |
| 4 | 110-A | 204 | NAP | C8A-N7A | 2.03 | 1.38 | 1.34 |
| 4 | 99-A | 204 | NAP | C6N-N1N | 2.03 | 1.41 | 1.35 |
| 4 | 134-A | 204 | NAP | O4D-C1D | 2.03 | 1.44 | 1.41 |
| 4 | 91-A | 204 | NAP | C6N-N1N | 2.03 | 1.41 | 1.35 |
| 4 | 22-A | 204 | NAP | C6N-N1N | 2.03 | 1.41 | 1.35 |
| 4 | 35-A | 204 | NAP | C5A-N7A | 2.03 | 1.46 | 1.39 |
| 4 | 14-A | 204 | NAP | C6N-N1N | 2.04 | 1.41 | 1.35 |
| 4 | 67-A | 204 | NAP | C5A-N7A | 2.04 | 1.46 | 1.39 |
| 4 | 41-A | 204 | NAP | C8A-N7A | 2.04 | 1.38 | 1.34 |
| 4 | 72-A | 204 | NAP | C6N-N1N | 2.04 | 1.41 | 1.35 |
| 2 | 150-A | 201 | FOL | C2-N3 | 2.05 | 1.36 | 1.33 |
| 4 | 7-A | 204 | NAP | O4D-C1D | 2.05 | 1.44 | 1.41 |
| 4 | 131-A | 204 | NAP | C2N-N1N | 2.05 | 1.38 | 1.35 |
| 2 | 56-A | 201 | FOL | CB-CA | 2.05 | 1.56 | 1.53 |
| 4 | 89-A | 204 | NAP | C8A-N7A | 2.06 | 1.38 | 1.34 |
| 2 | 46-A | 201 | FOL | C4A-C8A | 2.06 | 1.44 | 1.40 |
| 4 | 76-A | 204 | NAP | O4D-C1D | 2.06 | 1.44 | 1.41 |
| 2 | 83-A | 201 | FOL | CB-CA | 2.06 | 1.56 | 1.53 |
| 2 | 132-A | 201 | FOL | C2-N3 | 2.06 | 1.36 | 1.33 |
| 2 | 46-A | 201 | FOL | CB-CA | 2.06 | 1.56 | 1.53 |
| 4 | 106-A | 204 | NAP | C6N-N1N | 2.06 | 1.41 | 1.35 |
| 4 | 108-A | 204 | NAP | C6N-N1N | 2.06 | 1.41 | 1.35 |
| 2 | 25-A | 201 | FOL | C8A-N8 | 2.06 | 1.36 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 134-A | 201 | FOL | C2-N3 | 2.07 | 1.36 | 1.33 |
| 4 | 74-A | 204 | NAP | C5A-N7A | 2.07 | 1.46 | 1.39 |
| 4 | 106-A | 204 | NAP | C5A-N7A | 2.07 | 1.46 | 1.39 |
| 4 | 92-A | 204 | NAP | C6N-N1N | 2.07 | 1.41 | 1.35 |
| 4 | 100-A | 204 | NAP | C6N-N1N | 2.07 | 1.41 | 1.35 |
| 4 | 84-A | 204 | NAP | O4D-C1D | 2.07 | 1.44 | 1.41 |
| 4 | 143-A | 204 | NAP | O4D-C1D | 2.07 | 1.44 | 1.41 |
| 4 | 71-A | 204 | NAP | C6N-N1N | 2.07 | 1.41 | 1.35 |
| 4 | 31-A | 204 | NAP | O4D-C1D | 2.08 | 1.44 | 1.41 |
| 4 | 28-A | 204 | NAP | C5A-N7A | 2.08 | 1.46 | 1.39 |
| 4 | 29-A | 204 | NAP | C6N-N1N | 2.08 | 1.41 | 1.35 |
| 4 | 77-A | 204 | NAP | O4D-C1D | 2.08 | 1.44 | 1.41 |
| 2 | 34-A | 201 | FOL | C4A-C8A | 2.09 | 1.44 | 1.40 |
| 2 | 139-A | 201 | FOL | C4A-C8A | 2.09 | 1.44 | 1.40 |
| 2 | 151-A | 201 | FOL | C4A-C8A | 2.09 | 1.44 | 1.40 |
| 4 | 109-A | 204 | NAP | C6N-N1N | 2.09 | 1.41 | 1.35 |
| 4 | 145-A | 204 | NAP | C5A-N7A | 2.09 | 1.46 | 1.39 |
| 4 | 124-A | 204 | NAP | C8A-N7A | 2.09 | 1.38 | 1.34 |
| 4 | 68-A | 204 | NAP | C6N-N1N | 2.09 | 1.41 | 1.35 |
| 4 | 73-A | 204 | NAP | O4D-C1D | 2.09 | 1.44 | 1.41 |
| 4 | 115-A | 204 | NAP | C5A-N7A | 2.09 | 1.46 | 1.39 |
| 4 | 93-A | 204 | NAP | C6N-N1N | 2.09 | 1.41 | 1.35 |
| 2 | 18-A | 201 | FOL | C8A-N8 | 2.10 | 1.36 | 1.34 |
| 4 | 134-A | 204 | NAP | C2N-N1N | 2.10 | 1.38 | 1.35 |
| 2 | 23-A | 201 | FOL | C4-C4A | 2.10 | 1.45 | 1.41 |
| 4 | 28-A | 204 | NAP | C6N-N1N | 2.10 | 1.41 | 1.35 |
| 2 | 120-A | 201 | FOL | C7-N8 | 2.10 | 1.35 | 1.31 |
| 4 | 145-A | 204 | NAP | C8A-N7A | 2.10 | 1.38 | 1.34 |
| 4 | 93-A | 204 | NAP | O4D-C1D | 2.10 | 1.44 | 1.41 |
| 2 | 148-A | 201 | FOL | C2-N3 | 2.10 | 1.36 | 1.33 |
| 4 | 102-A | 204 | NAP | C6N-N1N | 2.11 | 1.41 | 1.35 |
| 4 | 36-A | 204 | NAP | C6N-N1N | 2.11 | 1.41 | 1.35 |
| 4 | 67-A | 204 | NAP | C6N-N1N | 2.11 | 1.41 | 1.35 |
| 2 | 116-A | 201 | FOL | C8A-N8 | 2.11 | 1.36 | 1.34 |
| 4 | 118-A | 204 | NAP | C2N-N1N | 2.11 | 1.38 | 1.35 |
| 4 | 116-A | 204 | NAP | C6N-N1N | 2.11 | 1.41 | 1.35 |
| 4 | 34-A | 204 | NAP | C2N-N1N | 2.11 | 1.38 | 1.35 |
| 4 | 7-A | 204 | NAP | C8A-N7A | 2.11 | 1.38 | 1.34 |
| 2 | 7-A | 201 | FOL | C4A-C8A | 2.11 | 1.44 | 1.40 |
| 2 | 55-A | 201 | FOL | CB-CA | 2.12 | 1.56 | 1.53 |
| 4 | 101-A | 204 | NAP | C6N-N1N | 2.12 | 1.41 | 1.35 |
| 4 | 73-A | 204 | NAP | C6N-N1N | 2.12 | 1.41 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 115-A | 204 | NAP | C6N-N1N | 2.12 | 1.41 | 1.35 |
| 4 | 39-A | 204 | NAP | C8A-N7A | 2.12 | 1.38 | 1.34 |
| 4 | 155-A | 204 | NAP | C8A-N7A | 2.12 | 1.38 | 1.34 |
| 4 | 18-A | 204 | NAP | C6N-N1N | 2.12 | 1.41 | 1.35 |
| 2 | 117-A | 201 | FOL | C2-N3 | 2.12 | 1.36 | 1.33 |
| 4 | 13-A | 204 | NAP | C8A-N7A | 2.12 | 1.38 | 1.34 |
| 4 | 82-A | 204 | NAP | C8A-N7A | 2.12 | 1.38 | 1.34 |
| 4 | 40-A | 204 | NAP | C6N-N1N | 2.13 | 1.41 | 1.35 |
| 4 | 153-A | 204 | NAP | C8A-N7A | 2.13 | 1.38 | 1.34 |
| 4 | 107-A | 204 | NAP | C6N-N1N | 2.13 | 1.41 | 1.35 |
| 4 | 32-A | 204 | NAP | C6N-N1N | 2.13 | 1.41 | 1.35 |
| 4 | 83-A | 204 | NAP | C2N-N1N | 2.13 | 1.38 | 1.35 |
| 2 | 57-A | 201 | FOL | CB-CA | 2.13 | 1.56 | 1.53 |
| 2 | 165-A | 201 | FOL | C8A-N8 | 2.13 | 1.36 | 1.34 |
| 2 | 126-A | 201 | FOL | C2-N3 | 2.13 | 1.36 | 1.33 |
| 4 | 114-A | 204 | NAP | C6N-N1N | 2.14 | 1.41 | 1.35 |
| 2 | 54-A | 201 | FOL | C8A-N8 | 2.14 | 1.36 | 1.34 |
| 2 | 145-A | 201 | FOL | C4A-C8A | 2.14 | 1.44 | 1.40 |
| 4 | 80-A | 204 | NAP | C8A-N7A | 2.14 | 1.38 | 1.34 |
| 2 | 16-A | 201 | FOL | C8A-N8 | 2.14 | 1.36 | 1.34 |
| 4 | 74-A | 204 | NAP | C8A-N7A | 2.14 | 1.38 | 1.34 |
| 4 | 124-A | 204 | NAP | C2N-N1N | 2.14 | 1.38 | 1.35 |
| 4 | 42-A | 204 | NAP | C6N-N1N | 2.14 | 1.41 | 1.35 |
| 4 | 112-A | 204 | NAP | C6N-N1N | 2.14 | 1.41 | 1.35 |
| 4 | 77-A | 204 | NAP | C6N-N1N | 2.14 | 1.41 | 1.35 |
| 4 | 88-A | 204 | NAP | O4D-C1D | 2.15 | 1.44 | 1.41 |
| 4 | 161-A | 204 | NAP | C8A-N7A | 2.15 | 1.38 | 1.34 |
| 4 | 101-A | 204 | NAP | C5A-N7A | 2.15 | 1.46 | 1.39 |
| 4 | 111-A | 204 | NAP | C6N-N1N | 2.15 | 1.41 | 1.35 |
| 4 | 98-A | 204 | NAP | C6N-N1N | 2.15 | 1.41 | 1.35 |
| 4 | 71-A | 204 | NAP | C8A-N7A | 2.15 | 1.38 | 1.34 |
| 4 | 67-A | 204 | NAP | O4D-C1D | 2.15 | 1.44 | 1.41 |
| 2 | 87-A | 201 | FOL | C2-N3 | 2.15 | 1.36 | 1.33 |
| 2 | 128-A | 201 | FOL | C4A-C8A | 2.16 | 1.44 | 1.40 |
| 4 | 19-A | 204 | NAP | C6N-N1N | 2.16 | 1.41 | 1.35 |
| 2 | 8-A | 201 | FOL | C4A-C8A | 2.16 | 1.44 | 1.40 |
| 4 | 119-A | 204 | NAP | C3B-C4B | 2.16 | 1.58 | 1.53 |
| 2 | 52-A | 201 | FOL | C8A-N8 | 2.16 | 1.36 | 1.34 |
| 2 | 82-A | 201 | FOL | C8A-N8 | 2.17 | 1.36 | 1.34 |
| 2 | 3-A | 201 | FOL | C4A-C8A | 2.17 | 1.44 | 1.40 |
| 4 | 120-A | 204 | NAP | C8A-N7A | 2.17 | 1.38 | 1.34 |
| 4 | 86-A | 204 | NAP | O4D-C1D | 2.17 | 1.44 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 27-A | 204 | NAP | C6N-N1N | 2.17 | 1.41 | 1.35 |
| 4 | 76-A | 204 | NAP | C6N-N1N | 2.17 | 1.41 | 1.35 |
| 4 | 112-A | 204 | NAP | C8A-N7A | 2.18 | 1.38 | 1.34 |
| 4 | 154-A | 204 | NAP | O4D-C1D | 2.18 | 1.44 | 1.41 |
| 4 | 113-A | 204 | NAP | C6N-N1N | 2.18 | 1.41 | 1.35 |
| 4 | 116-A | 204 | NAP | C8A-N7A | 2.18 | 1.38 | 1.34 |
| 4 | 139-A | 204 | NAP | C8A-N7A | 2.18 | 1.38 | 1.34 |
| 4 | 129-A | 204 | NAP | C2N-N1N | 2.18 | 1.38 | 1.35 |
| 4 | 31-A | 204 | NAP | C6N-N1N | 2.18 | 1.41 | 1.35 |
| 4 | 108-A | 204 | NAP | C7N-N7N | 2.18 | 1.37 | 1.33 |
| 4 | 59-A | 204 | NAP | C2N-N1N | 2.18 | 1.38 | 1.35 |
| 4 | 150-A | 204 | NAP | O4D-C1D | 2.18 | 1.44 | 1.41 |
| 4 | 117-A | 204 | NAP | O4D-C1D | 2.18 | 1.44 | 1.41 |
| 4 | 87-A | 204 | NAP | O4D-C1D | 2.18 | 1.44 | 1.41 |
| 4 | 117-A | 204 | NAP | C6N-N1N | 2.19 | 1.41 | 1.35 |
| 2 | 82-A | 201 | FOL | C4-C4A | 2.19 | 1.45 | 1.41 |
| 2 | 72-A | 201 | FOL | C4-C4A | 2.19 | 1.45 | 1.41 |
| 4 | 162-A | 204 | NAP | C8A-N7A | 2.20 | 1.38 | 1.34 |
| 4 | 107-A | 204 | NAP | C8A-N7A | 2.20 | 1.38 | 1.34 |
| 4 | 41-A | 204 | NAP | C6N-N1N | 2.20 | 1.41 | 1.35 |
| 2 | 75-A | 201 | FOL | C8A-N8 | 2.20 | 1.36 | 1.34 |
| 2 | 131-A | 201 | FOL | C4A-C8A | 2.20 | 1.44 | 1.40 |
| 4 | 35-A | 204 | NAP | C6N-N1N | 2.20 | 1.41 | 1.35 |
| 4 | 118-A | 204 | NAP | C8A-N7A | 2.20 | 1.38 | 1.34 |
| 4 | 70-A | 204 | NAP | C6N-N1N | 2.20 | 1.41 | 1.35 |
| 4 | 37-A | 204 | NAP | C6N-N1N | 2.20 | 1.41 | 1.35 |
| 4 | 142-A | 204 | NAP | O4D-C1D | 2.20 | 1.44 | 1.41 |
| 4 | 75-A | 204 | NAP | C6N-N1N | 2.21 | 1.41 | 1.35 |
| 4 | 165-A | 204 | NAP | C8A-N7A | 2.21 | 1.38 | 1.34 |
| 4 | 15-A | 204 | NAP | C2N-N1N | 2.21 | 1.38 | 1.35 |
| 4 | 79-A | 204 | NAP | C8A-N7A | 2.21 | 1.38 | 1.34 |
| 4 | 151-A | 204 | NAP | C8A-N7A | 2.21 | 1.38 | 1.34 |
| 2 | 85-A | 201 | FOL | C2-N3 | 2.21 | 1.36 | 1.33 |
| 4 | 45-A | 204 | NAP | C8A-N7A | 2.21 | 1.38 | 1.34 |
| 4 | 37-A | 204 | NAP | C8A-N7A | 2.21 | 1.38 | 1.34 |
| 4 | 74-A | 204 | NAP | O4D-C1D | 2.21 | 1.44 | 1.41 |
| 4 | 32-A | 204 | NAP | C8A-N7A | 2.21 | 1.38 | 1.34 |
| 2 | 35-A | 201 | FOL | C4A-C8A | 2.21 | 1.44 | 1.40 |
| 4 | 110-A | 204 | NAP | C6N-N1N | 2.21 | 1.41 | 1.35 |
| 4 | 42-A | 204 | NAP | C8A-N7A | 2.22 | 1.38 | 1.34 |
| 4 | 22-A | 204 | NAP | O4D-C1D | 2.22 | 1.44 | 1.41 |
| 2 | 24-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 161-A | 204 | NAP | C2N-N1N | 2.22 | 1.38 | 1.35 |
| 4 | 122-A | 204 | NAP | C8A-N7A | 2.22 | 1.38 | 1.34 |
| 4 | 16-A | 204 | NAP | C6N-N1N | 2.22 | 1.41 | 1.35 |
| 2 | 26-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 133-A | 201 | FOL | C4A-C8A | 2.22 | 1.44 | 1.40 |
| 2 | 82-A | 201 | FOL | C4A-C8A | 2.22 | 1.44 | 1.40 |
| 4 | 13-A | 204 | NAP | O4D-C1D | 2.23 | 1.44 | 1.41 |
| 4 | 87-A | 204 | NAP | C8A-N7A | 2.23 | 1.39 | 1.34 |
| 4 | 91-A | 204 | NAP | O4D-C1D | 2.23 | 1.44 | 1.41 |
| 4 | 39-A | 204 | NAP | C6N-N1N | 2.23 | 1.41 | 1.35 |
| 4 | 138-A | 204 | NAP | C8A-N7A | 2.23 | 1.39 | 1.34 |
| 4 | 147-A | 204 | NAP | O4D-C1D | 2.23 | 1.44 | 1.41 |
| 4 | 94-A | 204 | NAP | O4D-C1D | 2.23 | 1.44 | 1.41 |
| 4 | 136-A | 204 | NAP | O4D-C1D | 2.23 | 1.44 | 1.41 |
| 4 | 135-A | 204 | NAP | O4D-C1D | 2.23 | 1.44 | 1.41 |
| 4 | 66-A | 204 | NAP | O4D-C1D | 2.24 | 1.44 | 1.41 |
| 2 | 14-A | 201 | FOL | CB-CA | 2.24 | 1.56 | 1.53 |
| 4 | 69-A | 204 | NAP | C6N-N1N | 2.24 | 1.41 | 1.35 |
| 4 | 113-A | 204 | NAP | C8A-N7A | 2.24 | 1.39 | 1.34 |
| 4 | 148-A | 204 | NAP | O4D-C1D | 2.24 | 1.44 | 1.41 |
| 4 | 33-A | 204 | NAP | C8A-N7A | 2.24 | 1.39 | 1.34 |
| 2 | 32-A | 201 | FOL | C4A-C8A | 2.24 | 1.45 | 1.40 |
| 4 | 156-A | 204 | NAP | C8A-N7A | 2.24 | 1.39 | 1.34 |
| 4 | 29-A | 204 | NAP | C8A-N7A | 2.25 | 1.39 | 1.34 |
| 4 | 92-A | 204 | NAP | O4D-C1D | 2.25 | 1.44 | 1.41 |
| 2 | 41-A | 201 | FOL | C4A-C8A | 2.25 | 1.45 | 1.40 |
| 4 | 111-A | 204 | NAP | C8A-N7A | 2.25 | 1.39 | 1.34 |
| 4 | 138-A | 204 | NAP | O4D-C1D | 2.25 | 1.44 | 1.41 |
| 4 | 47-A | 204 | NAP | C8A-N7A | 2.25 | 1.39 | 1.34 |
| 4 | 164-A | 204 | NAP | C8A-N7A | 2.25 | 1.39 | 1.34 |
| 4 | 142-A | 204 | NAP | C2N-N1N | 2.25 | 1.38 | 1.35 |
| 4 | 137-A | 204 | NAP | O4D-C1D | 2.25 | 1.44 | 1.41 |
| 4 | 116-A | 204 | NAP | C2N-N1N | 2.25 | 1.38 | 1.35 |
| 4 | 5-A | 204 | NAP | C2N-N1N | 2.25 | 1.38 | 1.35 |
| 4 | 166-A | 204 | NAP | O4D-C1D | 2.25 | 1.44 | 1.41 |
| 4 | 95-A | 204 | NAP | O4D-C1D | 2.26 | 1.44 | 1.41 |
| 4 | 38-A | 204 | NAP | C6N-N1N | 2.26 | 1.41 | 1.35 |
| 4 | 72-A | 204 | NAP | C8A-N7A | 2.26 | 1.39 | 1.34 |
| 2 | 152-A | 201 | FOL | C2-N3 | 2.26 | 1.36 | 1.33 |
| 4 | 52-A | 204 | NAP | C8A-N7A | 2.26 | 1.39 | 1.34 |
| 4 | 117-A | 204 | NAP | C8A-N7A | 2.26 | 1.39 | 1.34 |
| 4 | 106-A | 204 | NAP | C8A-N7A | 2.26 | 1.39 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 44-A | 204 | NAP | C8A-N7A | 2.26 | 1.39 | 1.34 |
| 4 | 17-A | 204 | NAP | C6N-N1N | 2.26 | 1.41 | 1.35 |
| 4 | 123-A | 204 | NAP | C2N-N1N | 2.27 | 1.38 | 1.35 |
| 4 | 83-A | 204 | NAP | O4D-C1D | 2.27 | 1.44 | 1.41 |
| 4 | 144-A | 204 | NAP | C8A-N7A | 2.27 | 1.39 | 1.34 |
| 4 | 22-A | 204 | NAP | C8A-N7A | 2.27 | 1.39 | 1.34 |
| 4 | 77-A | 204 | NAP | C8A-N7A | 2.27 | 1.39 | 1.34 |
| 4 | 74-A | 204 | NAP | C6N-N1N | 2.27 | 1.41 | 1.35 |
| 4 | 54-A | 204 | NAP | C8A-N7A | 2.27 | 1.39 | 1.34 |
| 4 | 46-A | 204 | NAP | C8A-N7A | 2.28 | 1.39 | 1.34 |
| 4 | 75-A | 204 | NAP | O4D-C1D | 2.28 | 1.44 | 1.41 |
| 4 | 5-A | 204 | NAP | O4D-C1D | 2.28 | 1.44 | 1.41 |
| 4 | 79-A | 204 | NAP | O4D-C1D | 2.28 | 1.44 | 1.41 |
| 4 | 166-A | 204 | NAP | C2N-N1N | 2.28 | 1.38 | 1.35 |
| 2 | 1-A | 201 | FOL | C4-C4A | 2.28 | 1.45 | 1.41 |
| 4 | 157-A | 204 | NAP | C8A-N7A | 2.28 | 1.39 | 1.34 |
| 4 | 23-A | 204 | NAP | C6N-N1N | 2.28 | 1.42 | 1.35 |
| 4 | 1-A | 204 | NAP | O4D-C1D | 2.28 | 1.44 | 1.41 |
| 4 | 16-A | 204 | NAP | O4D-C1D | 2.28 | 1.44 | 1.41 |
| 4 | 141-A | 204 | NAP | C8A-N7A | 2.29 | 1.39 | 1.34 |
| 4 | 144-A | 204 | NAP | O4D-C1D | 2.29 | 1.44 | 1.41 |
| 4 | 26-A | 204 | NAP | C6N-N1N | 2.29 | 1.42 | 1.35 |
| 4 | 25-A | 204 | NAP | C6N-N1N | 2.29 | 1.42 | 1.35 |
| 4 | 3-A | 204 | NAP | O4D-C1D | 2.29 | 1.44 | 1.41 |
| 4 | 3-A | 204 | NAP | C8A-N7A | 2.30 | 1.39 | 1.34 |
| 4 | 12-A | 204 | NAP | C8A-N7A | 2.30 | 1.39 | 1.34 |
| 4 | 81-A | 204 | NAP | C2N-N1N | 2.30 | 1.38 | 1.35 |
| 2 | 81-A | 201 | FOL | C4-C4A | 2.30 | 1.45 | 1.41 |
| 2 | 109-A | 201 | FOL | C4A-C8A | 2.30 | 1.45 | 1.40 |
| 4 | 126-A | 204 | NAP | C8A-N7A | 2.30 | 1.39 | 1.34 |
| 2 | 157-A | 201 | FOL | C2-N3 | 2.30 | 1.36 | 1.33 |
| 2 | 165-A | 201 | FOL | C2-N3 | 2.30 | 1.36 | 1.33 |
| 4 | 63-A | 204 | NAP | C8A-N7A | 2.30 | 1.39 | 1.34 |
| 4 | 80-A | 204 | NAP | O4D-C1D | 2.30 | 1.44 | 1.41 |
| 4 | 92-A | 204 | NAP | C2N-N1N | 2.30 | 1.38 | 1.35 |
| 4 | 8-A | 204 | NAP | O4D-C1D | 2.31 | 1.44 | 1.41 |
| 4 | 104-A | 204 | NAP | C8A-N7A | 2.31 | 1.39 | 1.34 |
| 4 | 120-A | 204 | NAP | C6N-N1N | 2.31 | 1.42 | 1.35 |
| 2 | 132-A | 201 | FOL | C4A-C8A | 2.31 | 1.45 | 1.40 |
| 2 | 163-A | 201 | FOL | C2-N3 | 2.31 | 1.36 | 1.33 |
| 4 | 18-A | 204 | NAP | C8A-N7A | 2.31 | 1.39 | 1.34 |
| 4 | 12-A | 204 | NAP | C2N-N1N | 2.31 | 1.38 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 34-A | 204 | NAP | C8A-N7A | 2.31 | 1.39 | 1.34 |
| 4 | 20-A | 204 | NAP | C6N-N1N | 2.32 | 1.42 | 1.35 |
| 4 | 14-A | 204 | NAP | C8A-N7A | 2.32 | 1.39 | 1.34 |
| 4 | 118-A | 204 | NAP | C6N-N1N | 2.32 | 1.42 | 1.35 |
| 4 | 154-A | 204 | NAP | C8A-N7A | 2.32 | 1.39 | 1.34 |
| 4 | 65-A | 204 | NAP | O4D-C1D | 2.32 | 1.44 | 1.41 |
| 2 | 95-A | 201 | FOL | C4A-C8A | 2.32 | 1.45 | 1.40 |
| 4 | 123-A | 204 | NAP | O4D-C1D | 2.32 | 1.44 | 1.41 |
| 4 | 126-A | 204 | NAP | O4D-C1D | 2.32 | 1.44 | 1.41 |
| 2 | 161-A | 201 | FOL | C8A-N8 | 2.33 | 1.36 | 1.34 |
| 2 | 75-A | 201 | FOL | C4-C4A | 2.33 | 1.46 | 1.41 |
| 4 | 49-A | 204 | NAP | C8A-N7A | 2.33 | 1.39 | 1.34 |
| 4 | 98-A | 204 | NAP | O4D-C1D | 2.33 | 1.44 | 1.41 |
| 2 | 13-A | 201 | FOL | C4A-C8A | 2.33 | 1.45 | 1.40 |
| 2 | 159-A | 201 | FOL | C4-C4A | 2.33 | 1.46 | 1.41 |
| 4 | 30-A | 204 | NAP | C6N-N1N | 2.33 | 1.42 | 1.35 |
| 4 | 65-A | 204 | NAP | C8A-N7A | 2.33 | 1.39 | 1.34 |
| 4 | 76-A | 204 | NAP | C8A-N7A | 2.34 | 1.39 | 1.34 |
| 4 | 133-A | 204 | NAP | O4D-C1D | 2.34 | 1.44 | 1.41 |
| 4 | 163-A | 204 | NAP | C8A-N7A | 2.34 | 1.39 | 1.34 |
| 4 | 85-A | 204 | NAP | O4D-C1D | 2.34 | 1.44 | 1.41 |
| 2 | 15-A | 201 | FOL | CB-CA | 2.34 | 1.56 | 1.53 |
| 2 | 108-A | 201 | FOL | C4A-C8A | 2.34 | 1.45 | 1.40 |
| 2 | 136-A | 201 | FOL | C4A-C8A | 2.34 | 1.45 | 1.40 |
| 4 | 133-A | 204 | NAP | C2N-N1N | 2.34 | 1.38 | 1.35 |
| 2 | 113-A | 201 | FOL | C4A-C8A | 2.34 | 1.45 | 1.40 |
| 2 | 161-A | 201 | FOL | C4A-C8A | 2.34 | 1.45 | 1.40 |
| 4 | 30-A | 204 | NAP | C8A-N7A | 2.34 | 1.39 | 1.34 |
| 4 | 127-A | 204 | NAP | C2N-N1N | 2.34 | 1.38 | 1.35 |
| 2 | 29-A | 201 | FOL | C8A-N8 | 2.35 | 1.36 | 1.34 |
| 4 | 37-A | 204 | NAP | O4D-C1D | 2.35 | 1.44 | 1.41 |
| 4 | 24-A | 204 | NAP | O4D-C1D | 2.35 | 1.44 | 1.41 |
| 2 | 46-A | 201 | FOL | C8A-N8 | 2.36 | 1.36 | 1.34 |
| 4 | 51-A | 204 | NAP | C8A-N7A | 2.36 | 1.39 | 1.34 |
| 4 | 36-A | 204 | NAP | C8A-N7A | 2.36 | 1.39 | 1.34 |
| 2 | 101-A | 201 | FOL | C4A-C8A | 2.36 | 1.45 | 1.40 |
| 4 | 70-A | 204 | NAP | O4D-C1D | 2.36 | 1.44 | 1.41 |
| 2 | 116-A | 201 | FOL | C4A-C8A | 2.36 | 1.45 | 1.40 |
| 2 | 158-A | 201 | FOL | C4-C4A | 2.36 | 1.46 | 1.41 |
| 4 | 97-A | 204 | NAP | C8A-N7A | 2.36 | 1.39 | 1.34 |
| 4 | 61-A | 204 | NAP | O4D-C1D | 2.36 | 1.44 | 1.41 |
| 4 | 121-A | 204 | NAP | C8A-N7A | 2.36 | 1.39 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 158-A | 204 | NAP | C2A-N3A | 2.36 | 1.36 | 1.32 |
| 4 | 82-A | 204 | NAP | C2N-N1N | 2.37 | 1.38 | 1.35 |
| 4 | 51-A | 204 | NAP | C2N-N1N | 2.37 | 1.38 | 1.35 |
| 4 | 83-A | 204 | NAP | C2A-N3A | 2.37 | 1.36 | 1.32 |
| 4 | 130-A | 204 | NAP | O4D-C1D | 2.37 | 1.44 | 1.41 |
| 4 | 72-A | 204 | NAP | O4D-C1D | 2.37 | 1.44 | 1.41 |
| 4 | 119-A | 204 | NAP | C6N-N1N | 2.37 | 1.42 | 1.35 |
| 2 | 37-A | 201 | FOL | C4A-C8A | 2.37 | 1.45 | 1.40 |
| 4 | 11-A | 204 | NAP | C8A-N7A | 2.37 | 1.39 | 1.34 |
| 4 | 8-A | 204 | NAP | C7N-N7N | 2.37 | 1.37 | 1.33 |
| 2 | 33-A | 201 | FOL | CB-CA | 2.37 | 1.56 | 1.53 |
| 4 | 167-A | 204 | NAP | C8A-N7A | 2.37 | 1.39 | 1.34 |
| 4 | 86-A | 204 | NAP | C8A-N7A | 2.38 | 1.39 | 1.34 |
| 4 | 119-A | 204 | NAP | C8A-N7A | 2.38 | 1.39 | 1.34 |
| 2 | 162-A | 201 | FOL | C2-N3 | 2.38 | 1.36 | 1.33 |
| 2 | 1-A | 201 | FOL | C4A-C8A | 2.38 | 1.45 | 1.40 |
| 2 | 91-A | 201 | FOL | C4-C4A | 2.38 | 1.46 | 1.41 |
| 4 | 101-A | 204 | NAP | C8A-N7A | 2.38 | 1.39 | 1.34 |
| 4 | 155-A | 204 | NAP | O4D-C1D | 2.38 | 1.44 | 1.41 |
| 2 | 56-A | 201 | FOL | C4A-C8A | 2.39 | 1.45 | 1.40 |
| 2 | 110-A | 201 | FOL | C4A-C8A | 2.39 | 1.45 | 1.40 |
| 4 | 29-A | 204 | NAP | O4D-C1D | 2.39 | 1.44 | 1.41 |
| 4 | 166-A | 204 | NAP | C8A-N7A | 2.39 | 1.39 | 1.34 |
| 4 | 160-A | 204 | NAP | O4D-C1D | 2.39 | 1.44 | 1.41 |
| 2 | 11-A | 201 | FOL | C4A-C8A | 2.39 | 1.45 | 1.40 |
| 4 | 38-A | 204 | NAP | C8A-N7A | 2.39 | 1.39 | 1.34 |
| 4 | 24-A | 204 | NAP | C8A-N7A | 2.39 | 1.39 | 1.34 |
| 4 | 48-A | 204 | NAP | C8A-N7A | 2.39 | 1.39 | 1.34 |
| 4 | 20-A | 204 | NAP | C8A-N7A | 2.39 | 1.39 | 1.34 |
| 4 | 14-A | 204 | NAP | O4D-C1D | 2.39 | 1.44 | 1.41 |
| 4 | 75-A | 204 | NAP | C8A-N7A | 2.40 | 1.39 | 1.34 |
| 4 | 149-A | 204 | NAP | C8A-N7A | 2.40 | 1.39 | 1.34 |
| 4 | 19-A | 204 | NAP | C8A-N7A | 2.40 | 1.39 | 1.34 |
| 4 | 109-A | 204 | NAP | C8A-N7A | 2.40 | 1.39 | 1.34 |
| 4 | 146-A | 204 | NAP | C8A-N7A | 2.40 | 1.39 | 1.34 |
| 4 | 33-A | 204 | NAP | O4D-C1D | 2.40 | 1.44 | 1.41 |
| 2 | 69-A | 201 | FOL | CB-CA | 2.40 | 1.56 | 1.53 |
| 4 | 154-A | 204 | NAP | C2A-N3A | 2.40 | 1.36 | 1.32 |
| 4 | 69-A | 204 | NAP | C8A-N7A | 2.40 | 1.39 | 1.34 |
| 4 | 159-A | 204 | NAP | C8A-N7A | 2.40 | 1.39 | 1.34 |
| 4 | 121-A | 204 | NAP | C2N-N1N | 2.40 | 1.38 | 1.35 |
| 4 | 86-A | 204 | NAP | C2N-N1N | 2.40 | 1.38 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 128-A | 201 | FOL | C8A-N8 | 2.41 | 1.36 | 1.34 |
| 4 | 19-A | 204 | NAP | O4D-C1D | 2.41 | 1.44 | 1.41 |
| 4 | 125-A | 204 | NAP | C2N-N1N | 2.41 | 1.38 | 1.35 |
| 4 | 131-A | 204 | NAP | C8A-N7A | 2.41 | 1.39 | 1.34 |
| 4 | 100-A | 204 | NAP | C8A-N7A | 2.41 | 1.39 | 1.34 |
| 2 | 159-A | 201 | FOL | C2-N3 | 2.41 | 1.36 | 1.33 |
| 4 | 5-A | 204 | NAP | C8A-N7A | 2.41 | 1.39 | 1.34 |
| 2 | 156-A | 201 | FOL | C2-N3 | 2.41 | 1.36 | 1.33 |
| 2 | 77-A | 201 | FOL | C4-C4A | 2.41 | 1.46 | 1.41 |
| 2 | 125-A | 201 | FOL | C2-N3 | 2.41 | 1.36 | 1.33 |
| 4 | 1-A | 204 | NAP | C8A-N7A | 2.41 | 1.39 | 1.34 |
| 4 | 10-A | 204 | NAP | C8A-N7A | 2.41 | 1.39 | 1.34 |
| 2 | 16-A | 201 | FOL | C4-C4A | 2.42 | 1.46 | 1.41 |
| 4 | 68-A | 204 | NAP | C8A-N7A | 2.42 | 1.39 | 1.34 |
| 4 | 84-A | 204 | NAP | C8A-N7A | 2.42 | 1.39 | 1.34 |
| 4 | 35-A | 204 | NAP | O4D-C1D | 2.42 | 1.44 | 1.41 |
| 4 | 21-A | 204 | NAP | O4D-C1D | 2.42 | 1.44 | 1.41 |
| 2 | 71-A | 201 | FOL | C4-C4A | 2.42 | 1.46 | 1.41 |
| 4 | 52-A | 204 | NAP | O4D-C1D | 2.42 | 1.44 | 1.41 |
| 4 | 149-A | 204 | NAP | O4D-C1D | 2.42 | 1.44 | 1.41 |
| 2 | 125-A | 201 | FOL | C4A-C8A | 2.42 | 1.45 | 1.40 |
| 4 | 59-A | 204 | NAP | C8A-N7A | 2.43 | 1.39 | 1.34 |
| 4 | 88-A | 204 | NAP | C2N-N1N | 2.43 | 1.38 | 1.35 |
| 2 | 79-A | 201 | FOL | C4-C4A | 2.43 | 1.46 | 1.41 |
| 2 | 161-A | 201 | FOL | C2-N3 | 2.43 | 1.36 | 1.33 |
| 4 | 85-A | 204 | NAP | C2N-N1N | 2.44 | 1.38 | 1.35 |
| 4 | 114-A | 204 | NAP | C8A-N7A | 2.44 | 1.39 | 1.34 |
| 4 | 135-A | 204 | NAP | C2A-N3A | 2.44 | 1.36 | 1.32 |
| 4 | 91-A | 204 | NAP | C8A-N7A | 2.44 | 1.39 | 1.34 |
| 2 | 144-A | 201 | FOL | CB-CA | 2.44 | 1.56 | 1.53 |
| 4 | 50-A | 204 | NAP | C8A-N7A | 2.44 | 1.39 | 1.34 |
| 4 | 24-A | 204 | NAP | C6N-N1N | 2.44 | 1.42 | 1.35 |
| 4 | 71-A | 204 | NAP | O4D-C1D | 2.45 | 1.44 | 1.41 |
| 2 | 88-A | 201 | FOL | C4A-C8A | 2.45 | 1.45 | 1.40 |
| 4 | 117-A | 204 | NAP | C2N-N1N | 2.45 | 1.38 | 1.35 |
| 2 | 141-A | 201 | FOL | C4A-C8A | 2.45 | 1.45 | 1.40 |
| 4 | 123-A | 204 | NAP | C2A-N3A | 2.45 | 1.36 | 1.32 |
| 4 | 161-A | 204 | NAP | O4D-C1D | 2.45 | 1.44 | 1.41 |
| 4 | 77-A | 204 | NAP | C2A-N3A | 2.45 | 1.36 | 1.32 |
| 2 | 78-A | 201 | FOL | C4-C4A | 2.46 | 1.46 | 1.41 |
| 4 | 128-A | 204 | NAP | C2N-N1N | 2.46 | 1.38 | 1.35 |
| 4 | 46-A | 204 | NAP | C2N-N1N | 2.46 | 1.38 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 153-A | 201 | FOL | C4A-C8A | 2.46 | 1.45 | 1.40 |
| 4 | 130-A | 204 | NAP | C2N-N1N | 2.46 | 1.38 | 1.35 |
| 2 | 112-A | 201 | FOL | C4A-C8A | 2.46 | 1.45 | 1.40 |
| 4 | 33-A | 204 | NAP | C7N-N7N | 2.46 | 1.38 | 1.33 |
| 2 | 66-A | 201 | FOL | C4A-C8A | 2.47 | 1.45 | 1.40 |
| 4 | 55-A | 204 | NAP | C8A-N7A | 2.47 | 1.39 | 1.34 |
| 2 | 20-A | 201 | FOL | C4-C4A | 2.47 | 1.46 | 1.41 |
| 4 | 119-A | 204 | NAP | O4D-C1D | 2.47 | 1.44 | 1.41 |
| 4 | 98-A | 204 | NAP | C8A-N7A | 2.47 | 1.39 | 1.34 |
| 2 | 143-A | 201 | FOL | C4A-C8A | 2.47 | 1.45 | 1.40 |
| 4 | 17-A | 204 | NAP | C8A-N7A | 2.47 | 1.39 | 1.34 |
| 2 | 9-A | 201 | FOL | C4A-C8A | 2.47 | 1.45 | 1.40 |
| 4 | 99-A | 204 | NAP | O4D-C1D | 2.47 | 1.44 | 1.41 |
| 4 | 55-A | 204 | NAP | O4D-C1D | 2.47 | 1.44 | 1.41 |
| 4 | 20-A | 204 | NAP | O4D-C1D | 2.47 | 1.44 | 1.41 |
| 2 | 123-A | 201 | FOL | C4A-C8A | 2.47 | 1.45 | 1.40 |
| 4 | 40-A | 204 | NAP | C8A-N7A | 2.48 | 1.39 | 1.34 |
| 4 | 87-A | 204 | NAP | C2N-N1N | 2.48 | 1.38 | 1.35 |
| 4 | 88-A | 204 | NAP | C8A-N7A | 2.48 | 1.39 | 1.34 |
| 4 | 17-A | 204 | NAP | O4D-C1D | 2.48 | 1.44 | 1.41 |
| 2 | 140-A | 201 | FOL | C4-C4A | 2.48 | 1.46 | 1.41 |
| 4 | 61-A | 204 | NAP | C8A-N7A | 2.48 | 1.39 | 1.34 |
| 4 | 26-A | 204 | NAP | C8A-N7A | 2.48 | 1.39 | 1.34 |
| 4 | 69-A | 204 | NAP | O4D-C1D | 2.48 | 1.44 | 1.41 |
| 2 | 34-A | 201 | FOL | C4-C4A | 2.48 | 1.46 | 1.41 |
| 4 | 91-A | 204 | NAP | C2N-N1N | 2.48 | 1.38 | 1.35 |
| 4 | 67-A | 204 | NAP | C8A-N7A | 2.49 | 1.39 | 1.34 |
| 4 | 154-A | 204 | NAP | C2N-N1N | 2.49 | 1.38 | 1.35 |
| 2 | 145-A | 201 | FOL | C4-C4A | 2.49 | 1.46 | 1.41 |
| 4 | 67-A | 204 | NAP | C2A-N3A | 2.49 | 1.36 | 1.32 |
| 2 | 149-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 4 | 104-A | 204 | NAP | C2N-N1N | 2.49 | 1.38 | 1.35 |
| 2 | 166-A | 201 | FOL | C2-N3 | 2.49 | 1.36 | 1.33 |
| 2 | 22-A | 201 | FOL | C4A-C8A | 2.49 | 1.45 | 1.40 |
| 4 | 116-A | 204 | NAP | O4D-C1D | 2.49 | 1.44 | 1.41 |
| 2 | 161-A | 201 | FOL | C4-C4A | 2.49 | 1.46 | 1.41 |
| 4 | 136-A | 204 | NAP | C8A-N7A | 2.49 | 1.39 | 1.34 |
| 4 | 138-A | 204 | NAP | C2A-N3A | 2.49 | 1.36 | 1.32 |
| 4 | 23-A | 204 | NAP | O4D-C1D | 2.50 | 1.44 | 1.41 |
| 4 | 95-A | 204 | NAP | C2N-N1N | 2.50 | 1.38 | 1.35 |
| 2 | 36-A | 201 | FOL | C4A-C8A | 2.50 | 1.45 | 1.40 |
| 2 | 163-A | 201 | FOL | C8A-N8 | 2.50 | 1.36 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 118-A | 201 | FOL | C4A-C8A | 2.50 | 1.45 | 1.40 |
| 2 | 164-A | 201 | FOL | C2-N3 | 2.50 | 1.36 | 1.33 |
| 2 | 83-A | 201 | FOL | C4-C4A | 2.51 | 1.46 | 1.41 |
| 2 | 10-A | 201 | FOL | C4A-C8A | 2.51 | 1.45 | 1.40 |
| 4 | 126-A | 204 | NAP | C2N-N1N | 2.51 | 1.38 | 1.35 |
| 4 | 28-A | 204 | NAP | O4D-C1D | 2.51 | 1.44 | 1.41 |
| 2 | 114-A | 201 | FOL | C4A-C8A | 2.52 | 1.45 | 1.40 |
| 2 | 39-A | 201 | FOL | C4A-C8A | 2.52 | 1.45 | 1.40 |
| 4 | 125-A | 204 | NAP | C8A-N7A | 2.52 | 1.39 | 1.34 |
| 4 | 140-A | 204 | NAP | O4D-C1D | 2.52 | 1.44 | 1.41 |
| 4 | 150-A | 204 | NAP | C2A-N3A | 2.52 | 1.36 | 1.32 |
| 4 | 25-A | 204 | NAP | C8A-N7A | 2.52 | 1.39 | 1.34 |
| 2 | 14-A | 201 | FOL | C4A-C8A | 2.52 | 1.45 | 1.40 |
| 4 | 39-A | 204 | NAP | C2N-N1N | 2.52 | 1.38 | 1.35 |
| 4 | 127-A | 204 | NAP | C8A-N7A | 2.52 | 1.39 | 1.34 |
| 4 | 27-A | 204 | NAP | C8A-N7A | 2.53 | 1.39 | 1.34 |
| 4 | 81-A | 204 | NAP | C2A-N3A | 2.53 | 1.36 | 1.32 |
| 2 | 55-A | 201 | FOL | C4A-C8A | 2.53 | 1.45 | 1.40 |
| 2 | 154-A | 201 | FOL | C4A-C8A | 2.53 | 1.45 | 1.40 |
| 4 | 132-A | 204 | NAP | C8A-N7A | 2.53 | 1.39 | 1.34 |
| 2 | 75-A | 201 | FOL | C4A-C8A | 2.53 | 1.45 | 1.40 |
| 2 | 67-A | 201 | FOL | C4-C4A | 2.53 | 1.46 | 1.41 |
| 4 | 85-A | 204 | NAP | C8A-N7A | 2.54 | 1.39 | 1.34 |
| 4 | 148-A | 204 | NAP | C8A-N7A | 2.54 | 1.39 | 1.34 |
| 4 | 156-A | 204 | NAP | C2N-N1N | 2.54 | 1.38 | 1.35 |
| 4 | 129-A | 204 | NAP | C8A-N7A | 2.54 | 1.39 | 1.34 |
| 4 | 82-A | 204 | NAP | O4D-C1D | 2.54 | 1.44 | 1.41 |
| 2 | 43-A | 201 | FOL | C4A-C8A | 2.54 | 1.45 | 1.40 |
| 2 | 4-A | 201 | FOL | C4A-C8A | 2.54 | 1.45 | 1.40 |
| 4 | 36-A | 204 | NAP | O4D-C1D | 2.54 | 1.44 | 1.41 |
| 4 | 23-A | 204 | NAP | C8A-N7A | 2.54 | 1.39 | 1.34 |
| 4 | 122-A | 204 | NAP | O4D-C1D | 2.54 | 1.44 | 1.41 |
| 2 | 167-A | 201 | FOL | C4A-C8A | 2.54 | 1.45 | 1.40 |
| 4 | 95-A | 204 | NAP | C8A-N7A | 2.54 | 1.39 | 1.34 |
| 4 | 151-A | 204 | NAP | C2A-N3A | 2.54 | 1.36 | 1.32 |
| 4 | 2-A | 204 | NAP | C2N-N1N | 2.54 | 1.38 | 1.35 |
| 4 | 136-A | 204 | NAP | C2N-N1N | 2.55 | 1.38 | 1.35 |
| 4 | 58-A | 204 | NAP | C8A-N7A | 2.55 | 1.39 | 1.34 |
| 4 | 32-A | 204 | NAP | C2N-N1N | 2.55 | 1.38 | 1.35 |
| 4 | 128-A | 204 | NAP | O4D-C1D | 2.55 | 1.44 | 1.41 |
| 4 | 43-A | 204 | NAP | C2N-N1N | 2.55 | 1.38 | 1.35 |
| 4 | 158-A | 204 | NAP | C2N-N1N | 2.55 | 1.38 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 53-A | 204 | NAP | C8A-N7A | 2.55 | 1.39 | 1.34 |
| 4 | 157-A | 204 | NAP | C2A-N3A | 2.55 | 1.36 | 1.32 |
| 2 | 69-A | 201 | FOL | C4-C4A | 2.55 | 1.46 | 1.41 |
| 2 | 138-A | 201 | FOL | C4A-C8A | 2.55 | 1.45 | 1.40 |
| 4 | 80-A | 204 | NAP | C2N-N1N | 2.55 | 1.38 | 1.35 |
| 4 | 109-A | 204 | NAP | C2N-N1N | 2.55 | 1.38 | 1.35 |
| 2 | 74-A | 201 | FOL | C4-C4A | 2.56 | 1.46 | 1.41 |
| 2 | 160-A | 201 | FOL | C2-N3 | 2.56 | 1.36 | 1.33 |
| 4 | 39-A | 204 | NAP | O4D-C1D | 2.56 | 1.44 | 1.41 |
| 4 | 163-A | 204 | NAP | C2N-N1N | 2.56 | 1.38 | 1.35 |
| 4 | 26-A | 204 | NAP | O4D-C1D | 2.56 | 1.44 | 1.41 |
| 2 | 23-A | 201 | FOL | C4A-C8A | 2.56 | 1.45 | 1.40 |
| 4 | 105-A | 204 | NAP | C8A-N7A | 2.56 | 1.39 | 1.34 |
| 2 | 102-A | 201 | FOL | C4-C4A | 2.56 | 1.46 | 1.41 |
| 4 | 88-A | 204 | NAP | C2A-N3A | 2.57 | 1.36 | 1.32 |
| 4 | 34-A | 204 | NAP | C7N-N7N | 2.57 | 1.38 | 1.33 |
| 4 | 28-A | 204 | NAP | C8A-N7A | 2.57 | 1.39 | 1.34 |
| 2 | 156-A | 201 | FOL | C4A-C8A | 2.57 | 1.45 | 1.40 |
| 4 | 160-A | 204 | NAP | C8A-N7A | 2.57 | 1.39 | 1.34 |
| 4 | 157-A | 204 | NAP | C2N-N1N | 2.57 | 1.38 | 1.35 |
| 4 | 89-A | 204 | NAP | O4D-C1D | 2.57 | 1.44 | 1.41 |
| 2 | 54-A | 201 | FOL | C4A-C8A | 2.57 | 1.45 | 1.40 |
| 4 | 102-A | 204 | NAP | O4D-C1D | 2.58 | 1.44 | 1.41 |
| 4 | 143-A | 204 | NAP | C8A-N7A | 2.58 | 1.39 | 1.34 |
| 2 | 59-A | 201 | FOL | C4A-C8A | 2.58 | 1.45 | 1.40 |
| 2 | 126-A | 201 | FOL | C4A-C8A | 2.58 | 1.45 | 1.40 |
| 4 | 150-A | 204 | NAP | C8A-N7A | 2.58 | 1.39 | 1.34 |
| 4 | 139-A | 204 | NAP | C2A-N3A | 2.58 | 1.36 | 1.32 |
| 2 | 88-A | 201 | FOL | C4-C4A | 2.58 | 1.46 | 1.41 |
| 2 | 157-A | 201 | FOL | C4A-C8A | 2.58 | 1.45 | 1.40 |
| 4 | 86-A | 204 | NAP | C2A-N3A | 2.58 | 1.36 | 1.32 |
| 4 | 148-A | 204 | NAP | C2A-N3A | 2.58 | 1.36 | 1.32 |
| 4 | 92-A | 204 | NAP | C8A-N7A | 2.58 | 1.39 | 1.34 |
| 2 | 32-A | 201 | FOL | C4-C4A | 2.59 | 1.46 | 1.41 |
| 2 | 49-A | 201 | FOL | C4-C4A | 2.59 | 1.46 | 1.41 |
| 4 | 11-A | 204 | NAP | O4D-C1D | 2.59 | 1.44 | 1.41 |
| 4 | 64-A | 204 | NAP | C2A-N3A | 2.59 | 1.36 | 1.32 |
| 2 | 93-A | 201 | FOL | C4A-C8A | 2.59 | 1.45 | 1.40 |
| 2 | 104-A | 201 | FOL | C4A-C8A | 2.59 | 1.45 | 1.40 |
| 2 | 69-A | 201 | FOL | C4A-C8A | 2.59 | 1.45 | 1.40 |
| 4 | 9-A | 204 | NAP | C7N-N7N | 2.60 | 1.38 | 1.33 |
| 4 | 155-A | 204 | NAP | C2N-N1N | 2.60 | 1.38 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 148-A | 204 | NAP | C2N-N1N | 2.60 | 1.38 | 1.35 |
| 2 | 14-A | 201 | FOL | C4-C4A | 2.60 | 1.46 | 1.41 |
| 2 | 7-A | 201 | FOL | C4-C4A | 2.60 | 1.46 | 1.41 |
| 4 | 93-A | 204 | NAP | C2A-N3A | 2.60 | 1.36 | 1.32 |
| 4 | 31-A | 204 | NAP | C8A-N7A | 2.60 | 1.39 | 1.34 |
| 2 | 119-A | 201 | FOL | C4A-C8A | 2.60 | 1.45 | 1.40 |
| 4 | 49-A | 204 | NAP | O4D-C1D | 2.60 | 1.45 | 1.41 |
| 2 | 70-A | 201 | FOL | C4-C4A | 2.60 | 1.46 | 1.41 |
| 2 | 159-A | 201 | FOL | C8A-N8 | 2.60 | 1.37 | 1.34 |
| 2 | 127-A | 201 | FOL | C4A-C8A | 2.60 | 1.45 | 1.40 |
| 2 | 103-A | 201 | FOL | C4A-C8A | 2.60 | 1.45 | 1.40 |
| 2 | 68-A | 201 | FOL | C4-C4A | 2.60 | 1.46 | 1.41 |
| 2 | 58-A | 201 | FOL | C4-C4A | 2.61 | 1.46 | 1.41 |
| 4 | 108-A | 204 | NAP | O4D-C1D | 2.61 | 1.45 | 1.41 |
| 2 | 150-A | 201 | FOL | C4A-C8A | 2.61 | 1.45 | 1.40 |
| 4 | 81-A | 204 | NAP | O4D-C1D | 2.61 | 1.45 | 1.41 |
| 4 | 3-A | 204 | NAP | C2N-N1N | 2.61 | 1.38 | 1.35 |
| 4 | 93-A | 204 | NAP | C2N-N1N | 2.61 | 1.38 | 1.35 |
| 4 | 167-A | 204 | NAP | O4D-C1D | 2.61 | 1.45 | 1.41 |
| 4 | 12-A | 204 | NAP | O4D-C1D | 2.61 | 1.45 | 1.41 |
| 4 | 130-A | 204 | NAP | C2A-N3A | 2.61 | 1.36 | 1.32 |
| 4 | 132-A | 204 | NAP | C2A-N3A | 2.61 | 1.36 | 1.32 |
| 4 | 93-A | 204 | NAP | C8A-N7A | 2.61 | 1.39 | 1.34 |
| 4 | 152-A | 204 | NAP | C2N-N1N | 2.61 | 1.38 | 1.35 |
| 4 | 146-A | 204 | NAP | O4D-C1D | 2.62 | 1.45 | 1.41 |
| 4 | 60-A | 204 | NAP | C8A-N7A | 2.62 | 1.39 | 1.34 |
| 4 | 34-A | 204 | NAP | C2A-N3A | 2.62 | 1.36 | 1.32 |
| 2 | 5-A | 201 | FOL | C8A-N8 | 2.62 | 1.37 | 1.34 |
| 2 | 115-A | 201 | FOL | C4A-C8A | 2.62 | 1.45 | 1.40 |
| 4 | 94-A | 204 | NAP | C2N-N1N | 2.62 | 1.38 | 1.35 |
| 4 | 120-A | 204 | NAP | O4D-C1D | 2.62 | 1.45 | 1.41 |
| 4 | 15-A | 204 | NAP | O4D-C1D | 2.62 | 1.45 | 1.41 |
| 2 | 144-A | 201 | FOL | C4A-C8A | 2.62 | 1.45 | 1.40 |
| 4 | 50-A | 204 | NAP | C2N-N1N | 2.62 | 1.38 | 1.35 |
| 4 | 70-A | 204 | NAP | C8A-N7A | 2.62 | 1.39 | 1.34 |
| 2 | 47-A | 201 | FOL | C4A-C8A | 2.62 | 1.45 | 1.40 |
| 2 | 48-A | 201 | FOL | C4A-C8A | 2.62 | 1.45 | 1.40 |
| 2 | 132-A | 201 | FOL | C4-C4A | 2.62 | 1.46 | 1.41 |
| 4 | 51-A | 204 | NAP | O4D-C1D | 2.63 | 1.45 | 1.41 |
| 4 | 96-A | 204 | NAP | O4D-C1D | 2.63 | 1.45 | 1.41 |
| 4 | 128-A | 204 | NAP | C8A-N7A | 2.63 | 1.39 | 1.34 |
| 4 | 102-A | 204 | NAP | C8A-N7A | 2.63 | 1.39 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 105-A | 204 | NAP | C2N-N1N | 2.63 | 1.38 | 1.35 |
| 4 | 107-A | 204 | NAP | C2N-N1N | 2.63 | 1.38 | 1.35 |
| 4 | 4-A | 204 | NAP | O4D-C1D | 2.63 | 1.45 | 1.41 |
| 2 | 112-A | 201 | FOL | C4-C4A | 2.63 | 1.46 | 1.41 |
| 4 | 165-A | 204 | NAP | C2N-N1N | 2.63 | 1.38 | 1.35 |
| 2 | 142-A | 201 | FOL | C4-C4A | 2.63 | 1.46 | 1.41 |
| 4 | 73-A | 204 | NAP | C2A-N3A | 2.63 | 1.36 | 1.32 |
| 4 | 53-A | 204 | NAP | O4D-C1D | 2.64 | 1.45 | 1.41 |
| 4 | 89-A | 204 | NAP | C2N-N1N | 2.64 | 1.38 | 1.35 |
| 2 | 104-A | 201 | FOL | C4-C4A | 2.64 | 1.46 | 1.41 |
| 2 | 38-A | 201 | FOL | C4A-C8A | 2.64 | 1.45 | 1.40 |
| 4 | 103-A | 204 | NAP | C8A-N7A | 2.64 | 1.39 | 1.34 |
| 2 | 117-A | 201 | FOL | C4A-C8A | 2.64 | 1.45 | 1.40 |
| 4 | 61-A | 204 | NAP | C2A-N3A | 2.64 | 1.36 | 1.32 |
| 4 | 139-A | 204 | NAP | O4D-C1D | 2.64 | 1.45 | 1.41 |
| 4 | 62-A | 204 | NAP | C2A-N3A | 2.65 | 1.36 | 1.32 |
| 4 | 10-A | 204 | NAP | O4D-C1D | 2.65 | 1.45 | 1.41 |
| 2 | 102-A | 201 | FOL | C4A-C8A | 2.65 | 1.45 | 1.40 |
| 4 | 112-A | 204 | NAP | C2N-N1N | 2.65 | 1.38 | 1.35 |
| 4 | 57-A | 204 | NAP | C2A-N3A | 2.65 | 1.36 | 1.32 |
| 4 | 15-A | 204 | NAP | C2A-N3A | 2.65 | 1.36 | 1.32 |
| 2 | 120-A | 201 | FOL | C8A-N8 | 2.65 | 1.37 | 1.34 |
| 4 | 83-A | 204 | NAP | C8A-N7A | 2.65 | 1.39 | 1.34 |
| 2 | 163-A | 201 | FOL | C4A-C8A | 2.65 | 1.45 | 1.40 |
| 4 | 133-A | 204 | NAP | C2A-N3A | 2.65 | 1.36 | 1.32 |
| 2 | 2-A | 201 | FOL | C4A-C8A | 2.65 | 1.45 | 1.40 |
| 4 | 7-A | 204 | NAP | C2N-N1N | 2.65 | 1.38 | 1.35 |
| 4 | 53-A | 204 | NAP | C2N-N1N | 2.66 | 1.38 | 1.35 |
| 2 | 2-A | 201 | FOL | C4-C4A | 2.66 | 1.46 | 1.41 |
| 2 | 49-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 31-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 146-A | 201 | FOL | C4-C4A | 2.66 | 1.46 | 1.41 |
| 4 | 62-A | 204 | NAP | C2N-N1N | 2.66 | 1.38 | 1.35 |
| 4 | 96-A | 204 | NAP | C8A-N7A | 2.67 | 1.39 | 1.34 |
| 2 | 22-A | 201 | FOL | C4-C4A | 2.67 | 1.46 | 1.41 |
| 4 | 99-A | 204 | NAP | C8A-N7A | 2.67 | 1.39 | 1.34 |
| 4 | 64-A | 204 | NAP | C8A-N7A | 2.67 | 1.39 | 1.34 |
| 2 | 33-A | 201 | FOL | C4-C4A | 2.67 | 1.46 | 1.41 |
| 4 | 58-A | 204 | NAP | C2N-N1N | 2.67 | 1.38 | 1.35 |
| 4 | 48-A | 204 | NAP | C2N-N1N | 2.67 | 1.38 | 1.35 |
| 2 | 96-A | 201 | FOL | C4A-C8A | 2.67 | 1.45 | 1.40 |
| 4 | 135-A | 204 | NAP | C8A-N7A | 2.67 | 1.39 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 16-A | 201 | FOL | C4A-C8A | 2.67 | 1.45 | 1.40 |
| 4 | 4-A | 204 | NAP | C2N-N1N | 2.67 | 1.38 | 1.35 |
| 4 | 133-A | 204 | NAP | C8A-N7A | 2.67 | 1.39 | 1.34 |
| 4 | 54-A | 204 | NAP | O4D-C1D | 2.67 | 1.45 | 1.41 |
| 4 | 82-A | 204 | NAP | C2A-N3A | 2.67 | 1.36 | 1.32 |
| 2 | 105-A | 201 | FOL | CB-CA | 2.67 | 1.57 | 1.53 |
| 4 | 66-A | 204 | NAP | C8A-N7A | 2.68 | 1.39 | 1.34 |
| 4 | 61-A | 204 | NAP | C2N-N1N | 2.68 | 1.38 | 1.35 |
| 2 | 134-A | 201 | FOL | C4A-C8A | 2.68 | 1.45 | 1.40 |
| 4 | 130-A | 204 | NAP | C8A-N7A | 2.68 | 1.39 | 1.34 |
| 4 | 42-A | 204 | NAP | O4D-C1D | 2.68 | 1.45 | 1.41 |
| 2 | 62-A | 201 | FOL | C4-C4A | 2.68 | 1.46 | 1.41 |
| 4 | 114-A | 204 | NAP | O4D-C1D | 2.68 | 1.45 | 1.41 |
| 4 | 6-A | 204 | NAP | C2N-N1N | 2.68 | 1.38 | 1.35 |
| 4 | 108-A | 204 | NAP | C2N-N1N | 2.68 | 1.38 | 1.35 |
| 2 | 131-A | 201 | FOL | C8A-N8 | 2.68 | 1.37 | 1.34 |
| 2 | 84-A | 201 | FOL | C4-C4A | 2.68 | 1.46 | 1.41 |
| 2 | 99-A | 201 | FOL | C4A-C8A | 2.69 | 1.45 | 1.40 |
| 2 | 95-A | 201 | FOL | C4-C4A | 2.69 | 1.46 | 1.41 |
| 2 | 90-A | 201 | FOL | C4A-C8A | 2.69 | 1.45 | 1.40 |
| 2 | 5-A | 201 | FOL | C4A-C8A | 2.69 | 1.45 | 1.40 |
| 2 | 148-A | 201 | FOL | C4-C4A | 2.69 | 1.46 | 1.41 |
| 4 | 35-A | 204 | NAP | C2A-N3A | 2.69 | 1.36 | 1.32 |
| 4 | 43-A | 204 | NAP | C8A-N7A | 2.69 | 1.39 | 1.34 |
| 4 | 64-A | 204 | NAP | C2N-N1N | 2.69 | 1.38 | 1.35 |
| 4 | 109-A | 204 | NAP | C7N-N7N | 2.69 | 1.38 | 1.33 |
| 2 | 146-A | 201 | FOL | C4A-C8A | 2.69 | 1.45 | 1.40 |
| 4 | 27-A | 204 | NAP | O4D-C1D | 2.70 | 1.45 | 1.41 |
| 2 | 160-A | 201 | FOL | C4A-C8A | 2.70 | 1.45 | 1.40 |
| 4 | 129-A | 204 | NAP | O4D-C1D | 2.70 | 1.45 | 1.41 |
| 4 | 155-A | 204 | NAP | C2A-N3A | 2.70 | 1.36 | 1.32 |
| 2 | 93-A | 201 | FOL | CB-CA | 2.70 | 1.57 | 1.53 |
| 2 | 139-A | 201 | FOL | C4-C4A | 2.71 | 1.46 | 1.41 |
| 4 | 14-A | 204 | NAP | C2N-N1N | 2.71 | 1.38 | 1.35 |
| 4 | 65-A | 204 | NAP | C2N-N1N | 2.71 | 1.38 | 1.35 |
| 4 | 163-A | 204 | NAP | C2A-N3A | 2.71 | 1.36 | 1.32 |
| 2 | 116-A | 201 | FOL | C4-C4A | 2.71 | 1.46 | 1.41 |
| 4 | 16-A | 204 | NAP | C8A-N7A | 2.71 | 1.39 | 1.34 |
| 4 | 15-A | 204 | NAP | C8A-N7A | 2.71 | 1.39 | 1.34 |
| 2 | 50-A | 201 | FOL | C4-C4A | 2.71 | 1.46 | 1.41 |
| 4 | 119-A | 204 | NAP | C2A-N3A | 2.71 | 1.37 | 1.32 |
| 2 | 156-A | 201 | FOL | C4-C4A | 2.71 | 1.46 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 147-A | 204 | NAP | C8A-N7A | 2.71 | 1.39 | 1.34 |
| 2 | 12-A | 201 | FOL | C4A-C8A | 2.71 | 1.45 | 1.40 |
| 2 | 108-A | 201 | FOL | C4-C4A | 2.71 | 1.46 | 1.41 |
| 2 | 63-A | 201 | FOL | C4A-C8A | 2.72 | 1.45 | 1.40 |
| 2 | 57-A | 201 | FOL | C4-C4A | 2.72 | 1.46 | 1.41 |
| 2 | 25-A | 201 | FOL | C4A-C8A | 2.72 | 1.45 | 1.40 |
| 4 | 74-A | 204 | NAP | C2A-N3A | 2.72 | 1.37 | 1.32 |
| 2 | 131-A | 201 | FOL | C4-C4A | 2.72 | 1.46 | 1.41 |
| 2 | 63-A | 201 | FOL | C4-C4A | 2.72 | 1.46 | 1.41 |
| 4 | 115-A | 204 | NAP | C8A-N7A | 2.72 | 1.39 | 1.34 |
| 4 | 145-A | 204 | NAP | O4D-C1D | 2.72 | 1.45 | 1.41 |
| 4 | 123-A | 204 | NAP | C8A-N7A | 2.72 | 1.39 | 1.34 |
| 4 | 127-A | 204 | NAP | O4D-C1D | 2.72 | 1.45 | 1.41 |
| 4 | 140-A | 204 | NAP | C2A-N3A | 2.72 | 1.37 | 1.32 |
| 4 | 163-A | 204 | NAP | O4D-C1D | 2.72 | 1.45 | 1.41 |
| 2 | 122-A | 201 | FOL | C8A-N8 | 2.73 | 1.37 | 1.34 |
| 2 | 18-A | 201 | FOL | C4A-C8A | 2.73 | 1.45 | 1.40 |
| 2 | 40-A | 201 | FOL | C4A-C8A | 2.73 | 1.45 | 1.40 |
| 4 | 23-A | 204 | NAP | C2N-N1N | 2.73 | 1.39 | 1.35 |
| 4 | 73-A | 204 | NAP | C8A-N7A | 2.73 | 1.39 | 1.34 |
| 2 | 72-A | 201 | FOL | C4A-C8A | 2.74 | 1.45 | 1.40 |
| 4 | 165-A | 204 | NAP | C2A-N3A | 2.74 | 1.37 | 1.32 |
| 4 | 121-A | 204 | NAP | O4D-C1D | 2.74 | 1.45 | 1.41 |
| 2 | 130-A | 201 | FOL | C4A-C8A | 2.74 | 1.45 | 1.40 |
| 4 | 122-A | 204 | NAP | C2N-N1N | 2.74 | 1.39 | 1.35 |
| 2 | 155-A | 201 | FOL | C4-C4A | 2.74 | 1.46 | 1.41 |
| 4 | 153-A | 204 | NAP | C2A-N3A | 2.74 | 1.37 | 1.32 |
| 2 | 19-A | 201 | FOL | C4-C4A | 2.74 | 1.46 | 1.41 |
| 4 | 18-A | 204 | NAP | O4D-C1D | 2.74 | 1.45 | 1.41 |
| 4 | 81-A | 204 | NAP | C8A-N7A | 2.74 | 1.39 | 1.34 |
| 2 | 107-A | 201 | FOL | C4A-C8A | 2.74 | 1.45 | 1.40 |
| 4 | 17-A | 204 | NAP | C2A-N3A | 2.74 | 1.37 | 1.32 |
| 4 | 8-A | 204 | NAP | C8A-N7A | 2.74 | 1.39 | 1.34 |
| 4 | 9-A | 204 | NAP | C8A-N7A | 2.74 | 1.39 | 1.34 |
| 4 | 159-A | 204 | NAP | C7N-N7N | 2.74 | 1.38 | 1.33 |
| 4 | 29-A | 204 | NAP | C2A-N3A | 2.74 | 1.37 | 1.32 |
| 2 | 29-A | 201 | FOL | C4-C4A | 2.74 | 1.46 | 1.41 |
| 4 | 111-A | 204 | NAP | C2N-N1N | 2.75 | 1.39 | 1.35 |
| 2 | 147-A | 201 | FOL | C4A-C8A | 2.75 | 1.45 | 1.40 |
| 4 | 131-A | 204 | NAP | C2A-N3A | 2.75 | 1.37 | 1.32 |
| 4 | 119-A | 204 | NAP | C2N-N1N | 2.75 | 1.39 | 1.35 |
| 4 | 137-A | 204 | NAP | C2A-N3A | 2.75 | 1.37 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 38-A | 204 | NAP | C2A-N3A | 2.75 | 1.37 | 1.32 |
| 4 | 162-A | 204 | NAP | C2A-N3A | 2.75 | 1.37 | 1.32 |
| 4 | 25-A | 204 | NAP | O4D-C1D | 2.76 | 1.45 | 1.41 |
| 4 | 60-A | 204 | NAP | O4D-C1D | 2.76 | 1.45 | 1.41 |
| 4 | 101-A | 204 | NAP | O4D-C1D | 2.76 | 1.45 | 1.41 |
| 4 | 162-A | 204 | NAP | O4D-C1D | 2.76 | 1.45 | 1.41 |
| 4 | 162-A | 204 | NAP | C2N-N1N | 2.76 | 1.39 | 1.35 |
| 4 | 151-A | 204 | NAP | C2N-N1N | 2.76 | 1.39 | 1.35 |
| 4 | 135-A | 204 | NAP | C2N-N1N | 2.76 | 1.39 | 1.35 |
| 2 | 10-A | 201 | FOL | C4-C4A | 2.76 | 1.46 | 1.41 |
| 4 | 103-A | 204 | NAP | C2N-N1N | 2.76 | 1.39 | 1.35 |
| 2 | 35-A | 201 | FOL | C4-C4A | 2.76 | 1.46 | 1.41 |
| 4 | 9-A | 204 | NAP | C2N-N1N | 2.76 | 1.39 | 1.35 |
| 2 | 38-A | 201 | FOL | C4-C4A | 2.77 | 1.46 | 1.41 |
| 4 | 90-A | 204 | NAP | C8A-N7A | 2.77 | 1.40 | 1.34 |
| 2 | 55-A | 201 | FOL | C4-C4A | 2.77 | 1.46 | 1.41 |
| 4 | 120-A | 204 | NAP | C2N-N1N | 2.77 | 1.39 | 1.35 |
| 2 | 61-A | 201 | FOL | C4-C4A | 2.77 | 1.46 | 1.41 |
| 2 | 97-A | 201 | FOL | C4A-C8A | 2.77 | 1.46 | 1.40 |
| 4 | 50-A | 204 | NAP | O4D-C1D | 2.77 | 1.45 | 1.41 |
| 4 | 57-A | 204 | NAP | C2N-N1N | 2.77 | 1.39 | 1.35 |
| 2 | 36-A | 201 | FOL | C4-C4A | 2.77 | 1.46 | 1.41 |
| 4 | 125-A | 204 | NAP | C2A-N3A | 2.77 | 1.37 | 1.32 |
| 2 | 87-A | 201 | FOL | C4A-C8A | 2.77 | 1.46 | 1.40 |
| 2 | 19-A | 201 | FOL | C4A-C8A | 2.77 | 1.46 | 1.40 |
| 2 | 44-A | 201 | FOL | C4A-C8A | 2.78 | 1.46 | 1.40 |
| 4 | 10-A | 204 | NAP | C2N-N1N | 2.78 | 1.39 | 1.35 |
| 4 | 5-A | 204 | NAP | C2A-N3A | 2.78 | 1.37 | 1.32 |
| 4 | 94-A | 204 | NAP | C8A-N7A | 2.78 | 1.40 | 1.34 |
| 4 | 110-A | 204 | NAP | C2N-N1N | 2.78 | 1.39 | 1.35 |
| 2 | 85-A | 201 | FOL | C4A-C8A | 2.78 | 1.46 | 1.40 |
| 4 | 140-A | 204 | NAP | C8A-N7A | 2.78 | 1.40 | 1.34 |
| 2 | 94-A | 201 | FOL | C4A-C8A | 2.78 | 1.46 | 1.40 |
| 2 | 17-A | 201 | FOL | C4-C4A | 2.78 | 1.46 | 1.41 |
| 2 | 158-A | 201 | FOL | C4A-C8A | 2.78 | 1.46 | 1.40 |
| 4 | 107-A | 204 | NAP | O4D-C1D | 2.78 | 1.45 | 1.41 |
| 2 | 39-A | 201 | FOL | CB-CA | 2.79 | 1.57 | 1.53 |
| 4 | 164-A | 204 | NAP | O4D-C1D | 2.79 | 1.45 | 1.41 |
| 4 | 59-A | 204 | NAP | C2A-N3A | 2.79 | 1.37 | 1.32 |
| 4 | 115-A | 204 | NAP | O4D-C1D | 2.79 | 1.45 | 1.41 |
| 2 | 106-A | 201 | FOL | C4-C4A | 2.79 | 1.46 | 1.41 |
| 4 | 164-A | 204 | NAP | C2A-N3A | 2.79 | 1.37 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 18-A | 204 | NAP | C7N-N7N | 2.79 | 1.38 | 1.33 |
| 2 | 4-A | 201 | FOL | C4-C4A | 2.79 | 1.46 | 1.41 |
| 4 | 54-A | 204 | NAP | C2N-N1N | 2.79 | 1.39 | 1.35 |
| 4 | 21-A | 204 | NAP | C2A-N3A | 2.80 | 1.37 | 1.32 |
| 2 | 133-A | 201 | FOL | C4-C4A | 2.80 | 1.46 | 1.41 |
| 4 | 127-A | 204 | NAP | C2A-N3A | 2.80 | 1.37 | 1.32 |
| 4 | 90-A | 204 | NAP | C2A-N3A | 2.80 | 1.37 | 1.32 |
| 4 | 1-A | 204 | NAP | C2N-N1N | 2.80 | 1.39 | 1.35 |
| 4 | 73-A | 204 | NAP | C2N-N1N | 2.80 | 1.39 | 1.35 |
| 4 | 55-A | 204 | NAP | C2N-N1N | 2.80 | 1.39 | 1.35 |
| 2 | 3-A | 201 | FOL | C4-C4A | 2.80 | 1.47 | 1.41 |
| 4 | 56-A | 204 | NAP | C8A-N7A | 2.80 | 1.40 | 1.34 |
| 4 | 13-A | 204 | NAP | C2N-N1N | 2.80 | 1.39 | 1.35 |
| 2 | 153-A | 201 | FOL | C4-C4A | 2.80 | 1.47 | 1.41 |
| 4 | 141-A | 204 | NAP | O4D-C1D | 2.80 | 1.45 | 1.41 |
| 2 | 110-A | 201 | FOL | C4-C4A | 2.80 | 1.47 | 1.41 |
| 4 | 30-A | 204 | NAP | O4D-C1D | 2.80 | 1.45 | 1.41 |
| 2 | 121-A | 201 | FOL | C4A-C8A | 2.80 | 1.46 | 1.40 |
| 4 | 11-A | 204 | NAP | C2N-N1N | 2.80 | 1.39 | 1.35 |
| 4 | 149-A | 204 | NAP | C2N-N1N | 2.81 | 1.39 | 1.35 |
| 4 | 128-A | 204 | NAP | C2A-N3A | 2.81 | 1.37 | 1.32 |
| 2 | 20-A | 201 | FOL | C4A-C8A | 2.81 | 1.46 | 1.40 |
| 2 | 124-A | 201 | FOL | C4A-C8A | 2.81 | 1.46 | 1.40 |
| 4 | 166-A | 204 | NAP | C2A-N3A | 2.81 | 1.37 | 1.32 |
| 4 | 92-A | 204 | NAP | C2A-N3A | 2.81 | 1.37 | 1.32 |
| 4 | 165-A | 204 | NAP | O4D-C1D | 2.81 | 1.45 | 1.41 |
| 2 | 45-A | 201 | FOL | C4A-C8A | 2.81 | 1.46 | 1.40 |
| 2 | 122-A | 201 | FOL | C4A-C8A | 2.81 | 1.46 | 1.40 |
| 4 | 101-A | 204 | NAP | C2A-N3A | 2.81 | 1.37 | 1.32 |
| 2 | 42-A | 201 | FOL | C4A-C8A | 2.81 | 1.46 | 1.40 |
| 4 | 104-A | 204 | NAP | O4D-C1D | 2.81 | 1.45 | 1.41 |
| 2 | 120-A | 201 | FOL | C4A-C8A | 2.81 | 1.46 | 1.40 |
| 4 | 95-A | 204 | NAP | C2A-N3A | 2.81 | 1.37 | 1.32 |
| 4 | 78-A | 204 | NAP | C2N-N1N | 2.82 | 1.39 | 1.35 |
| 4 | 42-A | 204 | NAP | C2A-N3A | 2.82 | 1.37 | 1.32 |
| 4 | 36-A | 204 | NAP | C2A-N3A | 2.82 | 1.37 | 1.32 |
| 2 | 52-A | 201 | FOL | C4-C4A | 2.82 | 1.47 | 1.41 |
| 2 | 113-A | 201 | FOL | C4-C4A | 2.82 | 1.47 | 1.41 |
| 2 | 70-A | 201 | FOL | C4A-C8A | 2.82 | 1.46 | 1.40 |
| 2 | 73-A | 201 | FOL | C4A-C8A | 2.82 | 1.46 | 1.40 |
| 4 | 113-A | 204 | NAP | O4D-C1D | 2.82 | 1.45 | 1.41 |
| 4 | 97-A | 204 | NAP | C2N-N1N | 2.82 | 1.39 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 121-A | 204 | NAP | C2A-N3A | 2.82 | 1.37 | 1.32 |
| 4 | 40-A | 204 | NAP | C2A-N3A | 2.82 | 1.37 | 1.32 |
| 2 | 8-A | 201 | FOL | C4-C4A | 2.82 | 1.47 | 1.41 |
| 2 | 41-A | 201 | FOL | C4-C4A | 2.83 | 1.47 | 1.41 |
| 2 | 29-A | 201 | FOL | C4A-C8A | 2.83 | 1.46 | 1.40 |
| 4 | 47-A | 204 | NAP | O4D-C1D | 2.83 | 1.45 | 1.41 |
| 2 | 152-A | 201 | FOL | C4A-C8A | 2.83 | 1.46 | 1.40 |
| 2 | 61-A | 201 | FOL | C4A-C8A | 2.83 | 1.46 | 1.40 |
| 4 | 31-A | 204 | NAP | C7N-N7N | 2.84 | 1.38 | 1.33 |
| 4 | 79-A | 204 | NAP | C2N-N1N | 2.84 | 1.39 | 1.35 |
| 4 | 106-A | 204 | NAP | C2N-N1N | 2.84 | 1.39 | 1.35 |
| 2 | 45-A | 201 | FOL | C4-C4A | 2.84 | 1.47 | 1.41 |
| 2 | 81-A | 201 | FOL | C4A-C8A | 2.84 | 1.46 | 1.40 |
| 2 | 163-A | 201 | FOL | C4-C4A | 2.84 | 1.47 | 1.41 |
| 4 | 164-A | 204 | NAP | C7N-N7N | 2.84 | 1.38 | 1.33 |
| 2 | 111-A | 201 | FOL | C4A-C8A | 2.85 | 1.46 | 1.40 |
| 2 | 117-A | 201 | FOL | C4-C4A | 2.85 | 1.47 | 1.41 |
| 4 | 60-A | 204 | NAP | C2N-N1N | 2.85 | 1.39 | 1.35 |
| 2 | 64-A | 201 | FOL | C4A-C8A | 2.85 | 1.46 | 1.40 |
| 2 | 92-A | 201 | FOL | C4A-C8A | 2.85 | 1.46 | 1.40 |
| 4 | 96-A | 204 | NAP | C2A-N3A | 2.85 | 1.37 | 1.32 |
| 4 | 26-A | 204 | NAP | C2A-N3A | 2.85 | 1.37 | 1.32 |
| 2 | 78-A | 201 | FOL | C4A-C8A | 2.86 | 1.46 | 1.40 |
| 4 | 40-A | 204 | NAP | O4D-C1D | 2.86 | 1.45 | 1.41 |
| 4 | 124-A | 204 | NAP | C2A-N3A | 2.86 | 1.37 | 1.32 |
| 2 | 96-A | 201 | FOL | C4-C4A | 2.86 | 1.47 | 1.41 |
| 4 | 47-A | 204 | NAP | C2N-N1N | 2.86 | 1.39 | 1.35 |
| 4 | 28-A | 204 | NAP | C2N-N1N | 2.86 | 1.39 | 1.35 |
| 4 | 41-A | 204 | NAP | O4D-C1D | 2.86 | 1.45 | 1.41 |
| 2 | 103-A | 201 | FOL | C4-C4A | 2.86 | 1.47 | 1.41 |
| 4 | 46-A | 204 | NAP | O4D-C1D | 2.87 | 1.45 | 1.41 |
| 4 | 143-A | 204 | NAP | C2N-N1N | 2.87 | 1.39 | 1.35 |
| 2 | 129-A | 201 | FOL | C4A-C8A | 2.87 | 1.46 | 1.40 |
| 4 | 59-A | 204 | NAP | C7N-N7N | 2.87 | 1.38 | 1.33 |
| 2 | 71-A | 201 | FOL | C4A-C8A | 2.87 | 1.46 | 1.40 |
| 4 | 52-A | 204 | NAP | C2N-N1N | 2.87 | 1.39 | 1.35 |
| 4 | 66-A | 204 | NAP | C2N-N1N | 2.87 | 1.39 | 1.35 |
| 2 | 98-A | 201 | FOL | C4A-C8A | 2.87 | 1.46 | 1.40 |
| 2 | 165-A | 201 | FOL | C4A-C8A | 2.87 | 1.46 | 1.40 |
| 4 | 57-A | 204 | NAP | C8A-N7A | 2.87 | 1.40 | 1.34 |
| 4 | 48-A | 204 | NAP | O4D-C1D | 2.87 | 1.45 | 1.41 |
| 4 | 98-A | 204 | NAP | C2N-N1N | 2.88 | 1.39 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 102-A | 204 | NAP | C2N-N1N | 2.88 | 1.39 | 1.35 |
| 4 | 147-A | 204 | NAP | C2A-N3A | 2.88 | 1.37 | 1.32 |
| 4 | 14-A | 204 | NAP | C2A-N3A | 2.88 | 1.37 | 1.32 |
| 2 | 73-A | 201 | FOL | C4-C4A | 2.88 | 1.47 | 1.41 |
| 4 | 149-A | 204 | NAP | C2A-N3A | 2.88 | 1.37 | 1.32 |
| 4 | 72-A | 204 | NAP | C2A-N3A | 2.88 | 1.37 | 1.32 |
| 4 | 75-A | 204 | NAP | C2A-N3A | 2.88 | 1.37 | 1.32 |
| 4 | 103-A | 204 | NAP | O4D-C1D | 2.88 | 1.45 | 1.41 |
| 2 | 11-A | 201 | FOL | C4-C4A | 2.88 | 1.47 | 1.41 |
| 4 | 18-A | 204 | NAP | C2A-N3A | 2.88 | 1.37 | 1.32 |
| 4 | 76-A | 204 | NAP | C2N-N1N | 2.88 | 1.39 | 1.35 |
| 4 | 70-A | 204 | NAP | C2A-N3A | 2.89 | 1.37 | 1.32 |
| 4 | 11-A | 204 | NAP | C2A-N3A | 2.89 | 1.37 | 1.32 |
| 4 | 55-A | 204 | NAP | C2A-N3A | 2.89 | 1.37 | 1.32 |
| 2 | 86-A | 201 | FOL | C4-C4A | 2.89 | 1.47 | 1.41 |
| 2 | 66-A | 201 | FOL | C4-C4A | 2.89 | 1.47 | 1.41 |
| 4 | 21-A | 204 | NAP | C8A-N7A | 2.89 | 1.40 | 1.34 |
| 4 | 101-A | 204 | NAP | C2N-N1N | 2.89 | 1.39 | 1.35 |
| 2 | 86-A | 201 | FOL | C4A-C8A | 2.89 | 1.46 | 1.40 |
| 4 | 43-A | 204 | NAP | C2A-N3A | 2.90 | 1.37 | 1.32 |
| 4 | 25-A | 204 | NAP | C7N-N7N | 2.90 | 1.38 | 1.33 |
| 2 | 50-A | 201 | FOL | C4A-C8A | 2.90 | 1.46 | 1.40 |
| 4 | 137-A | 204 | NAP | C2N-N1N | 2.90 | 1.39 | 1.35 |
| 2 | 97-A | 201 | FOL | C4-C4A | 2.90 | 1.47 | 1.41 |
| 2 | 18-A | 201 | FOL | C4-C4A | 2.90 | 1.47 | 1.41 |
| 4 | 10-A | 204 | NAP | C2A-N3A | 2.90 | 1.37 | 1.32 |
| 4 | 85-A | 204 | NAP | C2A-N3A | 2.90 | 1.37 | 1.32 |
| 4 | 160-A | 204 | NAP | C2N-N1N | 2.91 | 1.39 | 1.35 |
| 2 | 52-A | 201 | FOL | C4A-C8A | 2.91 | 1.46 | 1.40 |
| 4 | 113-A | 204 | NAP | C2A-N3A | 2.91 | 1.37 | 1.32 |
| 4 | 6-A | 204 | NAP | C8A-N7A | 2.91 | 1.40 | 1.34 |
| 4 | 157-A | 204 | NAP | C7N-N7N | 2.91 | 1.38 | 1.33 |
| 2 | 138-A | 201 | FOL | C4-C4A | 2.91 | 1.47 | 1.41 |
| 4 | 150-A | 204 | NAP | C7N-N7N | 2.91 | 1.38 | 1.33 |
| 2 | 123-A | 201 | FOL | C4-C4A | 2.91 | 1.47 | 1.41 |
| 4 | 17-A | 204 | NAP | C2N-N1N | 2.91 | 1.39 | 1.35 |
| 4 | 77-A | 204 | NAP | C2N-N1N | 2.91 | 1.39 | 1.35 |
| 4 | 145-A | 204 | NAP | C2A-N3A | 2.92 | 1.37 | 1.32 |
| 4 | 158-A | 204 | NAP | C7N-N7N | 2.92 | 1.38 | 1.33 |
| 2 | 143-A | 201 | FOL | C4-C4A | 2.92 | 1.47 | 1.41 |
| 2 | 24-A | 201 | FOL | C4-C4A | 2.92 | 1.47 | 1.41 |
| 4 | 2-A | 204 | NAP | C2A-N3A | 2.92 | 1.37 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 32-A | 204 | NAP | C2A-N3A | 2.92 | 1.37 | 1.32 |
| 4 | 97-A | 204 | NAP | O4D-C1D | 2.92 | 1.45 | 1.41 |
| 4 | 153-A | 204 | NAP | C2N-N1N | 2.92 | 1.39 | 1.35 |
| 4 | 142-A | 204 | NAP | C8A-N7A | 2.92 | 1.40 | 1.34 |
| 2 | 79-A | 201 | FOL | C4A-C8A | 2.92 | 1.46 | 1.40 |
| 4 | 45-A | 204 | NAP | C2N-N1N | 2.92 | 1.39 | 1.35 |
| 2 | 6-A | 201 | FOL | C4A-C8A | 2.93 | 1.46 | 1.40 |
| 2 | 54-A | 201 | FOL | C4-C4A | 2.93 | 1.47 | 1.41 |
| 2 | 51-A | 201 | FOL | C4-C4A | 2.93 | 1.47 | 1.41 |
| 2 | 128-A | 201 | FOL | C4-C4A | 2.93 | 1.47 | 1.41 |
| 2 | 87-A | 201 | FOL | C4-C4A | 2.93 | 1.47 | 1.41 |
| 2 | 139-A | 201 | FOL | CB-CA | 2.93 | 1.57 | 1.53 |
| 4 | 110-A | 204 | NAP | O4D-C1D | 2.93 | 1.45 | 1.41 |
| 2 | 107-A | 201 | FOL | C4-C4A | 2.94 | 1.47 | 1.41 |
| 4 | 38-A | 204 | NAP | C2N-N1N | 2.94 | 1.39 | 1.35 |
| 2 | 85-A | 201 | FOL | C4-C4A | 2.94 | 1.47 | 1.41 |
| 2 | 31-A | 201 | FOL | C4-C4A | 2.94 | 1.47 | 1.41 |
| 4 | 37-A | 204 | NAP | C2N-N1N | 2.94 | 1.39 | 1.35 |
| 4 | 74-A | 204 | NAP | C2N-N1N | 2.94 | 1.39 | 1.35 |
| 4 | 44-A | 204 | NAP | O4D-C1D | 2.94 | 1.45 | 1.41 |
| 4 | 100-A | 204 | NAP | O4D-C1D | 2.94 | 1.45 | 1.41 |
| 2 | 134-A | 201 | FOL | C4-C4A | 2.95 | 1.47 | 1.41 |
| 2 | 58-A | 201 | FOL | CB-CA | 2.95 | 1.57 | 1.53 |
| 2 | 162-A | 201 | FOL | C4-C4A | 2.95 | 1.47 | 1.41 |
| 2 | 93-A | 201 | FOL | C4-C4A | 2.95 | 1.47 | 1.41 |
| 4 | 44-A | 204 | NAP | C2N-N1N | 2.95 | 1.39 | 1.35 |
| 4 | 141-A | 204 | NAP | C2N-N1N | 2.95 | 1.39 | 1.35 |
| 4 | 152-A | 204 | NAP | C2A-N3A | 2.95 | 1.37 | 1.32 |
| 4 | 32-A | 204 | NAP | C7N-N7N | 2.95 | 1.39 | 1.33 |
| 2 | 74-A | 201 | FOL | C4A-C8A | 2.95 | 1.46 | 1.40 |
| 4 | 163-A | 204 | NAP | C7N-N7N | 2.95 | 1.39 | 1.33 |
| 4 | 100-A | 204 | NAP | C2N-N1N | 2.95 | 1.39 | 1.35 |
| 4 | 8-A | 204 | NAP | C2A-N3A | 2.96 | 1.37 | 1.32 |
| 4 | 45-A | 204 | NAP | C2A-N3A | 2.96 | 1.37 | 1.32 |
| 4 | 113-A | 204 | NAP | C2N-N1N | 2.96 | 1.39 | 1.35 |
| 4 | 54-A | 204 | NAP | C2A-N3A | 2.96 | 1.37 | 1.32 |
| 4 | 120-A | 204 | NAP | C2A-N3A | 2.96 | 1.37 | 1.32 |
| 4 | 91-A | 204 | NAP | C2A-N3A | 2.96 | 1.37 | 1.32 |
| 4 | 142-A | 204 | NAP | C2A-N3A | 2.96 | 1.37 | 1.32 |
| 4 | 101-A | 204 | NAP | C7N-N7N | 2.96 | 1.39 | 1.33 |
| 2 | 106-A | 201 | FOL | C4A-C8A | 2.97 | 1.46 | 1.40 |
| 2 | 15-A | 201 | FOL | C4A-C8A | 2.97 | 1.46 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 11-A | 204 | NAP | C7N-N7N | 2.97 | 1.39 | 1.33 |
| 2 | 105-A | 201 | FOL | C4-C4A | 2.97 | 1.47 | 1.41 |
| 2 | 70-A | 201 | FOL | CB-CA | 2.97 | 1.57 | 1.53 |
| 4 | 89-A | 204 | NAP | C7N-N7N | 2.97 | 1.39 | 1.33 |
| 4 | 53-A | 204 | NAP | C2A-N3A | 2.97 | 1.37 | 1.32 |
| 4 | 138-A | 204 | NAP | C2N-N1N | 2.98 | 1.39 | 1.35 |
| 4 | 42-A | 204 | NAP | C2N-N1N | 2.98 | 1.39 | 1.35 |
| 4 | 109-A | 204 | NAP | O4D-C1D | 2.98 | 1.45 | 1.41 |
| 2 | 160-A | 201 | FOL | C4-C4A | 2.98 | 1.47 | 1.41 |
| 4 | 99-A | 204 | NAP | C2N-N1N | 2.98 | 1.39 | 1.35 |
| 2 | 137-A | 201 | FOL | C4A-C8A | 2.98 | 1.46 | 1.40 |
| 4 | 164-A | 204 | NAP | C2N-N1N | 2.98 | 1.39 | 1.35 |
| 2 | 135-A | 201 | FOL | C4A-C8A | 2.98 | 1.46 | 1.40 |
| 4 | 67-A | 204 | NAP | C2N-N1N | 2.99 | 1.39 | 1.35 |
| 4 | 131-A | 204 | NAP | C7N-N7N | 2.99 | 1.39 | 1.33 |
| 4 | 122-A | 204 | NAP | C2A-N3A | 2.99 | 1.37 | 1.32 |
| 2 | 37-A | 201 | FOL | C4-C4A | 2.99 | 1.47 | 1.41 |
| 2 | 44-A | 201 | FOL | C4-C4A | 2.99 | 1.47 | 1.41 |
| 4 | 75-A | 204 | NAP | C2N-N1N | 2.99 | 1.39 | 1.35 |
| 2 | 25-A | 201 | FOL | C4-C4A | 3.00 | 1.47 | 1.41 |
| 4 | 115-A | 204 | NAP | C2N-N1N | 3.00 | 1.39 | 1.35 |
| 2 | 51-A | 201 | FOL | C4A-C8A | 3.00 | 1.46 | 1.40 |
| 2 | 125-A | 201 | FOL | C4-C4A | 3.00 | 1.47 | 1.41 |
| 4 | 36-A | 204 | NAP | C2N-N1N | 3.00 | 1.39 | 1.35 |
| 2 | 144-A | 201 | FOL | C4-C4A | 3.00 | 1.47 | 1.41 |
| 2 | 47-A | 201 | FOL | C4-C4A | 3.00 | 1.47 | 1.41 |
| 4 | 132-A | 204 | NAP | C7N-N7N | 3.00 | 1.39 | 1.33 |
| 2 | 60-A | 201 | FOL | C4A-C8A | 3.01 | 1.46 | 1.40 |
| 4 | 161-A | 204 | NAP | C2A-N3A | 3.01 | 1.37 | 1.32 |
| 4 | 78-A | 204 | NAP | C2A-N3A | 3.01 | 1.37 | 1.32 |
| 2 | 39-A | 201 | FOL | C4-C4A | 3.01 | 1.47 | 1.41 |
| 4 | 6-A | 204 | NAP | C7N-N7N | 3.01 | 1.39 | 1.33 |
| 2 | 130-A | 201 | FOL | C4-C4A | 3.02 | 1.47 | 1.41 |
| 4 | 33-A | 204 | NAP | C2A-N3A | 3.02 | 1.37 | 1.32 |
| 2 | 141-A | 201 | FOL | C4-C4A | 3.02 | 1.47 | 1.41 |
| 4 | 78-A | 204 | NAP | C7N-N7N | 3.02 | 1.39 | 1.33 |
| 4 | 144-A | 204 | NAP | C2A-N3A | 3.02 | 1.37 | 1.32 |
| 4 | 110-A | 204 | NAP | C7N-N7N | 3.02 | 1.39 | 1.33 |
| 4 | 167-A | 204 | NAP | C2A-N3A | 3.02 | 1.37 | 1.32 |
| 4 | 63-A | 204 | NAP | C2A-N3A | 3.02 | 1.37 | 1.32 |
| 2 | 109-A | 201 | FOL | C4-C4A | 3.02 | 1.47 | 1.41 |
| 4 | 56-A | 204 | NAP | C2A-N3A | 3.02 | 1.37 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 105-A | 204 | NAP | C7N-N7N | 3.02 | 1.39 | 1.33 |
| 4 | 71-A | 204 | NAP | C2N-N1N | 3.02 | 1.39 | 1.35 |
| 4 | 71-A | 204 | NAP | C2A-N3A | 3.02 | 1.37 | 1.32 |
| 2 | 13-A | 201 | FOL | C4-C4A | 3.03 | 1.47 | 1.41 |
| 4 | 160-A | 204 | NAP | C2A-N3A | 3.03 | 1.37 | 1.32 |
| 2 | 164-A | 201 | FOL | C4A-C8A | 3.03 | 1.46 | 1.40 |
| 4 | 98-A | 204 | NAP | C2A-N3A | 3.03 | 1.37 | 1.32 |
| 2 | 27-A | 201 | FOL | C4A-C8A | 3.03 | 1.46 | 1.40 |
| 4 | 33-A | 204 | NAP | C2N-N1N | 3.04 | 1.39 | 1.35 |
| 4 | 146-A | 204 | NAP | C7N-N7N | 3.04 | 1.39 | 1.33 |
| 4 | 27-A | 204 | NAP | C2A-N3A | 3.04 | 1.37 | 1.32 |
| 4 | 126-A | 204 | NAP | C2A-N3A | 3.04 | 1.37 | 1.32 |
| 2 | 77-A | 201 | FOL | C4A-C8A | 3.04 | 1.46 | 1.40 |
| 4 | 79-A | 204 | NAP | C2A-N3A | 3.04 | 1.37 | 1.32 |
| 4 | 25-A | 204 | NAP | C2A-N3A | 3.04 | 1.37 | 1.32 |
| 4 | 96-A | 204 | NAP | C2N-N1N | 3.04 | 1.39 | 1.35 |
| 4 | 49-A | 204 | NAP | C2A-N3A | 3.04 | 1.37 | 1.32 |
| 4 | 15-A | 204 | NAP | C7N-N7N | 3.04 | 1.39 | 1.33 |
| 4 | 146-A | 204 | NAP | C2A-N3A | 3.04 | 1.37 | 1.32 |
| 2 | 99-A | 201 | FOL | C4-C4A | 3.05 | 1.47 | 1.41 |
| 2 | 149-A | 201 | FOL | C4-C4A | 3.05 | 1.47 | 1.41 |
| 4 | 45-A | 204 | NAP | O4D-C1D | 3.05 | 1.45 | 1.41 |
| 4 | 4-A | 204 | NAP | C2A-N3A | 3.05 | 1.37 | 1.32 |
| 2 | 115-A | 201 | FOL | C4-C4A | 3.05 | 1.47 | 1.41 |
| 4 | 22-A | 204 | NAP | C7N-N7N | 3.05 | 1.39 | 1.33 |
| 4 | 107-A | 204 | NAP | C2A-N3A | 3.05 | 1.37 | 1.32 |
| 4 | 147-A | 204 | NAP | C2N-N1N | 3.05 | 1.39 | 1.35 |
| 4 | 109-A | 204 | NAP | C2A-N3A | 3.05 | 1.37 | 1.32 |
| 4 | 58-A | 204 | NAP | C7N-N7N | 3.05 | 1.39 | 1.33 |
| 4 | 150-A | 204 | NAP | C2N-N1N | 3.05 | 1.39 | 1.35 |
| 4 | 112-A | 204 | NAP | C2A-N3A | 3.05 | 1.37 | 1.32 |
| 2 | 100-A | 201 | FOL | C4A-C8A | 3.06 | 1.46 | 1.40 |
| 2 | 118-A | 201 | FOL | C4-C4A | 3.06 | 1.47 | 1.41 |
| 4 | 140-A | 204 | NAP | C2N-N1N | 3.06 | 1.39 | 1.35 |
| 4 | 111-A | 204 | NAP | O4D-C1D | 3.06 | 1.45 | 1.41 |
| 4 | 10-A | 204 | NAP | C7N-N7N | 3.06 | 1.39 | 1.33 |
| 4 | 151-A | 204 | NAP | C7N-N7N | 3.06 | 1.39 | 1.33 |
| 4 | 156-A | 204 | NAP | C2A-N3A | 3.06 | 1.37 | 1.32 |
| 4 | 27-A | 204 | NAP | C7N-N7N | 3.07 | 1.39 | 1.33 |
| 2 | 21-A | 201 | FOL | C4-C4A | 3.07 | 1.47 | 1.41 |
| 2 | 162-A | 201 | FOL | C4A-C8A | 3.07 | 1.46 | 1.40 |
| 4 | 19-A | 204 | NAP | C7N-N7N | 3.07 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 112-A | 204 | NAP | O4D-C1D | 3.07 | 1.45 | 1.41 |
| 4 | 133-A | 204 | NAP | C7N-N7N | 3.07 | 1.39 | 1.33 |
| 4 | 40-A | 204 | NAP | C2N-N1N | 3.07 | 1.39 | 1.35 |
| 4 | 39-A | 204 | NAP | C2A-N3A | 3.07 | 1.37 | 1.32 |
| 2 | 5-A | 201 | FOL | C4-C4A | 3.07 | 1.47 | 1.41 |
| 4 | 114-A | 204 | NAP | C2A-N3A | 3.08 | 1.37 | 1.32 |
| 4 | 89-A | 204 | NAP | C2A-N3A | 3.08 | 1.37 | 1.32 |
| 2 | 167-A | 201 | FOL | C4-C4A | 3.08 | 1.47 | 1.41 |
| 2 | 46-A | 201 | FOL | C4-C4A | 3.08 | 1.47 | 1.41 |
| 2 | 24-A | 201 | FOL | C4A-C8A | 3.08 | 1.46 | 1.40 |
| 4 | 68-A | 204 | NAP | C2N-N1N | 3.08 | 1.39 | 1.35 |
| 2 | 89-A | 201 | FOL | C4A-C8A | 3.08 | 1.46 | 1.40 |
| 4 | 26-A | 204 | NAP | C7N-N7N | 3.08 | 1.39 | 1.33 |
| 4 | 12-A | 204 | NAP | C7N-N7N | 3.08 | 1.39 | 1.33 |
| 4 | 66-A | 204 | NAP | C7N-N7N | 3.08 | 1.39 | 1.33 |
| 2 | 80-A | 201 | FOL | C4-C4A | 3.08 | 1.47 | 1.41 |
| 4 | 129-A | 204 | NAP | C2A-N3A | 3.08 | 1.37 | 1.32 |
| 4 | 52-A | 204 | NAP | C2A-N3A | 3.08 | 1.37 | 1.32 |
| 2 | 67-A | 201 | FOL | C4A-C8A | 3.09 | 1.46 | 1.40 |
| 4 | 134-A | 204 | NAP | C2A-N3A | 3.09 | 1.37 | 1.32 |
| 2 | 92-A | 201 | FOL | C4-C4A | 3.09 | 1.47 | 1.41 |
| 4 | 31-A | 204 | NAP | C2A-N3A | 3.09 | 1.37 | 1.32 |
| 2 | 101-A | 201 | FOL | C4-C4A | 3.09 | 1.47 | 1.41 |
| 4 | 99-A | 204 | NAP | C2A-N3A | 3.09 | 1.37 | 1.32 |
| 2 | 151-A | 201 | FOL | C4-C4A | 3.09 | 1.47 | 1.41 |
| 4 | 62-A | 204 | NAP | C8A-N7A | 3.09 | 1.40 | 1.34 |
| 4 | 159-A | 204 | NAP | C2A-N3A | 3.09 | 1.37 | 1.32 |
| 4 | 23-A | 204 | NAP | C2A-N3A | 3.09 | 1.37 | 1.32 |
| 2 | 26-A | 201 | FOL | C4A-C8A | 3.09 | 1.46 | 1.40 |
| 4 | 145-A | 204 | NAP | C2N-N1N | 3.09 | 1.39 | 1.35 |
| 4 | 69-A | 204 | NAP | C2A-N3A | 3.09 | 1.37 | 1.32 |
| 4 | 22-A | 204 | NAP | C2A-N3A | 3.10 | 1.37 | 1.32 |
| 2 | 9-A | 201 | FOL | C4-C4A | 3.10 | 1.47 | 1.41 |
| 2 | 60-A | 201 | FOL | C4-C4A | 3.10 | 1.47 | 1.41 |
| 4 | 136-A | 204 | NAP | C2A-N3A | 3.10 | 1.37 | 1.32 |
| 2 | 136-A | 201 | FOL | C4-C4A | 3.10 | 1.47 | 1.41 |
| 4 | 30-A | 204 | NAP | C2N-N1N | 3.10 | 1.39 | 1.35 |
| 2 | 164-A | 201 | FOL | C4-C4A | 3.11 | 1.47 | 1.41 |
| 4 | 36-A | 204 | NAP | C7N-N7N | 3.11 | 1.39 | 1.33 |
| 2 | 137-A | 201 | FOL | C4-C4A | 3.11 | 1.47 | 1.41 |
| 4 | 71-A | 204 | NAP | C7N-N7N | 3.11 | 1.39 | 1.33 |
| 4 | 16-A | 204 | NAP | C2A-N3A | 3.11 | 1.37 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 139-A | 204 | NAP | C7N-N7N | 3.11 | 1.39 | 1.33 |
| 4 | 24-A | 204 | NAP | C2A-N3A | 3.11 | 1.37 | 1.32 |
| 4 | 154-A | 204 | NAP | C7N-N7N | 3.11 | 1.39 | 1.33 |
| 2 | 150-A | 201 | FOL | C4-C4A | 3.11 | 1.47 | 1.41 |
| 2 | 43-A | 201 | FOL | C4-C4A | 3.11 | 1.47 | 1.41 |
| 2 | 124-A | 201 | FOL | C4-C4A | 3.11 | 1.47 | 1.41 |
| 4 | 9-A | 204 | NAP | C2A-N3A | 3.11 | 1.37 | 1.32 |
| 4 | 22-A | 204 | NAP | C2N-N1N | 3.12 | 1.39 | 1.35 |
| 4 | 87-A | 204 | NAP | C2A-N3A | 3.12 | 1.37 | 1.32 |
| 2 | 90-A | 201 | FOL | C4-C4A | 3.12 | 1.47 | 1.41 |
| 2 | 12-A | 201 | FOL | C4-C4A | 3.12 | 1.47 | 1.41 |
| 2 | 166-A | 201 | FOL | C4A-C8A | 3.12 | 1.46 | 1.40 |
| 4 | 111-A | 204 | NAP | C7N-N7N | 3.12 | 1.39 | 1.33 |
| 4 | 27-A | 204 | NAP | C2N-N1N | 3.12 | 1.39 | 1.35 |
| 4 | 49-A | 204 | NAP | C2N-N1N | 3.13 | 1.39 | 1.35 |
| 4 | 7-A | 204 | NAP | C7N-N7N | 3.13 | 1.39 | 1.33 |
| 4 | 3-A | 204 | NAP | C2A-N3A | 3.13 | 1.37 | 1.32 |
| 2 | 15-A | 201 | FOL | C4-C4A | 3.14 | 1.47 | 1.41 |
| 4 | 30-A | 204 | NAP | C2A-N3A | 3.14 | 1.37 | 1.32 |
| 4 | 144-A | 204 | NAP | C2N-N1N | 3.14 | 1.39 | 1.35 |
| 2 | 17-A | 201 | FOL | C4A-C8A | 3.14 | 1.46 | 1.40 |
| 4 | 26-A | 204 | NAP | C2N-N1N | 3.14 | 1.39 | 1.35 |
| 4 | 162-A | 204 | NAP | C7N-N7N | 3.14 | 1.39 | 1.33 |
| 4 | 37-A | 204 | NAP | C2A-N3A | 3.14 | 1.37 | 1.32 |
| 2 | 83-A | 201 | FOL | C4A-C8A | 3.14 | 1.46 | 1.40 |
| 4 | 97-A | 204 | NAP | C7N-N7N | 3.15 | 1.39 | 1.33 |
| 2 | 28-A | 201 | FOL | C4A-C8A | 3.15 | 1.46 | 1.40 |
| 4 | 153-A | 204 | NAP | C7N-N7N | 3.15 | 1.39 | 1.33 |
| 2 | 165-A | 201 | FOL | C4-C4A | 3.15 | 1.47 | 1.41 |
| 4 | 35-A | 204 | NAP | C7N-N7N | 3.15 | 1.39 | 1.33 |
| 2 | 62-A | 201 | FOL | C4A-C8A | 3.15 | 1.46 | 1.40 |
| 2 | 27-A | 201 | FOL | C4-C4A | 3.15 | 1.47 | 1.41 |
| 2 | 84-A | 201 | FOL | C8A-N8 | 3.15 | 1.37 | 1.34 |
| 4 | 60-A | 204 | NAP | C2A-N3A | 3.15 | 1.37 | 1.32 |
| 4 | 16-A | 204 | NAP | C2N-N1N | 3.16 | 1.39 | 1.35 |
| 4 | 28-A | 204 | NAP | C2A-N3A | 3.16 | 1.37 | 1.32 |
| 4 | 17-A | 204 | NAP | C7N-N7N | 3.16 | 1.39 | 1.33 |
| 2 | 21-A | 201 | FOL | C4A-C8A | 3.16 | 1.46 | 1.40 |
| 4 | 68-A | 204 | NAP | C7N-N7N | 3.16 | 1.39 | 1.33 |
| 2 | 68-A | 201 | FOL | C4A-C8A | 3.16 | 1.46 | 1.40 |
| 2 | 100-A | 201 | FOL | C4-C4A | 3.16 | 1.47 | 1.41 |
| 4 | 19-A | 204 | NAP | C2N-N1N | 3.16 | 1.39 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 69-A | 204 | NAP | C2N-N1N | 3.16 | 1.39 | 1.35 |
| 2 | 152-A | 201 | FOL | C4-C4A | 3.17 | 1.47 | 1.41 |
| 4 | 107-A | 204 | NAP | C7N-N7N | 3.17 | 1.39 | 1.33 |
| 4 | 91-A | 204 | NAP | C7N-N7N | 3.17 | 1.39 | 1.33 |
| 4 | 116-A | 204 | NAP | C2A-N3A | 3.17 | 1.37 | 1.32 |
| 2 | 111-A | 201 | FOL | C4-C4A | 3.17 | 1.47 | 1.41 |
| 4 | 114-A | 204 | NAP | C2N-N1N | 3.17 | 1.39 | 1.35 |
| 4 | 129-A | 204 | NAP | C7N-N7N | 3.18 | 1.39 | 1.33 |
| 4 | 74-A | 204 | NAP | C7N-N7N | 3.18 | 1.39 | 1.33 |
| 4 | 117-A | 204 | NAP | C2A-N3A | 3.18 | 1.37 | 1.32 |
| 2 | 148-A | 201 | FOL | CB-CA | 3.19 | 1.57 | 1.53 |
| 4 | 94-A | 204 | NAP | C7N-N7N | 3.19 | 1.39 | 1.33 |
| 4 | 93-A | 204 | NAP | C7N-N7N | 3.19 | 1.39 | 1.33 |
| 4 | 100-A | 204 | NAP | C7N-N7N | 3.19 | 1.39 | 1.33 |
| 2 | 64-A | 201 | FOL | C4-C4A | 3.19 | 1.47 | 1.41 |
| 4 | 54-A | 204 | NAP | C7N-N7N | 3.19 | 1.39 | 1.33 |
| 4 | 56-A | 204 | NAP | C7N-N7N | 3.19 | 1.39 | 1.33 |
| 4 | 106-A | 204 | NAP | O4D-C1D | 3.20 | 1.45 | 1.41 |
| 2 | 147-A | 201 | FOL | C4-C4A | 3.20 | 1.47 | 1.41 |
| 4 | 49-A | 204 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 2 | 57-A | 201 | FOL | C4A-C8A | 3.20 | 1.46 | 1.40 |
| 4 | 115-A | 204 | NAP | C2A-N3A | 3.20 | 1.37 | 1.32 |
| 4 | 12-A | 204 | NAP | C2A-N3A | 3.20 | 1.37 | 1.32 |
| 2 | 121-A | 201 | FOL | C4-C4A | 3.20 | 1.47 | 1.41 |
| 2 | 126-A | 201 | FOL | C4-C4A | 3.20 | 1.47 | 1.41 |
| 4 | 160-A | 204 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 4 | 24-A | 204 | NAP | C7N-N7N | 3.20 | 1.39 | 1.33 |
| 4 | 102-A | 204 | NAP | C2A-N3A | 3.20 | 1.37 | 1.32 |
| 4 | 70-A | 204 | NAP | C2N-N1N | 3.20 | 1.39 | 1.35 |
| 4 | 77-A | 204 | NAP | C7N-N7N | 3.21 | 1.39 | 1.33 |
| 4 | 72-A | 204 | NAP | C2N-N1N | 3.21 | 1.39 | 1.35 |
| 2 | 155-A | 201 | FOL | C4A-C8A | 3.21 | 1.46 | 1.40 |
| 4 | 65-A | 204 | NAP | C2A-N3A | 3.21 | 1.37 | 1.32 |
| 4 | 25-A | 204 | NAP | C2N-N1N | 3.21 | 1.39 | 1.35 |
| 4 | 111-A | 204 | NAP | C2A-N3A | 3.21 | 1.37 | 1.32 |
| 4 | 20-A | 204 | NAP | C7N-N7N | 3.21 | 1.39 | 1.33 |
| 4 | 43-A | 204 | NAP | O4D-C1D | 3.21 | 1.45 | 1.41 |
| 4 | 166-A | 204 | NAP | C7N-N7N | 3.21 | 1.39 | 1.33 |
| 4 | 104-A | 204 | NAP | C2A-N3A | 3.21 | 1.37 | 1.32 |
| 4 | 165-A | 204 | NAP | C7N-N7N | 3.22 | 1.39 | 1.33 |
| 4 | 16-A | 204 | NAP | C7N-N7N | 3.22 | 1.39 | 1.33 |
| 4 | 21-A | 204 | NAP | C7N-N7N | 3.22 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 106-A | 204 | NAP | C7N-N7N | 3.22 | 1.39 | 1.33 |
| 4 | 81-A | 204 | NAP | C7N-N7N | 3.22 | 1.39 | 1.33 |
| 4 | 29-A | 204 | NAP | C2N-N1N | 3.22 | 1.39 | 1.35 |
| 4 | 24-A | 204 | NAP | C2N-N1N | 3.22 | 1.39 | 1.35 |
| 2 | 80-A | 201 | FOL | C4A-C8A | 3.22 | 1.46 | 1.40 |
| 4 | 28-A | 204 | NAP | C7N-N7N | 3.23 | 1.39 | 1.33 |
| 4 | 141-A | 204 | NAP | C2A-N3A | 3.23 | 1.37 | 1.32 |
| 2 | 154-A | 201 | FOL | C4-C4A | 3.23 | 1.47 | 1.41 |
| 4 | 41-A | 204 | NAP | C2N-N1N | 3.23 | 1.39 | 1.35 |
| 4 | 96-A | 204 | NAP | C7N-N7N | 3.23 | 1.39 | 1.33 |
| 4 | 41-A | 204 | NAP | C2A-N3A | 3.23 | 1.37 | 1.32 |
| 4 | 20-A | 204 | NAP | C2A-N3A | 3.23 | 1.37 | 1.32 |
| 2 | 65-A | 201 | FOL | C4-C4A | 3.23 | 1.47 | 1.41 |
| 2 | 135-A | 201 | FOL | C4-C4A | 3.23 | 1.47 | 1.41 |
| 4 | 23-A | 204 | NAP | C7N-N7N | 3.24 | 1.39 | 1.33 |
| 4 | 103-A | 204 | NAP | C2A-N3A | 3.24 | 1.37 | 1.32 |
| 2 | 76-A | 201 | FOL | C4A-C8A | 3.24 | 1.46 | 1.40 |
| 4 | 8-A | 204 | NAP | C2N-N1N | 3.24 | 1.39 | 1.35 |
| 4 | 21-A | 204 | NAP | C2N-N1N | 3.24 | 1.39 | 1.35 |
| 4 | 13-A | 204 | NAP | C2A-N3A | 3.24 | 1.37 | 1.32 |
| 4 | 82-A | 204 | NAP | C7N-N7N | 3.24 | 1.39 | 1.33 |
| 4 | 6-A | 204 | NAP | C2A-N3A | 3.24 | 1.37 | 1.32 |
| 4 | 20-A | 204 | NAP | C2N-N1N | 3.25 | 1.39 | 1.35 |
| 4 | 37-A | 204 | NAP | C7N-N7N | 3.25 | 1.39 | 1.33 |
| 4 | 94-A | 204 | NAP | C2A-N3A | 3.25 | 1.37 | 1.32 |
| 4 | 141-A | 204 | NAP | C7N-N7N | 3.25 | 1.39 | 1.33 |
| 2 | 129-A | 201 | FOL | C4-C4A | 3.25 | 1.47 | 1.41 |
| 2 | 98-A | 201 | FOL | C4-C4A | 3.25 | 1.47 | 1.41 |
| 4 | 63-A | 204 | NAP | C7N-N7N | 3.25 | 1.39 | 1.33 |
| 4 | 167-A | 204 | NAP | C2N-N1N | 3.26 | 1.39 | 1.35 |
| 4 | 146-A | 204 | NAP | C2N-N1N | 3.26 | 1.39 | 1.35 |
| 4 | 41-A | 204 | NAP | C7N-N7N | 3.26 | 1.39 | 1.33 |
| 4 | 83-A | 204 | NAP | C7N-N7N | 3.26 | 1.39 | 1.33 |
| 2 | 56-A | 201 | FOL | C4-C4A | 3.26 | 1.47 | 1.41 |
| 4 | 13-A | 204 | NAP | C7N-N7N | 3.26 | 1.39 | 1.33 |
| 4 | 31-A | 204 | NAP | C2N-N1N | 3.26 | 1.39 | 1.35 |
| 4 | 126-A | 204 | NAP | C7N-N7N | 3.26 | 1.39 | 1.33 |
| 2 | 122-A | 201 | FOL | C4-C4A | 3.26 | 1.47 | 1.41 |
| 4 | 143-A | 204 | NAP | C2A-N3A | 3.27 | 1.37 | 1.32 |
| 2 | 59-A | 201 | FOL | C4-C4A | 3.27 | 1.47 | 1.41 |
| 4 | 147-A | 204 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 4 | 105-A | 204 | NAP | C2A-N3A | 3.27 | 1.37 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 94-A | 201 | FOL | C4-C4A | 3.27 | 1.47 | 1.41 |
| 4 | 57-A | 204 | NAP | C7N-N7N | 3.28 | 1.39 | 1.33 |
| 2 | 42-A | 201 | FOL | C4-C4A | 3.28 | 1.47 | 1.41 |
| 4 | 99-A | 204 | NAP | C7N-N7N | 3.28 | 1.39 | 1.33 |
| 4 | 46-A | 204 | NAP | C2A-N3A | 3.28 | 1.38 | 1.32 |
| 2 | 76-A | 201 | FOL | C4-C4A | 3.28 | 1.47 | 1.41 |
| 4 | 95-A | 204 | NAP | C7N-N7N | 3.28 | 1.39 | 1.33 |
| 4 | 105-A | 204 | NAP | O4D-C1D | 3.29 | 1.45 | 1.41 |
| 4 | 155-A | 204 | NAP | C7N-N7N | 3.29 | 1.39 | 1.33 |
| 4 | 58-A | 204 | NAP | C2A-N3A | 3.29 | 1.38 | 1.32 |
| 2 | 6-A | 201 | FOL | C4-C4A | 3.29 | 1.48 | 1.41 |
| 4 | 134-A | 204 | NAP | C7N-N7N | 3.29 | 1.39 | 1.33 |
| 4 | 100-A | 204 | NAP | C2A-N3A | 3.29 | 1.38 | 1.32 |
| 2 | 30-A | 201 | FOL | C4A-C8A | 3.29 | 1.46 | 1.40 |
| 4 | 76-A | 204 | NAP | C2A-N3A | 3.30 | 1.38 | 1.32 |
| 4 | 88-A | 204 | NAP | C7N-N7N | 3.30 | 1.39 | 1.33 |
| 4 | 92-A | 204 | NAP | C7N-N7N | 3.30 | 1.39 | 1.33 |
| 4 | 51-A | 204 | NAP | C7N-N7N | 3.30 | 1.39 | 1.33 |
| 4 | 51-A | 204 | NAP | C2A-N3A | 3.31 | 1.38 | 1.32 |
| 4 | 14-A | 204 | NAP | C7N-N7N | 3.31 | 1.39 | 1.33 |
| 4 | 123-A | 204 | NAP | C7N-N7N | 3.31 | 1.39 | 1.33 |
| 4 | 128-A | 204 | NAP | C7N-N7N | 3.31 | 1.39 | 1.33 |
| 2 | 114-A | 201 | FOL | C4-C4A | 3.31 | 1.48 | 1.41 |
| 2 | 119-A | 201 | FOL | C4-C4A | 3.32 | 1.48 | 1.41 |
| 4 | 139-A | 204 | NAP | C2N-N1N | 3.32 | 1.39 | 1.35 |
| 4 | 84-A | 204 | NAP | C2A-N3A | 3.32 | 1.38 | 1.32 |
| 4 | 79-A | 204 | NAP | C7N-N7N | 3.33 | 1.39 | 1.33 |
| 4 | 108-A | 204 | NAP | C2A-N3A | 3.33 | 1.38 | 1.32 |
| 4 | 115-A | 204 | NAP | C7N-N7N | 3.33 | 1.39 | 1.33 |
| 2 | 53-A | 201 | FOL | C4A-C8A | 3.33 | 1.47 | 1.40 |
| 2 | 104-A | 201 | FOL | C8A-N8 | 3.33 | 1.37 | 1.34 |
| 4 | 127-A | 204 | NAP | C7N-N7N | 3.33 | 1.39 | 1.33 |
| 4 | 68-A | 204 | NAP | C2A-N3A | 3.33 | 1.38 | 1.32 |
| 2 | 89-A | 201 | FOL | C4-C4A | 3.34 | 1.48 | 1.41 |
| 4 | 65-A | 204 | NAP | C7N-N7N | 3.34 | 1.39 | 1.33 |
| 2 | 28-A | 201 | FOL | C4-C4A | 3.34 | 1.48 | 1.41 |
| 4 | 1-A | 204 | NAP | C2A-N3A | 3.34 | 1.38 | 1.32 |
| 2 | 53-A | 201 | FOL | C4-C4A | 3.35 | 1.48 | 1.41 |
| 4 | 112-A | 204 | NAP | C7N-N7N | 3.35 | 1.39 | 1.33 |
| 4 | 124-A | 204 | NAP | C7N-N7N | 3.36 | 1.39 | 1.33 |
| 4 | 84-A | 204 | NAP | C7N-N7N | 3.36 | 1.39 | 1.33 |
| 4 | 50-A | 204 | NAP | C2A-N3A | 3.36 | 1.38 | 1.32 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 117-A | 204 | NAP | C7N-N7N | 3.37 | 1.39 | 1.33 |
| 4 | 118-A | 204 | NAP | C7N-N7N | 3.37 | 1.39 | 1.33 |
| 2 | 166-A | 201 | FOL | C4-C4A | 3.37 | 1.48 | 1.41 |
| 4 | 75-A | 204 | NAP | C7N-N7N | 3.38 | 1.39 | 1.33 |
| 4 | 86-A | 204 | NAP | C7N-N7N | 3.38 | 1.39 | 1.33 |
| 4 | 145-A | 204 | NAP | C7N-N7N | 3.38 | 1.39 | 1.33 |
| 4 | 118-A | 204 | NAP | C2A-N3A | 3.39 | 1.38 | 1.32 |
| 4 | 148-A | 204 | NAP | C7N-N7N | 3.39 | 1.39 | 1.33 |
| 4 | 73-A | 204 | NAP | C7N-N7N | 3.39 | 1.39 | 1.33 |
| 2 | 127-A | 201 | FOL | C4-C4A | 3.39 | 1.48 | 1.41 |
| 4 | 161-A | 204 | NAP | C7N-N7N | 3.39 | 1.39 | 1.33 |
| 4 | 53-A | 204 | NAP | C7N-N7N | 3.40 | 1.39 | 1.33 |
| 4 | 103-A | 204 | NAP | C7N-N7N | 3.40 | 1.39 | 1.33 |
| 4 | 1-A | 204 | NAP | C7N-N7N | 3.40 | 1.39 | 1.33 |
| 4 | 114-A | 204 | NAP | C7N-N7N | 3.40 | 1.39 | 1.33 |
| 4 | 97-A | 204 | NAP | C2A-N3A | 3.41 | 1.38 | 1.32 |
| 4 | 80-A | 204 | NAP | C7N-N7N | 3.41 | 1.39 | 1.33 |
| 4 | 19-A | 204 | NAP | C2A-N3A | 3.41 | 1.38 | 1.32 |
| 4 | 44-A | 204 | NAP | C2A-N3A | 3.41 | 1.38 | 1.32 |
| 4 | 18-A | 204 | NAP | C2N-N1N | 3.41 | 1.39 | 1.35 |
| 4 | 122-A | 204 | NAP | C7N-N7N | 3.41 | 1.39 | 1.33 |
| 4 | 167-A | 204 | NAP | C7N-N7N | 3.42 | 1.39 | 1.33 |
| 4 | 80-A | 204 | NAP | C2A-N3A | 3.42 | 1.38 | 1.32 |
| 4 | 121-A | 204 | NAP | C7N-N7N | 3.42 | 1.39 | 1.33 |
| 4 | 67-A | 204 | NAP | C7N-N7N | 3.42 | 1.39 | 1.33 |
| 4 | 72-A | 204 | NAP | C7N-N7N | 3.42 | 1.39 | 1.33 |
| 4 | 2-A | 204 | NAP | C7N-N7N | 3.43 | 1.39 | 1.33 |
| 4 | 66-A | 204 | NAP | C2A-N3A | 3.43 | 1.38 | 1.32 |
| 4 | 144-A | 204 | NAP | C7N-N7N | 3.43 | 1.39 | 1.33 |
| 4 | 76-A | 204 | NAP | C7N-N7N | 3.44 | 1.39 | 1.33 |
| 2 | 40-A | 201 | FOL | C4-C4A | 3.44 | 1.48 | 1.41 |
| 4 | 110-A | 204 | NAP | C2A-N3A | 3.45 | 1.38 | 1.32 |
| 4 | 7-A | 204 | NAP | C2A-N3A | 3.45 | 1.38 | 1.32 |
| 4 | 64-A | 204 | NAP | C7N-N7N | 3.45 | 1.40 | 1.33 |
| 4 | 50-A | 204 | NAP | C7N-N7N | 3.45 | 1.40 | 1.33 |
| 4 | 120-A | 204 | NAP | C7N-N7N | 3.46 | 1.40 | 1.33 |
| 4 | 45-A | 204 | NAP | C7N-N7N | 3.46 | 1.40 | 1.33 |
| 2 | 120-A | 201 | FOL | C4-C4A | 3.46 | 1.48 | 1.41 |
| 2 | 65-A | 201 | FOL | C4A-C8A | 3.46 | 1.47 | 1.40 |
| 4 | 4-A | 204 | NAP | C7N-N7N | 3.47 | 1.40 | 1.33 |
| 4 | 156-A | 204 | NAP | C7N-N7N | 3.47 | 1.40 | 1.33 |
| 4 | 104-A | 204 | NAP | C7N-N7N | 3.47 | 1.40 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 38-A | 204 | NAP | C7N-N7N | 3.47 | 1.40 | 1.33 |
| 4 | 140-A | 204 | NAP | C7N-N7N | 3.48 | 1.40 | 1.33 |
| 4 | 48-A | 204 | NAP | C7N-N7N | 3.48 | 1.40 | 1.33 |
| 4 | 47-A | 204 | NAP | C2A-N3A | 3.48 | 1.38 | 1.32 |
| 4 | 69-A | 204 | NAP | C7N-N7N | 3.48 | 1.40 | 1.33 |
| 4 | 48-A | 204 | NAP | C2A-N3A | 3.48 | 1.38 | 1.32 |
| 4 | 98-A | 204 | NAP | C7N-N7N | 3.48 | 1.40 | 1.33 |
| 4 | 143-A | 204 | NAP | C7N-N7N | 3.49 | 1.40 | 1.33 |
| 4 | 47-A | 204 | NAP | C7N-N7N | 3.50 | 1.40 | 1.33 |
| 4 | 142-A | 204 | NAP | C7N-N7N | 3.51 | 1.40 | 1.33 |
| 2 | 105-A | 201 | FOL | C4A-C8A | 3.51 | 1.47 | 1.40 |
| 4 | 106-A | 204 | NAP | C2A-N3A | 3.52 | 1.38 | 1.32 |
| 4 | 119-A | 204 | NAP | C7N-N7N | 3.52 | 1.40 | 1.33 |
| 4 | 44-A | 204 | NAP | C7N-N7N | 3.52 | 1.40 | 1.33 |
| 4 | 149-A | 204 | NAP | C7N-N7N | 3.53 | 1.40 | 1.33 |
| 4 | 152-A | 204 | NAP | C7N-N7N | 3.53 | 1.40 | 1.33 |
| 2 | 81-A | 201 | FOL | CB-CA | 3.53 | 1.58 | 1.53 |
| 4 | 30-A | 204 | NAP | C7N-N7N | 3.55 | 1.40 | 1.33 |
| 4 | 85-A | 204 | NAP | C7N-N7N | 3.56 | 1.40 | 1.33 |
| 4 | 29-A | 204 | NAP | C7N-N7N | 3.56 | 1.40 | 1.33 |
| 4 | 116-A | 204 | NAP | C7N-N7N | 3.57 | 1.40 | 1.33 |
| 2 | 82-A | 201 | FOL | CB-CA | 3.58 | 1.58 | 1.53 |
| 4 | 62-A | 204 | NAP | C7N-N7N | 3.58 | 1.40 | 1.33 |
| 4 | 39-A | 204 | NAP | C7N-N7N | 3.58 | 1.40 | 1.33 |
| 4 | 55-A | 204 | NAP | C7N-N7N | 3.59 | 1.40 | 1.33 |
| 4 | 87-A | 204 | NAP | C7N-N7N | 3.60 | 1.40 | 1.33 |
| 4 | 125-A | 204 | NAP | C7N-N7N | 3.61 | 1.40 | 1.33 |
| 4 | 46-A | 204 | NAP | C7N-N7N | 3.61 | 1.40 | 1.33 |
| 4 | 130-A | 204 | NAP | C7N-N7N | 3.61 | 1.40 | 1.33 |
| 4 | 113-A | 204 | NAP | C7N-N7N | 3.61 | 1.40 | 1.33 |
| 4 | 42-A | 204 | NAP | C7N-N7N | 3.62 | 1.40 | 1.33 |
| 4 | 70-A | 204 | NAP | C7N-N7N | 3.63 | 1.40 | 1.33 |
| 2 | 48-A | 201 | FOL | C4-C4A | 3.64 | 1.48 | 1.41 |
| 4 | 90-A | 204 | NAP | C7N-N7N | 3.66 | 1.40 | 1.33 |
| 4 | 52-A | 204 | NAP | C7N-N7N | 3.66 | 1.40 | 1.33 |
| 4 | 61-A | 204 | NAP | C7N-N7N | 3.66 | 1.40 | 1.33 |
| 2 | 26-A | 201 | FOL | C4-C4A | 3.67 | 1.48 | 1.41 |
| 4 | 5-A | 204 | NAP | C7N-N7N | 3.68 | 1.40 | 1.33 |
| 2 | 13-A | 201 | FOL | CB-CA | 3.68 | 1.58 | 1.53 |
| 4 | 60-A | 204 | NAP | C7N-N7N | 3.70 | 1.40 | 1.33 |
| 4 | 35-A | 204 | NAP | C2N-N1N | 3.70 | 1.40 | 1.35 |
| 2 | 30-A | 201 | FOL | C4-C4A | 3.71 | 1.48 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 4 | 40-A | 204 | NAP | C7N-N7N | 3.79 | 1.40 | 1.33 |
| 4 | 43-A | 204 | NAP | C7N-N7N | 3.79 | 1.40 | 1.33 |
| 4 | 138-A | 204 | NAP | C7N-N7N | 3.81 | 1.40 | 1.33 |
| 4 | 3-A | 204 | NAP | C7N-N7N | 3.82 | 1.40 | 1.33 |
| 4 | 102-A | 204 | NAP | C7N-N7N | 3.87 | 1.40 | 1.33 |
| 4 | 135-A | 204 | NAP | C7N-N7N | 3.88 | 1.40 | 1.33 |
| 4 | 137-A | 204 | NAP | C7N-N7N | 3.96 | 1.41 | 1.33 |
| 4 | 136-A | 204 | NAP | C7N-N7N | 4.00 | 1.41 | 1.33 |

All (2601) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 4 | 118-A | 204 | NAP | O2N-PN-O3 | -11.07 | 57.84 | 105.27 |
| 4 | 57-A | 204 | NAP | O2N-PN-O3 | -10.58 | 59.95 | 105.27 |
| 4 | 56-A | 204 | NAP | O2N-PN-O3 | -9.07 | 66.38 | 105.27 |
| 2 | 156-A | 201 | FOL | CB-CA-N | -7.64 | 97.99 | 109.92 |
| 2 | 133-A | 201 | FOL | C4A-C4-N3 | -7.58 | 113.61 | 123.52 |
| 2 | 76-A | 201 | FOL | C4A-C4-N3 | -7.23 | 114.07 | 123.52 |
| 2 | 8-A | 201 | FOL | C4A-C4-N3 | -7.06 | 114.29 | 123.52 |
| 2 | 56-A | 201 | FOL | C4A-C4-N3 | -6.98 | 114.40 | 123.52 |
| 2 | 53-A | 201 | FOL | C4A-C4-N3 | -6.92 | 114.47 | 123.52 |
| 2 | 13-A | 201 | FOL | C4A-C4-N3 | -6.83 | 114.59 | 123.52 |
| 2 | 77-A | 201 | FOL | CB-CA-N | -6.79 | 99.32 | 109.92 |
| 2 | 98-A | 201 | FOL | C4A-C4-N3 | -6.77 | 114.68 | 123.52 |
| 4 | 118-A | 204 | NAP | O2N-PN-O5D | -6.63 | 76.64 | 108.24 |
| 2 | 154-A | 201 | FOL | C4A-C4-N3 | -6.61 | 114.88 | 123.52 |
| 2 | 160-A | 201 | FOL | C4A-C4-N3 | -6.57 | 114.93 | 123.52 |
| 2 | 111-A | 201 | FOL | C4A-C4-N3 | -6.54 | 114.97 | 123.52 |
| 2 | 136-A | 201 | FOL | C4A-C4-N3 | -6.49 | 115.04 | 123.52 |
| 2 | 167-A | 201 | FOL | C4A-C4-N3 | -6.42 | 115.12 | 123.52 |
| 2 | 51-A | 201 | FOL | C4A-C4-N3 | -6.40 | 115.16 | 123.52 |
| 2 | 134-A | 201 | FOL | C4A-C4-N3 | -6.38 | 115.18 | 123.52 |
| 2 | 164-A | 201 | FOL | C4A-C4-N3 | -6.36 | 115.21 | 123.52 |
| 2 | 151-A | 201 | FOL | C4A-C4-N3 | -6.35 | 115.22 | 123.52 |
| 2 | 107-A | 201 | FOL | C4A-C4-N3 | -6.33 | 115.24 | 123.52 |
| 2 | 126-A | 201 | FOL | C4A-C4-N3 | -6.31 | 115.27 | 123.52 |
| 2 | 6-A | 201 | FOL | C4A-C4-N3 | -6.20 | 115.42 | 123.52 |
| 2 | 27-A | 201 | FOL | C4A-C4-N3 | -6.19 | 115.43 | 123.52 |
| 2 | 138-A | 201 | FOL | CT-CA-N | -6.17 | 100.62 | 112.93 |
| 2 | 110-A | 201 | FOL | C4A-C4-N3 | -6.17 | 115.46 | 123.52 |
| 2 | 125-A | 201 | FOL | C4A-C4-N3 | -6.15 | 115.48 | 123.52 |
| 2 | 28-A | 201 | FOL | C4A-C4-N3 | -6.10 | 115.55 | 123.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | 105-A | 201 | FOL | C4A-C4-N3 | -6.09 | 115.56 | 123.52 |
| 2 | 113-A | 201 | FOL | C4A-C4-N3 | -6.08 | 115.58 | 123.52 |
| 2 | 77-A | 201 | FOL | C4A-C4-N3 | -6.06 | 115.60 | 123.52 |
| 2 | 15-A | 201 | FOL | C4A-C4-N3 | -6.05 | 115.61 | 123.52 |
| 2 | 44-A | 201 | FOL | C4A-C4-N3 | -6.04 | 115.63 | 123.52 |
| 4 | 56-A | 204 | NAP | O2N-PN-O5D | -6.02 | 79.54 | 108.24 |
| 2 | 19-A | 201 | FOL | C4A-C4-N3 | -6.01 | 115.67 | 123.52 |
| 2 | 118-A | 201 | FOL | C4A-C4-N3 | -6.00 | 115.68 | 123.52 |
| 2 | 36-A | 201 | FOL | C4A-C4-N3 | -5.99 | 115.69 | 123.52 |
| 2 | 7-A | 201 | FOL | C4A-C4-N3 | -5.97 | 115.71 | 123.52 |
| 2 | 83-A | 201 | FOL | C4A-C4-N3 | -5.97 | 115.72 | 123.52 |
| 2 | 143-A | 201 | FOL | C4A-C4-N3 | -5.94 | 115.76 | 123.52 |
| 2 | 121-A | 201 | FOL | C4A-C4-N3 | -5.93 | 115.77 | 123.52 |
| 2 | 119-A | 201 | FOL | C4A-C4-N3 | -5.92 | 115.78 | 123.52 |
| 2 | 66-A | 201 | FOL | C4A-C4-N3 | -5.91 | 115.80 | 123.52 |
| 2 | 4-A | 201 | FOL | C4A-C4-N3 | -5.88 | 115.83 | 123.52 |
| 2 | 115-A | 201 | FOL | C4A-C4-N3 | -5.88 | 115.83 | 123.52 |
| 2 | 123-A | 201 | FOL | C4A-C4-N3 | -5.84 | 115.89 | 123.52 |
| 2 | 57-A | 201 | FOL | C4A-C4-N3 | -5.83 | 115.90 | 123.52 |
| 4 | 57-A | 204 | NAP | O2N-PN-O5D | -5.82 | 80.48 | 108.24 |
| 2 | 68-A | 201 | FOL | C4A-C4-N3 | -5.81 | 115.92 | 123.52 |
| 2 | 74-A | 201 | FOL | C4A-C4-N3 | -5.81 | 115.93 | 123.52 |
| 2 | 54-A | 201 | FOL | C4A-C4-N3 | -5.79 | 115.95 | 123.52 |
| 2 | 155-A | 201 | FOL | C4A-C4-N3 | -5.79 | 115.95 | 123.52 |
| 2 | 165-A | 201 | FOL | CT-CA-N | -5.78 | 101.39 | 112.93 |
| 2 | 42-A | 201 | FOL | C4A-C4-N3 | -5.76 | 115.99 | 123.52 |
| 2 | 14-A | 201 | FOL | C4A-C4-N3 | -5.76 | 116.00 | 123.52 |
| 2 | 67-A | 201 | FOL | C4A-C4-N3 | -5.74 | 116.01 | 123.52 |
| 2 | 69-A | 201 | FOL | C4A-C4-N3 | -5.74 | 116.01 | 123.52 |
| 2 | 112-A | 201 | FOL | C4A-C4-N3 | -5.74 | 116.03 | 123.52 |
| 2 | 146-A | 201 | FOL | C4A-C4-N3 | -5.74 | 116.03 | 123.52 |
| 2 | 152-A | 201 | FOL | C4A-C4-N3 | -5.71 | 116.06 | 123.52 |
| 2 | 100-A | 201 | FOL | C4A-C4-N3 | -5.67 | 116.11 | 123.52 |
| 2 | 163-A | 201 | FOL | C4A-C4-N3 | -5.66 | 116.12 | 123.52 |
| 2 | 55-A | 201 | FOL | C4A-C4-N3 | -5.64 | 116.16 | 123.52 |
| 2 | 148-A | 201 | FOL | C4A-C4-N3 | -5.62 | 116.17 | 123.52 |
| 2 | 25-A | 201 | FOL | C4A-C4-N3 | -5.62 | 116.18 | 123.52 |
| 2 | 145-A | 201 | FOL | C4A-C4-N3 | -5.61 | 116.19 | 123.52 |
| 2 | 72-A | 201 | FOL | C4A-C4-N3 | -5.60 | 116.20 | 123.52 |
| 2 | 50-A | 201 | FOL | C4A-C4-N3 | -5.60 | 116.20 | 123.52 |
| 2 | 108-A | 201 | FOL | C4A-C4-N3 | -5.57 | 116.23 | 123.52 |
| 2 | 38-A | 201 | FOL | C4A-C4-N3 | -5.57 | 116.24 | 123.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 18-A | 201 | FOL | C4A-C4-N3 | -5.56 | 116.25 | 123.52 |
| 2 | 49-A | 201 | FOL | C4A-C4-N3 | -5.55 | 116.26 | 123.52 |
| 2 | 61-A | 201 | FOL | C4A-C4-N3 | -5.55 | 116.27 | 123.52 |
| 4 | 119-A | 204 | NAP | C1B-N9A-C4A | -5.53 | 120.64 | 126.81 |
| 4 | 119-A | 204 | NAP | O2N-PN-O3 | -5.52 | 81.63 | 105.27 |
| 2 | 99-A | 201 | FOL | C4A-C4-N3 | -5.51 | 116.31 | 123.52 |
| 2 | 22-A | 201 | FOL | C4A-C4-N3 | -5.51 | 116.31 | 123.52 |
| 2 | 130-A | 201 | FOL | C4A-C4-N3 | -5.51 | 116.31 | 123.52 |
| 2 | 128-A | 201 | FOL | C4A-C4-N3 | -5.51 | 116.32 | 123.52 |
| 2 | 62-A | 201 | FOL | C4A-C4-N3 | -5.50 | 116.33 | 123.52 |
| 2 | 132-A | 201 | FOL | C4A-C4-N3 | -5.48 | 116.36 | 123.52 |
| 2 | 41-A | 201 | FOL | C4A-C4-N3 | -5.47 | 116.37 | 123.52 |
| 2 | 104-A | 201 | FOL | C4A-C4-N3 | -5.47 | 116.37 | 123.52 |
| 2 | 47-A | 201 | FOL | C4A-C4-N3 | -5.47 | 116.38 | 123.52 |
| 2 | 63-A | 201 | FOL | C4A-C4-N3 | -5.46 | 116.38 | 123.52 |
| 2 | 109-A | 201 | FOL | C4A-C4-N3 | -5.46 | 116.39 | 123.52 |
| 2 | 29-A | 201 | FOL | C4A-C4-N3 | -5.44 | 116.41 | 123.52 |
| 2 | 60-A | 201 | FOL | C4A-C4-N3 | -5.44 | 116.42 | 123.52 |
| 2 | 79-A | 201 | FOL | C4A-C4-N3 | -5.43 | 116.42 | 123.52 |
| 2 | 166-A | 201 | FOL | C4A-C4-N3 | -5.43 | 116.42 | 123.52 |
| 2 | 150-A | 201 | FOL | C4A-C4-N3 | -5.43 | 116.42 | 123.52 |
| 2 | 117-A | 201 | FOL | C4A-C4-N3 | -5.43 | 116.43 | 123.52 |
| 2 | 75-A | 201 | FOL | C4A-C4-N3 | -5.41 | 116.44 | 123.52 |
| 2 | 135-A | 201 | FOL | C4A-C4-N3 | -5.41 | 116.45 | 123.52 |
| 2 | 78-A | 201 | FOL | C4A-C4-N3 | -5.40 | 116.46 | 123.52 |
| 2 | 124-A | 201 | FOL | C4A-C4-N3 | -5.40 | 116.46 | 123.52 |
| 2 | 103-A | 201 | FOL | C4A-C4-N3 | -5.40 | 116.46 | 123.52 |
| 2 | 97-A | 201 | FOL | C4A-C4-N3 | -5.39 | 116.47 | 123.52 |
| 2 | 100-A | 201 | FOL | CB-CA-N | -5.39 | 101.51 | 109.92 |
| 2 | 122-A | 201 | FOL | C4A-C4-N3 | -5.38 | 116.49 | 123.52 |
| 2 | 1-A | 201 | FOL | C4A-C4-N3 | -5.38 | 116.49 | 123.52 |
| 2 | 70-A | 201 | FOL | C4A-C4-N3 | -5.37 | 116.51 | 123.52 |
| 2 | 84-A | 201 | FOL | C4A-C4-N3 | -5.35 | 116.52 | 123.52 |
| 2 | 156-A | 201 | FOL | C4A-C4-N3 | -5.35 | 116.53 | 123.52 |
| 2 | 129-A | 201 | FOL | C4A-C4-N3 | -5.35 | 116.53 | 123.52 |
| 2 | 39-A | 201 | FOL | CT-CA-N | -5.35 | 102.26 | 112.93 |
| 2 | 71-A | 201 | FOL | C4A-C4-N3 | -5.32 | 116.56 | 123.52 |
| 2 | 39-A | 201 | FOL | C4A-C4-N3 | -5.30 | 116.59 | 123.52 |
| 2 | 26-A | 201 | FOL | C4A-C4-N3 | -5.30 | 116.59 | 123.52 |
| 2 | 11-A | 201 | FOL | C4A-C4-N3 | -5.28 | 116.62 | 123.52 |
| 2 | 45-A | 201 | FOL | C4A-C4-N3 | -5.27 | 116.63 | 123.52 |
| 2 | 82-A | 201 | FOL | C4A-C4-N3 | -5.26 | 116.64 | 123.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | 161-A | 201 | FOL | C4A-C4-N3 | -5.21 | 116.71 | 123.52 |
| 2 | 31-A | 201 | FOL | C4A-C4-N3 | -5.20 | 116.72 | 123.52 |
| 2 | 88-A | 201 | FOL | C4A-C4-N3 | -5.19 | 116.74 | 123.52 |
| 2 | 85-A | 201 | FOL | C4A-C4-N3 | -5.18 | 116.76 | 123.52 |
| 2 | 141-A | 201 | FOL | C4A-C4-N3 | -5.16 | 116.77 | 123.52 |
| 2 | 106-A | 201 | FOL | C4A-C4-N3 | -5.15 | 116.79 | 123.52 |
| 2 | 144-A | 201 | FOL | C4A-C4-N3 | -5.15 | 116.79 | 123.52 |
| 2 | 32-A | 201 | FOL | C4A-C4-N3 | -5.14 | 116.80 | 123.52 |
| 2 | 65-A | 201 | FOL | C4A-C4-N3 | -5.13 | 116.81 | 123.52 |
| 2 | 116-A | 201 | FOL | C4A-C4-N3 | -5.13 | 116.81 | 123.52 |
| 2 | 37-A | 201 | FOL | C4A-C4-N3 | -5.12 | 116.83 | 123.52 |
| 2 | 93-A | 201 | FOL | C4A-C4-N3 | -5.08 | 116.88 | 123.52 |
| 2 | 91-A | 201 | FOL | C4A-C4-N3 | -5.07 | 116.90 | 123.52 |
| 2 | 46-A | 201 | FOL | C4A-C4-N3 | -5.05 | 116.92 | 123.52 |
| 2 | 40-A | 201 | FOL | C4A-C4-N3 | -5.05 | 116.92 | 123.52 |
| 2 | 80-A | 201 | FOL | NA2-C2-N3 | -5.05 | 113.83 | 120.29 |
| 2 | 94-A | 201 | FOL | C4A-C4-N3 | -5.05 | 116.93 | 123.52 |
| 2 | 58-A | 201 | FOL | C4A-C4-N3 | -5.02 | 116.96 | 123.52 |
| 2 | 59-A | 201 | FOL | C4A-C4-N3 | -5.01 | 116.97 | 123.52 |
| 2 | 21-A | 201 | FOL | C4A-C4-N3 | -5.00 | 116.99 | 123.52 |
| 2 | 64-A | 201 | FOL | C4A-C4-N3 | -4.98 | 117.01 | 123.52 |
| 2 | 12-A | 201 | FOL | C4A-C4-N3 | -4.98 | 117.01 | 123.52 |
| 2 | 89-A | 201 | FOL | C4A-C4-N3 | -4.97 | 117.03 | 123.52 |
| 2 | 114-A | 201 | FOL | C4A-C4-N3 | -4.97 | 117.03 | 123.52 |
| 2 | 142-A | 201 | FOL | C4A-C4-N3 | -4.96 | 117.03 | 123.52 |
| 2 | 165-A | 201 | FOL | C4A-C4-N3 | -4.96 | 117.04 | 123.52 |
| 2 | 35-A | 201 | FOL | C4A-C4-N3 | -4.96 | 117.04 | 123.52 |
| 2 | 137-A | 201 | FOL | C4A-C4-N3 | -4.95 | 117.05 | 123.52 |
| 2 | 81-A | 201 | FOL | C4A-C4-N3 | -4.94 | 117.06 | 123.52 |
| 2 | 43-A | 201 | FOL | C4A-C4-N3 | -4.94 | 117.07 | 123.52 |
| 2 | 3-A | 201 | FOL | C4A-C4-N3 | -4.94 | 117.07 | 123.52 |
| 2 | 138-A | 201 | FOL | C4A-C4-N3 | -4.93 | 117.08 | 123.52 |
| 2 | 87-A | 201 | FOL | C4A-C4-N3 | -4.91 | 117.11 | 123.52 |
| 2 | 102-A | 201 | FOL | C4A-C4-N3 | -4.90 | 117.11 | 123.52 |
| 2 | 110-A | 201 | FOL | CT-CA-N | -4.89 | 103.17 | 112.93 |
| 2 | 13-A | 201 | FOL | CT-CA-N | -4.88 | 103.19 | 112.93 |
| 2 | 149-A | 201 | FOL | C4A-C4-N3 | -4.88 | 117.14 | 123.52 |
| 2 | 20-A | 201 | FOL | C4A-C4-N3 | -4.87 | 117.16 | 123.52 |
| 2 | 17-A | 201 | FOL | C4A-C4-N3 | -4.85 | 117.18 | 123.52 |
| 2 | 86-A | 201 | FOL | C4A-C4-N3 | -4.85 | 117.18 | 123.52 |
| 2 | 16-A | 201 | FOL | CB-CA-N | -4.85 | 102.35 | 109.92 |
| 2 | 52-A | 201 | FOL | CT-CA-N | -4.83 | 103.29 | 112.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 159-A | 201 | FOL | C4A-C4-N3 | -4.82 | 117.23 | 123.52 |
| 2 | 80-A | 201 | FOL | C4A-C4-N3 | -4.79 | 117.26 | 123.52 |
| 2 | 43-A | 201 | FOL | NA2-C2-N3 | -4.79 | 114.15 | 120.29 |
| 2 | 101-A | 201 | FOL | C4A-C4-N3 | -4.78 | 117.27 | 123.52 |
| 2 | 34-A | 201 | FOL | C4A-C4-N3 | -4.75 | 117.31 | 123.52 |
| 2 | 5-A | 201 | FOL | C4A-C4-N3 | -4.75 | 117.31 | 123.52 |
| 2 | 48-A | 201 | FOL | C4A-C4-N3 | -4.75 | 117.31 | 123.52 |
| 2 | 2-A | 201 | FOL | C4A-C4-N3 | -4.75 | 117.32 | 123.52 |
| 2 | 147-A | 201 | FOL | C4A-C4-N3 | -4.73 | 117.34 | 123.52 |
| 2 | 48-A | 201 | FOL | NA2-C2-N3 | -4.72 | 114.25 | 120.29 |
| 2 | 90-A | 201 | FOL | C4A-C4-N3 | -4.69 | 117.40 | 123.52 |
| 2 | 158-A | 201 | FOL | C4A-C4-N3 | -4.67 | 117.41 | 123.52 |
| 2 | 120-A | 201 | FOL | NA2-C2-N3 | -4.66 | 114.32 | 120.29 |
| 2 | 9-A | 201 | FOL | C4A-C4-N3 | -4.65 | 117.44 | 123.52 |
| 2 | 10-A | 201 | FOL | C4A-C4-N3 | -4.65 | 117.44 | 123.52 |
| 2 | 92-A | 201 | FOL | C4A-C4-N3 | -4.62 | 117.48 | 123.52 |
| 2 | 21-A | 201 | FOL | CB-CA-N | -4.61 | 102.73 | 109.92 |
| 2 | 162-A | 201 | FOL | C4A-C4-N3 | -4.60 | 117.51 | 123.52 |
| 2 | 167-A | 201 | FOL | CT-CA-N | -4.58 | 103.79 | 112.93 |
| 2 | 120-A | 201 | FOL | C4A-C4-N3 | -4.57 | 117.55 | 123.52 |
| 2 | 139-A | 201 | FOL | CT-CA-N | -4.53 | 103.89 | 112.93 |
| 2 | 142-A | 201 | FOL | CT-CA-N | -4.51 | 103.94 | 112.93 |
| 2 | 157-A | 201 | FOL | C4A-C4-N3 | -4.49 | 117.66 | 123.52 |
| 2 | 131-A | 201 | FOL | NA2-C2-N3 | -4.47 | 114.57 | 120.29 |
| 2 | 60-A | 201 | FOL | CT-CA-N | -4.47 | 104.02 | 112.93 |
| 2 | 139-A | 201 | FOL | C4A-C4-N3 | -4.46 | 117.69 | 123.52 |
| 2 | 93-A | 201 | FOL | CT-CA-N | -4.45 | 104.06 | 112.93 |
| 2 | 30-A | 201 | FOL | C4A-C4-N3 | -4.43 | 117.73 | 123.52 |
| 2 | 105-A | 201 | FOL | CT-CA-N | -4.40 | 104.15 | 112.93 |
| 2 | 153-A | 201 | FOL | CT-CA-N | -4.36 | 104.23 | 112.93 |
| 2 | 96-A | 201 | FOL | C4A-C4-N3 | -4.36 | 117.83 | 123.52 |
| 4 | 108-A | 204 | NAP | O3D-C3D-C2D | -4.34 | 97.82 | 111.86 |
| 2 | 73-A | 201 | FOL | C4A-C4-N3 | -4.34 | 117.86 | 123.52 |
| 2 | 7-A | 201 | FOL | CT-CA-N | -4.32 | 104.31 | 112.93 |
| 2 | 131-A | 201 | FOL | C4A-C4-N3 | -4.30 | 117.90 | 123.52 |
| 2 | 24-A | 201 | FOL | C4A-C4-N3 | -4.28 | 117.92 | 123.52 |
| 2 | 95-A | 201 | FOL | C4A-C4-N3 | -4.27 | 117.94 | 123.52 |
| 2 | 118-A | 201 | FOL | CT-CA-N | -4.27 | 104.41 | 112.93 |
| 2 | 126-A | 201 | FOL | O-C-C11 | -4.25 | 113.67 | 120.95 |
| 2 | 52-A | 201 | FOL | CB-CA-N | -4.23 | 103.31 | 109.92 |
| 2 | 127-A | 201 | FOL | C4A-C4-N3 | -4.22 | 118.01 | 123.52 |
| 2 | 52-A | 201 | FOL | C4A-C4-N3 | -4.19 | 118.05 | 123.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 99-A | 201 | FOL | CT-CA-N | -4.16 | 104.62 | 112.93 |
| 2 | 40-A | 201 | FOL | NA2-C2-N3 | -4.15 | 114.97 | 120.29 |
| 2 | 62-A | 201 | FOL | CT-CA-N | -4.14 | 104.67 | 112.93 |
| 4 | 56-A | 204 | NAP | O4D-C1D-N1N | -4.09 | 103.69 | 108.10 |
| 2 | 165-A | 201 | FOL | NA2-C2-N3 | -4.04 | 115.12 | 120.29 |
| 2 | 16-A | 201 | FOL | NA2-C2-N3 | -4.04 | 115.12 | 120.29 |
| 2 | 16-A | 201 | FOL | C4A-C4-N3 | -4.03 | 118.25 | 123.52 |
| 2 | 153-A | 201 | FOL | C4A-C4-N3 | -4.03 | 118.25 | 123.52 |
| 2 | 149-A | 201 | FOL | NA2-C2-N3 | -4.01 | 115.16 | 120.29 |
| 2 | 147-A | 201 | FOL | NA2-C2-N3 | -3.98 | 115.19 | 120.29 |
| 4 | 117-A | 204 | NAP | O2N-PN-O3 | -3.97 | 88.26 | 105.27 |
| 2 | 90-A | 201 | FOL | CT-CA-N | -3.96 | 105.03 | 112.93 |
| 4 | 118-A | 204 | NAP | N3A-C2A-N1A | -3.95 | 125.77 | 128.87 |
| 2 | 25-A | 201 | FOL | CT-CA-N | -3.94 | 105.07 | 112.93 |
| 2 | 140-A | 201 | FOL | C4A-C4-N3 | -3.92 | 118.40 | 123.52 |
| 2 | 23-A | 201 | FOL | CT-CA-N | -3.91 | 105.13 | 112.93 |
| 4 | 119-A | 204 | NAP | O2N-PN-O5D | -3.90 | 89.66 | 108.24 |
| 2 | 5-A | 201 | FOL | NA2-C2-N3 | -3.89 | 115.31 | 120.29 |
| 2 | 131-A | 201 | FOL | CT-CA-N | -3.88 | 105.18 | 112.93 |
| 2 | 57-A | 201 | FOL | CT-CA-N | -3.88 | 105.19 | 112.93 |
| 2 | 53-A | 201 | FOL | CB-CA-N | -3.87 | 103.88 | 109.92 |
| 2 | 5-A | 201 | FOL | CT-CA-N | -3.86 | 105.23 | 112.93 |
| 2 | 80-A | 201 | FOL | O-C-N | -3.81 | 115.56 | 122.45 |
| 2 | 64-A | 201 | FOL | NA2-C2-N3 | -3.80 | 115.42 | 120.29 |
| 2 | 126-A | 201 | FOL | CB-CG-CD | -3.79 | 97.58 | 113.05 |
| 4 | 90-A | 204 | NAP | O7N-C7N-N7N | -3.79 | 117.18 | 122.58 |
| 2 | 9-A | 201 | FOL | CT-CA-N | -3.78 | 105.39 | 112.93 |
| 2 | 161-A | 201 | FOL | CT-CA-N | -3.78 | 105.39 | 112.93 |
| 2 | 33-A | 201 | FOL | C4A-C4-N3 | -3.76 | 118.60 | 123.52 |
| 4 | 135-A | 204 | NAP | C1B-N9A-C4A | -3.76 | 122.61 | 126.81 |
| 4 | 42-A | 204 | NAP | C1B-N9A-C4A | -3.74 | 122.63 | 126.81 |
| 2 | 129-A | 201 | FOL | C16-C11-C12 | -3.74 | 113.49 | 118.61 |
| 4 | 85-A | 204 | NAP | O4D-C1D-N1N | -3.73 | 104.08 | 108.10 |
| 2 | 127-A | 201 | FOL | NA2-C2-N3 | -3.72 | 115.52 | 120.29 |
| 2 | 135-A | 201 | FOL | NA2-C2-N3 | -3.72 | 115.53 | 120.29 |
| 2 | 63-A | 201 | FOL | CT-CA-N | -3.71 | 105.53 | 112.93 |
| 2 | 115-A | 201 | FOL | CT-CA-N | -3.71 | 105.53 | 112.93 |
| 4 | 156-A | 204 | NAP | O4D-C1D-N1N | -3.70 | 104.11 | 108.10 |
| 4 | 139-A | 204 | NAP | C1B-N9A-C4A | -3.68 | 122.70 | 126.81 |
| 4 | 156-A | 204 | NAP | N3A-C2A-N1A | -3.68 | 125.98 | 128.87 |
| 2 | 72-A | 201 | FOL | O-C-C11 | -3.66 | 114.68 | 120.95 |
| 2 | 89-A | 201 | FOL | NA2-C2-N3 | -3.64 | 115.63 | 120.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 144-A | 201 | FOL | CT-CA-N | -3.61 | 105.72 | 112.93 |
| 4 | 151-A | 204 | NAP | C1B-N9A-C4A | -3.61 | 122.78 | 126.81 |
| 4 | 115-A | 204 | NAP | O7N-C7N-N7N | -3.60 | 117.44 | 122.58 |
| 2 | 155-A | 201 | FOL | NA2-C2-N3 | -3.60 | 115.68 | 120.29 |
| 2 | 157-A | 201 | FOL | NA2-C2-N3 | -3.59 | 115.69 | 120.29 |
| 2 | 46-A | 201 | FOL | CT-CA-N | -3.59 | 105.77 | 112.93 |
| 2 | 113-A | 201 | FOL | CT-CA-N | -3.59 | 105.77 | 112.93 |
| 4 | 102-A | 204 | NAP | C1B-N9A-C4A | -3.56 | 122.83 | 126.81 |
| 4 | 155-A | 204 | NAP | O4D-C1D-N1N | -3.56 | 104.26 | 108.10 |
| 2 | 26-A | 201 | FOL | CT-CA-N | -3.53 | 105.88 | 112.93 |
| 2 | 49-A | 201 | FOL | CT-CA-N | -3.53 | 105.89 | 112.93 |
| 2 | 108-A | 201 | FOL | CT-CA-N | -3.52 | 105.90 | 112.93 |
| 2 | 78-A | 201 | FOL | CT-CA-N | -3.52 | 105.91 | 112.93 |
| 4 | 131-A | 204 | NAP | O4D-C1D-N1N | -3.51 | 104.32 | 108.10 |
| 2 | 144-A | 201 | FOL | NA2-C2-N3 | -3.51 | 115.80 | 120.29 |
| 4 | 118-A | 204 | NAP | O4D-C1D-N1N | -3.47 | 104.35 | 108.10 |
| 2 | 20-A | 201 | FOL | NA2-C2-N3 | -3.47 | 115.84 | 120.29 |
| 2 | 70-A | 201 | FOL | CT-CA-N | -3.47 | 106.01 | 112.93 |
| 4 | 79-A | 204 | NAP | N3A-C2A-N1A | -3.47 | 126.15 | 128.87 |
| 2 | 24-A | 201 | FOL | CT-CA-N | -3.47 | 106.01 | 112.93 |
| 2 | 140-A | 201 | FOL | CT-CA-N | -3.47 | 106.02 | 112.93 |
| 2 | 127-A | 201 | FOL | O-C-C11 | -3.47 | 115.01 | 120.95 |
| 2 | 37-A | 201 | FOL | CB-CA-N | -3.46 | 104.53 | 109.92 |
| 2 | 31-A | 201 | FOL | NA2-C2-N3 | -3.45 | 115.87 | 120.29 |
| 2 | 15-A | 201 | FOL | CT-CA-N | -3.44 | 106.06 | 112.93 |
| 4 | 79-A | 204 | NAP | O4D-C1D-N1N | -3.44 | 104.39 | 108.10 |
| 4 | 115-A | 204 | NAP | N3A-C2A-N1A | -3.44 | 126.17 | 128.87 |
| 4 | 35-A | 204 | NAP | O4D-C1D-N1N | -3.43 | 104.40 | 108.10 |
| 2 | 63-A | 201 | FOL | O-C-C11 | -3.43 | 115.08 | 120.95 |
| 4 | 132-A | 204 | NAP | O4D-C1D-N1N | -3.42 | 104.41 | 108.10 |
| 2 | 23-A | 201 | FOL | C4A-C4-N3 | -3.42 | 119.05 | 123.52 |
| 2 | 158-A | 201 | FOL | CT-CA-N | -3.42 | 106.12 | 112.93 |
| 2 | 112-A | 201 | FOL | CT-CA-N | -3.41 | 106.13 | 112.93 |
| 2 | 122-A | 201 | FOL | NA2-C2-N3 | -3.40 | 115.93 | 120.29 |
| 4 | 59-A | 204 | NAP | O4D-C1D-N1N | -3.39 | 104.44 | 108.10 |
| 2 | 66-A | 201 | FOL | C13-C14-N10 | -3.39 | 114.30 | 121.04 |
| 2 | 61-A | 201 | FOL | CT-CA-N | -3.39 | 106.17 | 112.93 |
| 2 | 34-A | 201 | FOL | C15-C14-C13 | -3.39 | 114.34 | 119.06 |
| 2 | 129-A | 201 | FOL | CT-CA-N | -3.39 | 106.18 | 112.93 |
| 4 | 114-A | 204 | NAP | N3A-C2A-N1A | -3.38 | 126.21 | 128.87 |
| 4 | 18-A | 204 | NAP | O7N-C7N-N7N | -3.38 | 117.76 | 122.58 |
| 2 | 56-A | 201 | FOL | CT-CA-N | -3.36 | 106.23 | 112.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 92-A | 201 | FOL | CB-CG-CD | -3.35 | 99.38 | 113.05 |
| 2 | 81-A | 201 | FOL | CT-CA-N | -3.34 | 106.28 | 112.93 |
| 2 | 41-A | 201 | FOL | O-C-N | -3.33 | 116.43 | 122.45 |
| 2 | 83-A | 201 | FOL | CT-CA-N | -3.32 | 106.31 | 112.93 |
| 4 | 57-A | 204 | NAP | O4D-C1D-N1N | -3.31 | 104.53 | 108.10 |
| 2 | 69-A | 201 | FOL | CT-CA-N | -3.31 | 106.34 | 112.93 |
| 4 | 29-A | 204 | NAP | C1B-N9A-C4A | -3.29 | 123.14 | 126.81 |
| 2 | 121-A | 201 | FOL | CT-CA-N | -3.29 | 106.37 | 112.93 |
| 4 | 78-A | 204 | NAP | O2N-PN-O3 | -3.28 | 91.20 | 105.27 |
| 2 | 10-A | 201 | FOL | NA2-C2-N3 | -3.28 | 116.09 | 120.29 |
| 2 | 59-A | 201 | FOL | NA2-C2-N3 | -3.27 | 116.10 | 120.29 |
| 2 | 124-A | 201 | FOL | CB-CG-CD | -3.27 | 99.69 | 113.05 |
| 2 | 14-A | 201 | FOL | CT-CA-N | -3.27 | 106.40 | 112.93 |
| 4 | 104-A | 204 | NAP | O3D-C3D-C2D | -3.27 | 101.28 | 111.86 |
| 2 | 157-A | 201 | FOL | CT-CA-N | -3.27 | 106.41 | 112.93 |
| 2 | 38-A | 201 | FOL | CT-CA-N | -3.26 | 106.42 | 112.93 |
| 2 | 29-A | 201 | FOL | CT-CA-N | -3.26 | 106.43 | 112.93 |
| 4 | 63-A | 204 | NAP | O4D-C1D-N1N | -3.24 | 104.60 | 108.10 |
| 4 | 148-A | 204 | NAP | C1B-N9A-C4A | -3.23 | 123.20 | 126.81 |
| 2 | 51-A | 201 | FOL | O-C-C11 | -3.23 | 115.42 | 120.95 |
| 2 | 148-A | 201 | FOL | CT-CA-N | -3.23 | 106.50 | 112.93 |
| 4 | 119-A | 204 | NAP | N3A-C2A-N1A | -3.22 | 126.34 | 128.87 |
| 4 | 123-A | 204 | NAP | N3A-C2A-N1A | -3.22 | 126.34 | 128.87 |
| 4 | 99-A | 204 | NAP | O4D-C1D-N1N | -3.21 | 104.63 | 108.10 |
| 2 | 3-A | 201 | FOL | CT-CA-N | -3.21 | 106.52 | 112.93 |
| 4 | 84-A | 204 | NAP | O4D-C1D-N1N | -3.20 | 104.64 | 108.10 |
| 2 | 74-A | 201 | FOL | C16-C11-C12 | -3.20 | 114.23 | 118.61 |
| 2 | 94-A | 201 | FOL | O-C-C11 | -3.20 | 115.47 | 120.95 |
| 4 | 26-A | 204 | NAP | O2N-PN-O3 | -3.20 | 91.56 | 105.27 |
| 2 | 162-A | 201 | FOL | NA2-C2-N3 | -3.19 | 116.20 | 120.29 |
| 4 | 121-A | 204 | NAP | N3A-C2A-N1A | -3.19 | 126.36 | 128.87 |
| 4 | 129-A | 204 | NAP | O2A-PA-O5B | -3.19 | 93.04 | 108.24 |
| 4 | 119-A | 204 | NAP | O4B-C4B-C5B | -3.18 | 97.90 | 109.29 |
| 2 | 58-A | 201 | FOL | CT-CA-N | -3.18 | 106.59 | 112.93 |
| 4 | 52-A | 204 | NAP | O2N-PN-O3 | -3.18 | 91.65 | 105.27 |
| 2 | 147-A | 201 | FOL | CT-CA-N | -3.18 | 106.59 | 112.93 |
| 2 | 33-A | 201 | FOL | CT-CA-N | -3.17 | 106.61 | 112.93 |
| 4 | 80-A | 204 | NAP | O4D-C1D-N1N | -3.16 | 104.69 | 108.10 |
| 4 | 117-A | 204 | NAP | N3A-C2A-N1A | -3.16 | 126.39 | 128.87 |
| 2 | 110-A | 201 | FOL | CB-CG-CD | -3.16 | 100.17 | 113.05 |
| 4 | 83-A | 204 | NAP | O4D-C1D-N1N | -3.15 | 104.70 | 108.10 |
| 2 | 70-A | 201 | FOL | O-C-C11 | -3.15 | 115.56 | 120.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 5-A | 204 | NAP | O4D-C1D-N1N | -3.14 | 104.71 | 108.10 |
| 4 | 82-A | 204 | NAP | O4B-C4B-C5B | -3.13 | 98.08 | 109.29 |
| 2 | 135-A | 201 | FOL | CB-CA-N | -3.13 | 105.03 | 109.92 |
| 4 | 101-A | 204 | NAP | C1B-N9A-C4A | -3.12 | 123.32 | 126.81 |
| 2 | 75-A | 201 | FOL | CT-CA-N | -3.12 | 106.71 | 112.93 |
| 4 | 1-A | 204 | NAP | N3A-C2A-N1A | -3.11 | 126.43 | 128.87 |
| 2 | 10-A | 201 | FOL | CT-CA-N | -3.11 | 106.73 | 112.93 |
| 2 | 64-A | 201 | FOL | C13-C14-N10 | -3.11 | 114.86 | 121.04 |
| 4 | 30-A | 204 | NAP | O4D-C1D-N1N | -3.10 | 104.76 | 108.10 |
| 2 | 141-A | 201 | FOL | O-C-C11 | -3.10 | 115.65 | 120.95 |
| 2 | 128-A | 201 | FOL | CT-CA-N | -3.09 | 106.76 | 112.93 |
| 2 | 151-A | 201 | FOL | CT-CA-N | -3.09 | 106.76 | 112.93 |
| 4 | 70-A | 204 | NAP | C1B-N9A-C4A | -3.09 | 123.36 | 126.81 |
| 2 | 93-A | 201 | FOL | NA2-C2-N3 | -3.09 | 116.34 | 120.29 |
| 4 | 21-A | 204 | NAP | O4D-C1D-N1N | -3.08 | 104.78 | 108.10 |
| 2 | 81-A | 201 | FOL | NA2-C2-N3 | -3.08 | 116.34 | 120.29 |
| 4 | 138-A | 204 | NAP | C1B-N9A-C4A | -3.08 | 123.37 | 126.81 |
| 4 | 71-A | 204 | NAP | N3A-C2A-N1A | -3.08 | 126.45 | 128.87 |
| 4 | 1-A | 204 | NAP | O2N-PN-O3 | -3.08 | 92.09 | 105.27 |
| 4 | 12-A | 204 | NAP | N3A-C2A-N1A | -3.07 | 126.46 | 128.87 |
| 4 | 75-A | 204 | NAP | O4D-C1D-N1N | -3.07 | 104.79 | 108.10 |
| 4 | 130-A | 204 | NAP | C1B-N9A-C4A | -3.07 | 123.38 | 126.81 |
| 4 | 77-A | 204 | NAP | O2N-PN-O3 | -3.06 | 92.15 | 105.27 |
| 4 | 128-A | 204 | NAP | O2A-PA-O5B | -3.06 | 93.65 | 108.24 |
| 4 | 104-A | 204 | NAP | O4D-C1D-N1N | -3.06 | 104.80 | 108.10 |
| 2 | 86-A | 201 | FOL | CT-CA-N | -3.06 | 106.83 | 112.93 |
| 2 | 55-A | 201 | FOL | CT-CA-N | -3.06 | 106.83 | 112.93 |
| 4 | 166-A | 204 | NAP | O4D-C1D-N1N | -3.05 | 104.81 | 108.10 |
| 4 | 40-A | 204 | NAP | N3A-C2A-N1A | -3.05 | 126.47 | 128.87 |
| 2 | 143-A | 201 | FOL | CT-CA-N | -3.05 | 106.85 | 112.93 |
| 4 | 74-A | 204 | NAP | O4D-C1D-N1N | -3.05 | 104.81 | 108.10 |
| 4 | 95-A | 204 | NAP | C1B-N9A-C4A | -3.04 | 123.41 | 126.81 |
| 2 | 114-A | 201 | FOL | NA2-C2-N3 | -3.04 | 116.39 | 120.29 |
| 4 | 111-A | 204 | NAP | C1B-N9A-C4A | -3.04 | 123.42 | 126.81 |
| 4 | 96-A | 204 | NAP | C1B-N9A-C4A | -3.03 | 123.42 | 126.81 |
| 4 | 73-A | 204 | NAP | C1B-N9A-C4A | -3.03 | 123.42 | 126.81 |
| 4 | 19-A | 204 | NAP | N3A-C2A-N1A | -3.03 | 126.49 | 128.87 |
| 2 | 79-A | 201 | FOL | CT-CA-N | -3.03 | 106.88 | 112.93 |
| 4 | 34-A | 204 | NAP | C1B-N9A-C4A | -3.03 | 123.42 | 126.81 |
| 4 | 51-A | 204 | NAP | O2N-PN-O3 | -3.02 | 92.30 | 105.27 |
| 2 | 22-A | 201 | FOL | CT-CA-N | -3.02 | 106.90 | 112.93 |
| 2 | 163-A | 201 | FOL | CT-CA-N | -3.02 | 106.90 | 112.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 32-A | 204 | NAP | C1B-N9A-C4A | -3.02 | 123.43 | 126.81 |
| 2 | 12-A | 201 | FOL | CT-CA-N | -3.02 | 106.92 | 112.93 |
| 2 | 35-A | 201 | FOL | CT-CA-N | -3.02 | 106.92 | 112.93 |
| 2 | 82-A | 201 | FOL | CT-CA-N | -3.01 | 106.92 | 112.93 |
| 4 | 12-A | 204 | NAP | O4D-C1D-N1N | -3.01 | 104.86 | 108.10 |
| 2 | 167-A | 201 | FOL | CB-CA-N | -3.01 | 105.23 | 109.92 |
| 4 | 49-A | 204 | NAP | O2N-PN-O3 | -3.00 | 92.39 | 105.27 |
| 2 | 30-A | 201 | FOL | NA2-C2-N3 | -3.00 | 116.45 | 120.29 |
| 4 | 11-A | 204 | NAP | N3A-C2A-N1A | -2.98 | 126.53 | 128.87 |
| 4 | 125-A | 204 | NAP | N3A-C2A-N1A | -2.98 | 126.53 | 128.87 |
| 4 | 53-A | 204 | NAP | O2N-PN-O3 | -2.98 | 92.50 | 105.27 |
| 4 | 17-A | 204 | NAP | C1B-N9A-C4A | -2.98 | 123.48 | 126.81 |
| 2 | 163-A | 201 | FOL | NA2-C2-N3 | -2.98 | 116.48 | 120.29 |
| 4 | 158-A | 204 | NAP | O4D-C1D-N1N | -2.97 | 104.89 | 108.10 |
| 2 | 153-A | 201 | FOL | NA2-C2-N3 | -2.97 | 116.49 | 120.29 |
| 2 | 104-A | 201 | FOL | NA2-C2-N3 | -2.97 | 116.49 | 120.29 |
| 4 | 113-A | 204 | NAP | C1B-N9A-C4A | -2.97 | 123.49 | 126.81 |
| 4 | 117-A | 204 | NAP | O2N-PN-O5D | -2.97 | 94.10 | 108.24 |
| 4 | 48-A | 204 | NAP | O2N-PN-O3 | -2.97 | 92.55 | 105.27 |
| 2 | 57-A | 201 | FOL | C6-N5-C4A | -2.97 | 114.72 | 118.43 |
| 4 | 106-A | 204 | NAP | N3A-C2A-N1A | -2.96 | 126.55 | 128.87 |
| 2 | 153-A | 201 | FOL | O-C-C11 | -2.96 | 115.89 | 120.95 |
| 2 | 99-A | 201 | FOL | O-C-N | -2.95 | 117.10 | 122.45 |
| 2 | 130-A | 201 | FOL | CT-CA-N | -2.95 | 107.04 | 112.93 |
| 2 | 137-A | 201 | FOL | CT-CA-N | -2.95 | 107.05 | 112.93 |
| 4 | 15-A | 204 | NAP | O2N-PN-O3 | -2.94 | 92.66 | 105.27 |
| 2 | 159-A | 201 | FOL | NA2-C2-N3 | -2.94 | 116.52 | 120.29 |
| 2 | 27-A | 201 | FOL | CT-CA-N | -2.94 | 107.06 | 112.93 |
| 4 | 3-A | 204 | NAP | O2N-PN-O3 | -2.94 | 92.66 | 105.27 |
| 2 | 108-A | 201 | FOL | NA2-C2-N3 | -2.93 | 116.53 | 120.29 |
| 4 | 33-A | 204 | NAP | C1B-N9A-C4A | -2.93 | 123.53 | 126.81 |
| 4 | 100-A | 204 | NAP | O4D-C1D-N1N | -2.93 | 104.94 | 108.10 |
| 4 | 67-A | 204 | NAP | C1B-N9A-C4A | -2.93 | 123.53 | 126.81 |
| 2 | 4-A | 201 | FOL | C16-C11-C12 | -2.93 | 114.60 | 118.61 |
| 2 | 9-A | 201 | FOL | NA2-C2-N3 | -2.92 | 116.55 | 120.29 |
| 2 | 143-A | 201 | FOL | CB-CA-N | -2.92 | 105.36 | 109.92 |
| 4 | 90-A | 204 | NAP | N3A-C2A-N1A | -2.92 | 126.58 | 128.87 |
| 2 | 94-A | 201 | FOL | NA2-C2-N3 | -2.92 | 116.55 | 120.29 |
| 4 | 33-A | 204 | NAP | O4B-C4B-C5B | -2.92 | 98.85 | 109.29 |
| 4 | 4-A | 204 | NAP | O2N-PN-O3 | -2.92 | 92.77 | 105.27 |
| 4 | 31-A | 204 | NAP | O4D-C1D-N1N | -2.91 | 104.96 | 108.10 |
| 4 | 100-A | 204 | NAP | N3A-C2A-N1A | -2.91 | 126.58 | 128.87 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 102-A | 201 | FOL | NA2-C2-N3 | -2.91 | 116.56 | 120.29 |
| 4 | 122-A | 204 | NAP | N3A-C2A-N1A | -2.91 | 126.59 | 128.87 |
| 4 | 79-A | 204 | NAP | O2A-PA-O5B | -2.90 | 94.42 | 108.24 |
| 4 | 120-A | 204 | NAP | N3A-C2A-N1A | -2.90 | 126.59 | 128.87 |
| 4 | 28-A | 204 | NAP | O2A-PA-O5B | -2.90 | 94.42 | 108.24 |
| 4 | 2-A | 204 | NAP | O2N-PN-O3 | -2.90 | 92.85 | 105.27 |
| 4 | 127-A | 204 | NAP | C1B-N9A-C4A | -2.89 | 123.58 | 126.81 |
| 2 | 102-A | 201 | FOL | O-C-C11 | -2.89 | 116.00 | 120.95 |
| 2 | 41-A | 201 | FOL | C7-C6-N5 | -2.89 | 117.67 | 120.51 |
| 4 | 73-A | 204 | NAP | N3A-C2A-N1A | -2.89 | 126.60 | 128.87 |
| 4 | 27-A | 204 | NAP | O2N-PN-O3 | -2.88 | 92.92 | 105.27 |
| 4 | 43-A | 204 | NAP | C1B-N9A-C4A | -2.87 | 123.60 | 126.81 |
| 4 | 38-A | 204 | NAP | O2D-C2D-C3D | -2.87 | 102.57 | 111.86 |
| 4 | 42-A | 204 | NAP | O2A-PA-O5B | -2.87 | 94.55 | 108.24 |
| 2 | 80-A | 201 | FOL | CT-CA-N | -2.87 | 107.21 | 112.93 |
| 4 | 62-A | 204 | NAP | N3A-C2A-N1A | -2.87 | 126.62 | 128.87 |
| 4 | 31-A | 204 | NAP | O2X-P2B-O1X | -2.87 | 101.27 | 110.63 |
| 2 | 66-A | 201 | FOL | CT-CA-N | -2.86 | 107.23 | 112.93 |
| 4 | 98-A | 204 | NAP | C1B-N9A-C4A | -2.86 | 123.62 | 126.81 |
| 4 | 113-A | 204 | NAP | N3A-C2A-N1A | -2.86 | 126.63 | 128.87 |
| 4 | 76-A | 204 | NAP | O2N-PN-O3 | -2.85 | 93.05 | 105.27 |
| 2 | 115-A | 201 | FOL | NA2-C2-N3 | -2.85 | 116.64 | 120.29 |
| 2 | 44-A | 201 | FOL | CT-CA-N | -2.84 | 107.26 | 112.93 |
| 2 | 57-A | 201 | FOL | C16-C11-C12 | -2.83 | 114.73 | 118.61 |
| 4 | 79-A | 204 | NAP | C1B-N9A-C4A | -2.83 | 123.64 | 126.81 |
| 2 | 166-A | 201 | FOL | NA2-C2-N3 | -2.83 | 116.66 | 120.29 |
| 4 | 129-A | 204 | NAP | O2A-PA-O3 | -2.83 | 93.14 | 105.27 |
| 4 | 92-A | 204 | NAP | O4D-C1D-N1N | -2.83 | 105.05 | 108.10 |
| 4 | 5-A | 204 | NAP | C1B-N9A-C4A | -2.83 | 123.65 | 126.81 |
| 2 | 112-A | 201 | FOL | NA2-C2-N3 | -2.83 | 116.67 | 120.29 |
| 4 | 105-A | 204 | NAP | C1B-N9A-C4A | -2.83 | 123.65 | 126.81 |
| 4 | 160-A | 204 | NAP | C1B-N9A-C4A | -2.83 | 123.65 | 126.81 |
| 4 | 75-A | 204 | NAP | N3A-C2A-N1A | -2.83 | 126.65 | 128.87 |
| 4 | 79-A | 204 | NAP | O2N-PN-O3 | -2.83 | 93.16 | 105.27 |
| 4 | 134-A | 204 | NAP | O4D-C1D-N1N | -2.82 | 105.06 | 108.10 |
| 2 | 39-A | 201 | FOL | NA2-C2-N3 | -2.82 | 116.68 | 120.29 |
| 2 | 117-A | 201 | FOL | CT-CA-N | -2.82 | 107.31 | 112.93 |
| 2 | 128-A | 201 | FOL | NA2-C2-N3 | -2.82 | 116.68 | 120.29 |
| 4 | 3-A | 204 | NAP | O2A-PA-O5B | -2.82 | 94.81 | 108.24 |
| 4 | 140-A | 204 | NAP | C1B-N9A-C4A | -2.81 | 123.66 | 126.81 |
| 4 | 45-A | 204 | NAP | C1B-N9A-C4A | -2.81 | 123.67 | 126.81 |
| 4 | 147-A | 204 | NAP | C1B-N9A-C4A | -2.81 | 123.67 | 126.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 23-A | 204 | NAP | O2N-PN-O3 | -2.81 | 93.25 | 105.27 |
| 4 | 25-A | 204 | NAP | O2N-PN-O3 | -2.80 | 93.25 | 105.27 |
| 4 | 29-A | 204 | NAP | O2A-PA-O5B | -2.80 | 94.89 | 108.24 |
| 2 | 29-A | 201 | FOL | NA2-C2-N3 | -2.80 | 116.71 | 120.29 |
| 2 | 115-A | 201 | FOL | C13-C14-N10 | -2.80 | 115.47 | 121.04 |
| 4 | 163-A | 204 | NAP | C1B-N9A-C4A | -2.80 | 123.68 | 126.81 |
| 4 | 80-A | 204 | NAP | O2A-PA-O5B | -2.80 | 94.91 | 108.24 |
| 4 | 42-A | 204 | NAP | O4B-C4B-C5B | -2.79 | 99.30 | 109.29 |
| 4 | 98-A | 204 | NAP | O4D-C1D-N1N | -2.79 | 105.09 | 108.10 |
| 4 | 64-A | 204 | NAP | C1B-N9A-C4A | -2.79 | 123.69 | 126.81 |
| 2 | 97-A | 201 | FOL | NA2-C2-N3 | -2.79 | 116.72 | 120.29 |
| 2 | 9-A | 201 | FOL | O-C-C11 | -2.79 | 116.18 | 120.95 |
| 4 | 128-A | 204 | NAP | O2N-PN-O3 | -2.79 | 93.33 | 105.27 |
| 4 | 69-A | 204 | NAP | N3A-C2A-N1A | -2.78 | 126.69 | 128.87 |
| 2 | 90-A | 201 | FOL | NA2-C2-N3 | -2.77 | 116.74 | 120.29 |
| 2 | 86-A | 201 | FOL | NA2-C2-N3 | -2.77 | 116.74 | 120.29 |
| 4 | 49-A | 204 | NAP | O2A-PA-O5B | -2.77 | 95.02 | 108.24 |
| 4 | 138-A | 204 | NAP | O2N-PN-O3 | -2.77 | 93.40 | 105.27 |
| 4 | 43-A | 204 | NAP | N3A-C2A-N1A | -2.77 | 126.70 | 128.87 |
| 4 | 28-A | 204 | NAP | O2A-PA-O3 | -2.77 | 93.41 | 105.27 |
| 4 | 31-A | 204 | NAP | C1B-N9A-C4A | -2.76 | 123.72 | 126.81 |
| 2 | 116-A | 201 | FOL | CT-CA-N | -2.76 | 107.42 | 112.93 |
| 4 | 153-A | 204 | NAP | O2N-PN-O3 | -2.76 | 93.44 | 105.27 |
| 4 | 18-A | 204 | NAP | N3A-C2A-N1A | -2.76 | 126.70 | 128.87 |
| 4 | 159-A | 204 | NAP | O4D-C1D-N1N | -2.75 | 105.13 | 108.10 |
| 4 | 70-A | 204 | NAP | N3A-C2A-N1A | -2.75 | 126.71 | 128.87 |
| 2 | 19-A | 201 | FOL | CT-CA-N | -2.75 | 107.44 | 112.93 |
| 2 | 144-A | 201 | FOL | C13-C14-N10 | -2.75 | 115.56 | 121.04 |
| 4 | 159-A | 204 | NAP | N3A-C2A-N1A | -2.75 | 126.71 | 128.87 |
| 4 | 49-A | 204 | NAP | O4D-C1D-N1N | -2.74 | 105.14 | 108.10 |
| 4 | 90-A | 204 | NAP | O4D-C1D-N1N | -2.74 | 105.14 | 108.10 |
| 2 | 32-A | 201 | FOL | NA2-C2-N3 | -2.74 | 116.78 | 120.29 |
| 4 | 99-A | 204 | NAP | O2A-PA-O5B | -2.74 | 95.17 | 108.24 |
| 4 | 42-A | 204 | NAP | O4D-C1D-N1N | -2.74 | 105.15 | 108.10 |
| 2 | 120-A | 201 | FOL | CT-CA-N | -2.74 | 107.47 | 112.93 |
| 4 | 16-A | 204 | NAP | O4D-C1D-N1N | -2.73 | 105.16 | 108.10 |
| 4 | 29-A | 204 | NAP | O2A-PA-O3 | -2.73 | 93.57 | 105.27 |
| 4 | 109-A | 204 | NAP | C1B-N9A-C4A | -2.73 | 123.76 | 126.81 |
| 4 | 27-A | 204 | NAP | O2A-PA-O5B | -2.73 | 95.24 | 108.24 |
| 4 | 114-A | 204 | NAP | C1B-N9A-C4A | -2.73 | 123.76 | 126.81 |
| 4 | 77-A | 204 | NAP | C1B-N9A-C4A | -2.73 | 123.76 | 126.81 |
| 2 | 42-A | 201 | FOL | CT-CA-N | -2.73 | 107.49 | 112.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 6-A | 204 | NAP | N3A-C2A-N1A | -2.72 | 126.73 | 128.87 |
| 2 | 100-A | 201 | FOL | C9-C6-C7 | -2.72 | 116.60 | 121.39 |
| 4 | 154-A | 204 | NAP | O2N-PN-O3 | -2.72 | 93.60 | 105.27 |
| 4 | 93-A | 204 | NAP | O2A-PA-O5B | -2.72 | 95.26 | 108.24 |
| 4 | 103-A | 204 | NAP | O2N-PN-O3 | -2.72 | 93.62 | 105.27 |
| 4 | 161-A | 204 | NAP | C1B-N9A-C4A | -2.72 | 123.77 | 126.81 |
| 4 | 127-A | 204 | NAP | O2A-PA-O5B | -2.72 | 95.29 | 108.24 |
| 4 | 117-A | 204 | NAP | O4D-C1D-N1N | -2.71 | 105.17 | 108.10 |
| 2 | 72-A | 201 | FOL | CT-CA-N | -2.71 | 107.53 | 112.93 |
| 4 | 130-A | 204 | NAP | O2A-PA-O5B | -2.71 | 95.34 | 108.24 |
| 4 | 128-A | 204 | NAP | O2A-PA-O3 | -2.71 | 93.67 | 105.27 |
| 4 | 49-A | 204 | NAP | O7N-C7N-N7N | -2.70 | 118.73 | 122.58 |
| 4 | 114-A | 204 | NAP | O2N-PN-O3 | -2.70 | 93.71 | 105.27 |
| 2 | 83-A | 201 | FOL | C16-C11-C12 | -2.70 | 114.92 | 118.61 |
| 2 | 4-A | 201 | FOL | CT-CA-N | -2.69 | 107.56 | 112.93 |
| 4 | 154-A | 204 | NAP | O2A-PA-O5B | -2.69 | 95.41 | 108.24 |
| 2 | 103-A | 201 | FOL | NA2-C2-N3 | -2.69 | 116.84 | 120.29 |
| 4 | 104-A | 204 | NAP | C1B-N9A-C4A | -2.69 | 123.81 | 126.81 |
| 4 | 162-A | 204 | NAP | C1B-N9A-C4A | -2.69 | 123.81 | 126.81 |
| 4 | 112-A | 204 | NAP | N3A-C2A-N1A | -2.69 | 126.76 | 128.87 |
| 4 | 111-A | 204 | NAP | N3A-C2A-N1A | -2.68 | 126.77 | 128.87 |
| 4 | 89-A | 204 | NAP | O2N-PN-O3 | -2.68 | 93.79 | 105.27 |
| 4 | 121-A | 204 | NAP | O4D-C1D-N1N | -2.68 | 105.21 | 108.10 |
| 4 | 122-A | 204 | NAP | O2A-PA-O5B | -2.68 | 95.48 | 108.24 |
| 2 | 25-A | 201 | FOL | CB-CG-CD | -2.68 | 102.13 | 113.05 |
| 4 | 103-A | 204 | NAP | C1B-N9A-C4A | -2.68 | 123.82 | 126.81 |
| 4 | 3-A | 204 | NAP | O2A-PA-O3 | -2.68 | 93.80 | 105.27 |
| 4 | 164-A | 204 | NAP | O2N-PN-O3 | -2.68 | 93.80 | 105.27 |
| 2 | 104-A | 201 | FOL | CT-CA-N | -2.67 | 107.60 | 112.93 |
| 4 | 4-A | 204 | NAP | O2A-PA-O5B | -2.67 | 95.52 | 108.24 |
| 4 | 30-A | 204 | NAP | C1B-N9A-C4A | -2.67 | 123.83 | 126.81 |
| 4 | 48-A | 204 | NAP | O4D-C1D-N1N | -2.67 | 105.23 | 108.10 |
| 4 | 14-A | 204 | NAP | O2N-PN-O3 | -2.66 | 93.85 | 105.27 |
| 4 | 110-A | 204 | NAP | N3A-C2A-N1A | -2.66 | 126.78 | 128.87 |
| 4 | 94-A | 204 | NAP | O2A-PA-O5B | -2.66 | 95.57 | 108.24 |
| 2 | 134-A | 201 | FOL | O-C-N | -2.66 | 117.64 | 122.45 |
| 4 | 40-A | 204 | NAP | C1B-N9A-C4A | -2.66 | 123.84 | 126.81 |
| 2 | 50-A | 201 | FOL | CT-CA-N | -2.66 | 107.63 | 112.93 |
| 4 | 138-A | 204 | NAP | O2A-PA-O5B | -2.65 | 95.59 | 108.24 |
| 2 | 18-A | 201 | FOL | CT-CA-N | -2.65 | 107.64 | 112.93 |
| 2 | 24-A | 201 | FOL | NA2-C2-N3 | -2.65 | 116.89 | 120.29 |
| 2 | 160-A | 201 | FOL | CT-CA-N | -2.65 | 107.64 | 112.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 162-A | 204 | NAP | O4D-C1D-N1N | -2.65 | 105.24 | 108.10 |
| 2 | 65-A | 201 | FOL | C9-C6-C7 | -2.65 | 116.73 | 121.39 |
| 2 | 134-A | 201 | FOL | CB-CG-CD | -2.65 | 102.25 | 113.05 |
| 4 | 54-A | 204 | NAP | O2A-PA-O5B | -2.65 | 95.62 | 108.24 |
| 4 | 129-A | 204 | NAP | O2N-PN-O3 | -2.64 | 93.93 | 105.27 |
| 4 | 28-A | 204 | NAP | O2N-PN-O3 | -2.64 | 93.94 | 105.27 |
| 4 | 150-A | 204 | NAP | O2N-PN-O3 | -2.64 | 93.94 | 105.27 |
| 4 | 104-A | 204 | NAP | O2N-PN-O3 | -2.64 | 93.94 | 105.27 |
| 4 | 131-A | 204 | NAP | C1B-N9A-C4A | -2.64 | 123.86 | 126.81 |
| 4 | 107-A | 204 | NAP | C1B-N9A-C4A | -2.64 | 123.86 | 126.81 |
| 4 | 72-A | 204 | NAP | C1B-N9A-C4A | -2.64 | 123.86 | 126.81 |
| 4 | 54-A | 204 | NAP | O2N-PN-O3 | -2.64 | 93.96 | 105.27 |
| 4 | 123-A | 204 | NAP | O2A-PA-O5B | -2.64 | 95.67 | 108.24 |
| 4 | 23-A | 204 | NAP | N3A-C2A-N1A | -2.64 | 126.80 | 128.87 |
| 4 | 137-A | 204 | NAP | O2A-PA-O5B | -2.64 | 95.67 | 108.24 |
| 2 | 26-A | 201 | FOL | O-C-N | -2.63 | 117.68 | 122.45 |
| 4 | 123-A | 204 | NAP | C1B-N9A-C4A | -2.63 | 123.87 | 126.81 |
| 4 | 123-A | 204 | NAP | O4D-C1D-N1N | -2.63 | 105.26 | 108.10 |
| 4 | 81-A | 204 | NAP | N3A-C2A-N1A | -2.63 | 126.81 | 128.87 |
| 4 | 38-A | 204 | NAP | N3A-C2A-N1A | -2.63 | 126.81 | 128.87 |
| 2 | 20-A | 201 | FOL | CT-CA-N | -2.63 | 107.69 | 112.93 |
| 2 | 154-A | 201 | FOL | CT-CA-N | -2.63 | 107.69 | 112.93 |
| 2 | 109-A | 201 | FOL | CB-CG-CD | -2.62 | 102.35 | 113.05 |
| 4 | 129-A | 204 | NAP | N3A-C2A-N1A | -2.62 | 126.81 | 128.87 |
| 2 | 73-A | 201 | FOL | CT-CA-N | -2.62 | 107.70 | 112.93 |
| 4 | 10-A | 204 | NAP | C1B-N9A-C4A | -2.62 | 123.88 | 126.81 |
| 4 | 89-A | 204 | NAP | O4D-C1D-N1N | -2.61 | 105.28 | 108.10 |
| 4 | 149-A | 204 | NAP | O2N-PN-O3 | -2.61 | 94.07 | 105.27 |
| 2 | 62-A | 201 | FOL | NA2-C2-N3 | -2.61 | 116.95 | 120.29 |
| 4 | 163-A | 204 | NAP | O4D-C1D-N1N | -2.61 | 105.29 | 108.10 |
| 2 | 54-A | 201 | FOL | CT-CA-N | -2.61 | 107.73 | 112.93 |
| 2 | 91-A | 201 | FOL | CT-CA-N | -2.61 | 107.73 | 112.93 |
| 4 | 61-A | 204 | NAP | O2A-PA-O5B | -2.61 | 95.81 | 108.24 |
| 4 | 5-A | 204 | NAP | N3A-C2A-N1A | -2.61 | 126.82 | 128.87 |
| 4 | 93-A | 204 | NAP | C1B-N9A-C4A | -2.60 | 123.90 | 126.81 |
| 4 | 25-A | 204 | NAP | O4D-C1D-N1N | -2.60 | 105.29 | 108.10 |
| 2 | 21-A | 201 | FOL | C16-C11-C12 | -2.60 | 115.05 | 118.61 |
| 2 | 76-A | 201 | FOL | C9-C6-C7 | -2.60 | 116.81 | 121.39 |
| 2 | 68-A | 201 | FOL | NA2-C2-N3 | -2.60 | 116.96 | 120.29 |
| 2 | 87-A | 201 | FOL | C16-C11-C12 | -2.60 | 115.05 | 118.61 |
| 2 | 95-A | 201 | FOL | NA2-C2-N3 | -2.60 | 116.96 | 120.29 |
| 2 | 126-A | 201 | FOL | C9-C6-C7 | -2.60 | 116.82 | 121.39 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 17-A | 204 | NAP | O4D-C1D-N1N | -2.59 | 105.30 | 108.10 |
| 2 | 36-A | 201 | FOL | CB-CA-N | -2.59 | 105.88 | 109.92 |
| 4 | 140-A | 204 | NAP | O2N-PN-O3 | -2.59 | 94.16 | 105.27 |
| 4 | 4-A | 204 | NAP | O4D-C1D-N1N | -2.59 | 105.31 | 108.10 |
| 2 | 78-A | 201 | FOL | CB-CA-N | -2.59 | 105.88 | 109.92 |
| 4 | 81-A | 204 | NAP | C1B-N9A-C4A | -2.59 | 123.92 | 126.81 |
| 4 | 44-A | 204 | NAP | O2A-PA-O5B | -2.59 | 95.90 | 108.24 |
| 4 | 15-A | 204 | NAP | O2A-PA-O5B | -2.58 | 95.94 | 108.24 |
| 2 | 130-A | 201 | FOL | NA2-C2-N3 | -2.58 | 116.99 | 120.29 |
| 4 | 54-A | 204 | NAP | O2A-PA-O3 | -2.58 | 94.22 | 105.27 |
| 4 | 120-A | 204 | NAP | O2N-PN-O3 | -2.58 | 94.22 | 105.27 |
| 4 | 124-A | 204 | NAP | O2A-PA-O5B | -2.58 | 95.95 | 108.24 |
| 4 | 103-A | 204 | NAP | O2A-PA-O5B | -2.58 | 95.96 | 108.24 |
| 4 | 115-A | 204 | NAP | O2N-PN-O3 | -2.57 | 94.24 | 105.27 |
| 4 | 86-A | 204 | NAP | C1B-N9A-C4A | -2.57 | 123.94 | 126.81 |
| 4 | 128-A | 204 | NAP | C1B-N9A-C4A | -2.57 | 123.94 | 126.81 |
| 4 | 126-A | 204 | NAP | N3A-C2A-N1A | -2.57 | 126.85 | 128.87 |
| 4 | 165-A | 204 | NAP | O2A-PA-O5B | -2.57 | 96.01 | 108.24 |
| 4 | 144-A | 204 | NAP | N3A-C2A-N1A | -2.57 | 126.86 | 128.87 |
| 2 | 155-A | 201 | FOL | CT-CA-N | -2.56 | 107.81 | 112.93 |
| 2 | 158-A | 201 | FOL | C16-C11-C12 | -2.56 | 115.10 | 118.61 |
| 4 | 60-A | 204 | NAP | O2A-PA-O5B | -2.56 | 96.01 | 108.24 |
| 4 | 165-A | 204 | NAP | O2N-PN-O3 | -2.56 | 94.28 | 105.27 |
| 4 | 75-A | 204 | NAP | O2A-PA-O5B | -2.56 | 96.02 | 108.24 |
| 4 | 107-A | 204 | NAP | O4D-C1D-N1N | -2.56 | 105.34 | 108.10 |
| 4 | 52-A | 204 | NAP | C1B-N9A-C4A | -2.56 | 123.95 | 126.81 |
| 4 | 81-A | 204 | NAP | O4D-C1D-N1N | -2.56 | 105.34 | 108.10 |
| 2 | 2-A | 201 | FOL | CT-CA-N | -2.56 | 107.82 | 112.93 |
| 4 | 87-A | 204 | NAP | O2A-PA-O5B | -2.56 | 96.04 | 108.24 |
| 2 | 92-A | 201 | FOL | NA2-C2-N3 | -2.56 | 117.01 | 120.29 |
| 4 | 50-A | 204 | NAP | O2N-PN-O3 | -2.56 | 94.30 | 105.27 |
| 4 | 145-A | 204 | NAP | C1B-N9A-C4A | -2.56 | 123.95 | 126.81 |
| 4 | 63-A | 204 | NAP | O2A-PA-O5B | -2.56 | 96.05 | 108.24 |
| 4 | 136-A | 204 | NAP | O2A-PA-O5B | -2.56 | 96.05 | 108.24 |
| 2 | 109-A | 201 | FOL | NA2-C2-N3 | -2.56 | 117.02 | 120.29 |
| 4 | 137-A | 204 | NAP | O2N-PN-O3 | -2.56 | 94.31 | 105.27 |
| 4 | 154-A | 204 | NAP | C1B-N9A-C4A | -2.56 | 123.95 | 126.81 |
| 4 | 107-A | 204 | NAP | N3A-C2A-N1A | -2.55 | 126.86 | 128.87 |
| 4 | 88-A | 204 | NAP | C1B-N9A-C4A | -2.55 | 123.95 | 126.81 |
| 4 | 72-A | 204 | NAP | N3A-C2A-N1A | -2.55 | 126.86 | 128.87 |
| 4 | 68-A | 204 | NAP | N3A-C2A-N1A | -2.55 | 126.86 | 128.87 |
| 2 | 84-A | 201 | FOL | NA2-C2-N3 | -2.55 | 117.02 | 120.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 2-A | 204 | NAP | O2A-PA-O3 | -2.55 | 94.34 | 105.27 |
| 4 | 122-A | 204 | NAP | O4D-C1D-N1N | -2.55 | 105.35 | 108.10 |
| 4 | 130-A | 204 | NAP | O2N-PN-O3 | -2.55 | 94.35 | 105.27 |
| 4 | 70-A | 204 | NAP | O2N-PN-O3 | -2.55 | 94.35 | 105.27 |
| 4 | 38-A | 204 | NAP | C1B-N9A-C4A | -2.55 | 123.96 | 126.81 |
| 4 | 146-A | 204 | NAP | N3A-C2A-N1A | -2.55 | 126.87 | 128.87 |
| 2 | 123-A | 201 | FOL | CT-CA-N | -2.54 | 107.86 | 112.93 |
| 2 | 105-A | 201 | FOL | NA2-C2-N3 | -2.54 | 117.04 | 120.29 |
| 4 | 62-A | 204 | NAP | O2A-PA-O5B | -2.54 | 96.12 | 108.24 |
| 4 | 156-A | 204 | NAP | O2A-PA-O5B | -2.54 | 96.12 | 108.24 |
| 4 | 10-A | 204 | NAP | N3A-C2A-N1A | -2.54 | 126.88 | 128.87 |
| 4 | 104-A | 204 | NAP | O2A-PA-O5B | -2.54 | 96.13 | 108.24 |
| 2 | 65-A | 201 | FOL | C6-N5-C4A | -2.54 | 115.25 | 118.43 |
| 4 | 82-A | 204 | NAP | C1B-N9A-C4A | -2.54 | 123.97 | 126.81 |
| 2 | 8-A | 201 | FOL | CT-CA-N | -2.54 | 107.87 | 112.93 |
| 4 | 67-A | 204 | NAP | O2N-PN-O3 | -2.53 | 94.41 | 105.27 |
| 4 | 152-A | 204 | NAP | O2N-PN-O3 | -2.53 | 94.41 | 105.27 |
| 4 | 123-A | 204 | NAP | O2A-PA-O3 | -2.53 | 94.41 | 105.27 |
| 4 | 124-A | 204 | NAP | O4D-C1D-N1N | -2.53 | 105.37 | 108.10 |
| 4 | 145-A | 204 | NAP | N3A-C2A-N1A | -2.53 | 126.88 | 128.87 |
| 2 | 34-A | 201 | FOL | NA2-C2-N3 | -2.53 | 117.05 | 120.29 |
| 4 | 130-A | 204 | NAP | N3A-C2A-N1A | -2.53 | 126.88 | 128.87 |
| 4 | 49-A | 204 | NAP | C1B-N9A-C4A | -2.53 | 123.98 | 126.81 |
| 2 | 144-A | 201 | FOL | O-C-C11 | -2.53 | 116.62 | 120.95 |
| 4 | 5-A | 204 | NAP | O2N-PN-O3 | -2.52 | 94.46 | 105.27 |
| 4 | 142-A | 204 | NAP | C1B-N9A-C4A | -2.52 | 123.99 | 126.81 |
| 4 | 164-A | 204 | NAP | C1B-N9A-C4A | -2.52 | 123.99 | 126.81 |
| 4 | 127-A | 204 | NAP | N3A-C2A-N1A | -2.52 | 126.89 | 128.87 |
| 4 | 81-A | 204 | NAP | N6A-C6A-N1A | -2.52 | 114.28 | 118.52 |
| 4 | 2-A | 204 | NAP | O3D-C3D-C2D | -2.52 | 103.70 | 111.86 |
| 4 | 167-A | 204 | NAP | O2A-PA-O5B | -2.52 | 96.22 | 108.24 |
| 4 | 150-A | 204 | NAP | O7N-C7N-N7N | -2.52 | 118.99 | 122.58 |
| 4 | 16-A | 204 | NAP | O2A-PA-O5B | -2.52 | 96.24 | 108.24 |
| 2 | 47-A | 201 | FOL | C6-C9-N10 | -2.52 | 107.67 | 113.30 |
| 4 | 55-A | 204 | NAP | C1B-N9A-C4A | -2.51 | 124.00 | 126.81 |
| 4 | 95-A | 204 | NAP | O4D-C1D-N1N | -2.51 | 105.39 | 108.10 |
| 4 | 69-A | 204 | NAP | C1B-N9A-C4A | -2.51 | 124.00 | 126.81 |
| 4 | 148-A | 204 | NAP | O2N-PN-O3 | -2.51 | 94.50 | 105.27 |
| 4 | 122-A | 204 | NAP | O2N-PN-O3 | -2.51 | 94.51 | 105.27 |
| 4 | 150-A | 204 | NAP | O2A-PA-O5B | -2.51 | 96.28 | 108.24 |
| 2 | 31-A | 201 | FOL | CB-CG-CD | -2.51 | 102.82 | 113.05 |
| 2 | 162-A | 201 | FOL | CT-CA-N | -2.51 | 107.93 | 112.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 35-A | 204 | NAP | O2N-PN-O3 | -2.51 | 94.52 | 105.27 |
| 4 | 136-A | 204 | NAP | O4D-C1D-N1N | -2.51 | 105.40 | 108.10 |
| 4 | 166-A | 204 | NAP | O2N-PN-O3 | -2.51 | 94.53 | 105.27 |
| 4 | 37-A | 204 | NAP | O4D-C1D-N1N | -2.51 | 105.40 | 108.10 |
| 4 | 157-A | 204 | NAP | O4D-C1D-N1N | -2.50 | 105.40 | 108.10 |
| 4 | 41-A | 204 | NAP | O2A-PA-O5B | -2.50 | 96.31 | 108.24 |
| 4 | 13-A | 204 | NAP | O2A-PA-O5B | -2.50 | 96.31 | 108.24 |
| 2 | 51-A | 201 | FOL | CT-CA-N | -2.50 | 107.94 | 112.93 |
| 4 | 117-A | 204 | NAP | O2A-PA-O5B | -2.50 | 96.31 | 108.24 |
| 4 | 143-A | 204 | NAP | O2N-PN-O3 | -2.50 | 94.54 | 105.27 |
| 4 | 123-A | 204 | NAP | O2N-PN-O3 | -2.50 | 94.55 | 105.27 |
| 4 | 129-A | 204 | NAP | C1B-N9A-C4A | -2.50 | 124.01 | 126.81 |
| 4 | 113-A | 204 | NAP | O2A-PA-O5B | -2.50 | 96.32 | 108.24 |
| 4 | 116-A | 204 | NAP | O2N-PN-O3 | -2.50 | 94.55 | 105.27 |
| 4 | 5-A | 204 | NAP | O2A-PA-O5B | -2.50 | 96.33 | 108.24 |
| 2 | 23-A | 201 | FOL | NA2-C2-N3 | -2.50 | 117.09 | 120.29 |
| 4 | 126-A | 204 | NAP | O2N-PN-O3 | -2.50 | 94.56 | 105.27 |
| 2 | 64-A | 201 | FOL | O-C-C11 | -2.50 | 116.67 | 120.95 |
| 4 | 78-A | 204 | NAP | O2A-PA-O5B | -2.50 | 96.33 | 108.24 |
| 4 | 128-A | 204 | NAP | N3A-C2A-N1A | -2.50 | 126.91 | 128.87 |
| 4 | 18-A | 204 | NAP | C1B-N9A-C4A | -2.49 | 124.02 | 126.81 |
| 2 | 54-A | 201 | FOL | C13-C14-N10 | -2.49 | 116.08 | 121.04 |
| 4 | 39-A | 204 | NAP | O2N-PN-O3 | -2.49 | 94.58 | 105.27 |
| 4 | 112-A | 204 | NAP | C1B-N9A-C4A | -2.49 | 124.02 | 126.81 |
| 4 | 144-A | 204 | NAP | O2N-PN-O3 | -2.49 | 94.59 | 105.27 |
| 4 | 139-A | 204 | NAP | O7N-C7N-N7N | -2.49 | 119.03 | 122.58 |
| 2 | 83-A | 201 | FOL | C6-N5-C4A | -2.49 | 115.31 | 118.43 |
| 2 | 75-A | 201 | FOL | NA2-C2-N3 | -2.49 | 117.10 | 120.29 |
| 4 | 111-A | 204 | NAP | O4D-C1D-N1N | -2.49 | 105.42 | 108.10 |
| 4 | 36-A | 204 | NAP | C1B-N9A-C4A | -2.48 | 124.03 | 126.81 |
| 4 | 17-A | 204 | NAP | O2N-PN-O3 | -2.48 | 94.64 | 105.27 |
| 4 | 130-A | 204 | NAP | O4D-C1D-N1N | -2.48 | 105.43 | 108.10 |
| 4 | 95-A | 204 | NAP | O2A-PA-O5B | -2.48 | 96.43 | 108.24 |
| 4 | 141-A | 204 | NAP | N3A-C2A-N1A | -2.48 | 126.92 | 128.87 |
| 4 | 167-A | 204 | NAP | O2N-PN-O3 | -2.48 | 94.66 | 105.27 |
| 4 | 23-A | 204 | NAP | O2N-PN-O5D | -2.47 | 96.45 | 108.24 |
| 4 | 147-A | 204 | NAP | N3A-C2A-N1A | -2.47 | 126.93 | 128.87 |
| 4 | 15-A | 204 | NAP | C1B-N9A-C4A | -2.47 | 124.05 | 126.81 |
| 2 | 57-A | 201 | FOL | NA2-C2-N3 | -2.47 | 117.13 | 120.29 |
| 4 | 151-A | 204 | NAP | N3A-C2A-N1A | -2.47 | 126.93 | 128.87 |
| 4 | 78-A | 204 | NAP | O2A-PA-O3 | -2.47 | 94.70 | 105.27 |
| 2 | 158-A | 201 | FOL | C6-N5-C4A | -2.47 | 115.34 | 118.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 60-A | 204 | NAP | O2N-PN-O3 | -2.46 | 94.71 | 105.27 |
| 4 | 12-A | 204 | NAP | O2A-PA-O5B | -2.46 | 96.49 | 108.24 |
| 4 | 4-A | 204 | NAP | O2A-PA-O3 | -2.46 | 94.72 | 105.27 |
| 4 | 98-A | 204 | NAP | O2A-PA-O5B | -2.46 | 96.50 | 108.24 |
| 4 | 140-A | 204 | NAP | N3A-C2A-N1A | -2.46 | 126.94 | 128.87 |
| 4 | 45-A | 204 | NAP | O2A-PA-O5B | -2.46 | 96.52 | 108.24 |
| 4 | 125-A | 204 | NAP | O2A-PA-O5B | -2.46 | 96.52 | 108.24 |
| 4 | 74-A | 204 | NAP | O2A-PA-O5B | -2.46 | 96.52 | 108.24 |
| 4 | 43-A | 204 | NAP | O2N-PN-O3 | -2.45 | 94.75 | 105.27 |
| 4 | 145-A | 204 | NAP | O2N-PN-O3 | -2.45 | 94.76 | 105.27 |
| 2 | 167-A | 201 | FOL | C13-C14-N10 | -2.45 | 116.16 | 121.04 |
| 4 | 136-A | 204 | NAP | O2N-PN-O3 | -2.45 | 94.76 | 105.27 |
| 2 | 138-A | 201 | FOL | NA2-C2-N3 | -2.45 | 117.15 | 120.29 |
| 4 | 14-A | 204 | NAP | O2A-PA-O5B | -2.45 | 96.56 | 108.24 |
| 4 | 108-A | 204 | NAP | O7N-C7N-N7N | -2.45 | 119.09 | 122.58 |
| 4 | 92-A | 204 | NAP | C1B-N9A-C4A | -2.44 | 124.08 | 126.81 |
| 4 | 77-A | 204 | NAP | O2A-PA-O5B | -2.44 | 96.59 | 108.24 |
| 4 | 56-A | 204 | NAP | O7N-C7N-C3N | -2.44 | 116.89 | 119.60 |
| 4 | 139-A | 204 | NAP | O2A-PA-O5B | -2.44 | 96.59 | 108.24 |
| 4 | 41-A | 204 | NAP | O2N-PN-O3 | -2.44 | 94.80 | 105.27 |
| 2 | 37-A | 201 | FOL | C9-C6-C7 | -2.44 | 117.09 | 121.39 |
| 2 | 124-A | 201 | FOL | NA2-C2-N3 | -2.44 | 117.16 | 120.29 |
| 4 | 124-A | 204 | NAP | O2A-PA-O3 | -2.44 | 94.81 | 105.27 |
| 4 | 25-A | 204 | NAP | O2A-PA-O5B | -2.44 | 96.60 | 108.24 |
| 4 | 42-A | 204 | NAP | O2N-PN-O3 | -2.44 | 94.81 | 105.27 |
| 4 | 158-A | 204 | NAP | C1B-N9A-C4A | -2.44 | 124.08 | 126.81 |
| 2 | 87-A | 201 | FOL | CT-CA-N | -2.44 | 108.06 | 112.93 |
| 4 | 37-A | 204 | NAP | C1B-N9A-C4A | -2.44 | 124.08 | 126.81 |
| 4 | 43-A | 204 | NAP | O2A-PA-O5B | -2.44 | 96.62 | 108.24 |
| 4 | 106-A | 204 | NAP | C1B-N9A-C4A | -2.44 | 124.08 | 126.81 |
| 4 | 116-A | 204 | NAP | O2A-PA-O5B | -2.44 | 96.62 | 108.24 |
| 4 | 34-A | 204 | NAP | O4D-C1D-N1N | -2.44 | 105.47 | 108.10 |
| 2 | 145-A | 201 | FOL | CT-CA-N | -2.44 | 108.07 | 112.93 |
| 2 | 52-A | 201 | FOL | C13-C14-N10 | -2.43 | 116.20 | 121.04 |
| 4 | 127-A | 204 | NAP | O2N-PN-O3 | -2.43 | 94.84 | 105.27 |
| 4 | 165-A | 204 | NAP | C1B-N9A-C4A | -2.43 | 124.09 | 126.81 |
| 4 | 73-A | 204 | NAP | O2A-PA-O5B | -2.43 | 96.64 | 108.24 |
| 4 | 116-A | 204 | NAP | N3A-C2A-N1A | -2.43 | 126.96 | 128.87 |
| 4 | 91-A | 204 | NAP | O2A-PA-O5B | -2.43 | 96.65 | 108.24 |
| 4 | 80-A | 204 | NAP | O2N-PN-O3 | -2.43 | 94.85 | 105.27 |
| 2 | 52-A | 201 | FOL | NA2-C2-N3 | -2.43 | 117.18 | 120.29 |
| 4 | 6-A | 204 | NAP | O3D-C3D-C2D | -2.43 | 104.00 | 111.86 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 154-A | 204 | NAP | N3A-C2A-N1A | -2.43 | 126.97 | 128.87 |
| 4 | 41-A | 204 | NAP | C1B-N9A-C4A | -2.43 | 124.10 | 126.81 |
| 2 | 42-A | 201 | FOL | C16-C11-C12 | -2.43 | 115.29 | 118.61 |
| 4 | 160-A | 204 | NAP | O2N-PN-O3 | -2.43 | 94.87 | 105.27 |
| 4 | 166-A | 204 | NAP | O2A-PA-O5B | -2.42 | 96.68 | 108.24 |
| 4 | 79-A | 204 | NAP | O2A-PA-O3 | -2.42 | 94.89 | 105.27 |
| 4 | 1-A | 204 | NAP | O2A-PA-O5B | -2.42 | 96.70 | 108.24 |
| 4 | 11-A | 204 | NAP | C1B-N9A-C4A | -2.42 | 124.11 | 126.81 |
| 4 | 77-A | 204 | NAP | O2A-PA-O3 | -2.42 | 94.90 | 105.27 |
| 4 | 111-A | 204 | NAP | O2A-PA-O5B | -2.42 | 96.72 | 108.24 |
| 4 | 148-A | 204 | NAP | O2A-PA-O5B | -2.42 | 96.72 | 108.24 |
| 4 | 55-A | 204 | NAP | O2A-PA-O5B | -2.42 | 96.72 | 108.24 |
| 4 | 100-A | 204 | NAP | O2N-PN-O3 | -2.42 | 94.92 | 105.27 |
| 4 | 32-A | 204 | NAP | O4D-C1D-N1N | -2.41 | 105.50 | 108.10 |
| 4 | 146-A | 204 | NAP | O2N-PN-O3 | -2.41 | 94.92 | 105.27 |
| 4 | 35-A | 204 | NAP | C1B-N9A-C4A | -2.41 | 124.11 | 126.81 |
| 4 | 86-A | 204 | NAP | O2A-PA-O5B | -2.41 | 96.75 | 108.24 |
| 4 | 110-A | 204 | NAP | C1B-N9A-C4A | -2.41 | 124.11 | 126.81 |
| 4 | 118-A | 204 | NAP | O2A-PA-O5B | -2.41 | 96.75 | 108.24 |
| 2 | 106-A | 201 | FOL | NA2-C2-N3 | -2.41 | 117.21 | 120.29 |
| 2 | 119-A | 201 | FOL | CT-CA-N | -2.41 | 108.13 | 112.93 |
| 4 | 62-A | 204 | NAP | O2N-PN-O3 | -2.41 | 94.96 | 105.27 |
| 4 | 149-A | 204 | NAP | O2A-PA-O5B | -2.40 | 96.79 | 108.24 |
| 2 | 21-A | 201 | FOL | C9-C6-C7 | -2.40 | 117.17 | 121.39 |
| 4 | 12-A | 204 | NAP | O2N-PN-O3 | -2.40 | 94.99 | 105.27 |
| 4 | 50-A | 204 | NAP | O2A-PA-O5B | -2.40 | 96.81 | 108.24 |
| 4 | 151-A | 204 | NAP | O4D-C1D-N1N | -2.40 | 105.52 | 108.10 |
| 2 | 136-A | 201 | FOL | CT-CA-N | -2.40 | 108.15 | 112.93 |
| 4 | 32-A | 204 | NAP | O2X-P2B-O2B | -2.39 | 99.46 | 106.62 |
| 4 | 90-A | 204 | NAP | O2A-PA-O5B | -2.39 | 96.83 | 108.24 |
| 4 | 135-A | 204 | NAP | O2N-PN-O3 | -2.39 | 95.01 | 105.27 |
| 4 | 91-A | 204 | NAP | O2N-PN-O3 | -2.39 | 95.02 | 105.27 |
| 4 | 30-A | 204 | NAP | O2A-PA-O5B | -2.39 | 96.85 | 108.24 |
| 4 | 17-A | 204 | NAP | O2A-PA-O5B | -2.39 | 96.86 | 108.24 |
| 4 | 10-A | 204 | NAP | O2N-PN-O3 | -2.39 | 95.04 | 105.27 |
| 4 | 102-A | 204 | NAP | O2N-PN-O3 | -2.39 | 95.04 | 105.27 |
| 4 | 109-A | 204 | NAP | N3A-C2A-N1A | -2.39 | 127.00 | 128.87 |
| 4 | 66-A | 204 | NAP | O2N-PN-O3 | -2.39 | 95.04 | 105.27 |
| 4 | 125-A | 204 | NAP | O2A-PA-O3 | -2.38 | 95.05 | 105.27 |
| 4 | 76-A | 204 | NAP | O2A-PA-O5B | -2.38 | 96.88 | 108.24 |
| 4 | 77-A | 204 | NAP | N3A-C2A-N1A | -2.38 | 127.00 | 128.87 |
| 4 | 147-A | 204 | NAP | O2N-PN-O3 | -2.38 | 95.07 | 105.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 23-A | 204 | NAP | O2A-PA-O3 | -2.38 | 95.07 | 105.27 |
| 2 | 138-A | 201 | FOL | C15-C14-C13 | -2.38 | 115.75 | 119.06 |
| 4 | 156-A | 204 | NAP | O2X-P2B-O2B | -2.38 | 99.51 | 106.62 |
| 4 | 40-A | 204 | NAP | O2N-PN-O3 | -2.38 | 95.08 | 105.27 |
| 4 | 68-A | 204 | NAP | O2N-PN-O3 | -2.38 | 95.09 | 105.27 |
| 4 | 66-A | 204 | NAP | O2A-PA-O5B | -2.38 | 96.92 | 108.24 |
| 4 | 36-A | 204 | NAP | O2A-PA-O5B | -2.37 | 96.92 | 108.24 |
| 2 | 107-A | 201 | FOL | CB-CG-CD | -2.37 | 103.37 | 113.05 |
| 4 | 67-A | 204 | NAP | O2A-PA-O5B | -2.37 | 96.93 | 108.24 |
| 4 | 164-A | 204 | NAP | O7N-C7N-N7N | -2.37 | 119.20 | 122.58 |
| 2 | 96-A | 201 | FOL | CT-CA-N | -2.37 | 108.20 | 112.93 |
| 4 | 72-A | 204 | NAP | O2N-PN-O3 | -2.37 | 95.11 | 105.27 |
| 4 | 53-A | 204 | NAP | O2A-PA-O5B | -2.37 | 96.94 | 108.24 |
| 4 | 23-A | 204 | NAP | O2A-PA-O5B | -2.37 | 96.94 | 108.24 |
| 4 | 137-A | 204 | NAP | C1B-N9A-C4A | -2.37 | 124.16 | 126.81 |
| 4 | 74-A | 204 | NAP | O2N-PN-O3 | -2.37 | 95.12 | 105.27 |
| 4 | 13-A | 204 | NAP | O2N-PN-O3 | -2.37 | 95.12 | 105.27 |
| 4 | 119-A | 204 | NAP | O2A-PA-O5B | -2.37 | 96.96 | 108.24 |
| 4 | 126-A | 204 | NAP | O2A-PA-O5B | -2.37 | 96.96 | 108.24 |
| 4 | 112-A | 204 | NAP | O2A-PA-O5B | -2.37 | 96.96 | 108.24 |
| 2 | 23-A | 201 | FOL | C13-C14-N10 | -2.36 | 116.34 | 121.04 |
| 2 | 118-A | 201 | FOL | O-C-N | -2.36 | 118.17 | 122.45 |
| 4 | 85-A | 204 | NAP | O2A-PA-O5B | -2.36 | 96.98 | 108.24 |
| 4 | 46-A | 204 | NAP | O2A-PA-O5B | -2.36 | 96.99 | 108.24 |
| 4 | 61-A | 204 | NAP | O2N-PN-O3 | -2.36 | 95.17 | 105.27 |
| 4 | 164-A | 204 | NAP | O2A-PA-O5B | -2.36 | 97.00 | 108.24 |
| 2 | 73-A | 201 | FOL | CB-CG-CD | -2.36 | 103.44 | 113.05 |
| 4 | 11-A | 204 | NAP | O2A-PA-O5B | -2.36 | 97.00 | 108.24 |
| 4 | 48-A | 204 | NAP | O2A-PA-O5B | -2.36 | 97.01 | 108.24 |
| 4 | 96-A | 204 | NAP | O4D-C1D-N1N | -2.36 | 105.56 | 108.10 |
| 4 | 111-A | 204 | NAP | O2N-PN-O3 | -2.35 | 95.18 | 105.27 |
| 4 | 71-A | 204 | NAP | O2N-PN-O3 | -2.35 | 95.18 | 105.27 |
| 4 | 142-A | 204 | NAP | O2A-PA-O5B | -2.35 | 97.03 | 108.24 |
| 4 | 97-A | 204 | NAP | O2A-PA-O5B | -2.35 | 97.03 | 108.24 |
| 2 | 136-A | 201 | FOL | CB-CA-N | -2.35 | 106.25 | 109.92 |
| 4 | 29-A | 204 | NAP | O2N-PN-O3 | -2.35 | 95.20 | 105.27 |
| 4 | 115-A | 204 | NAP | O2A-PA-O5B | -2.35 | 97.04 | 108.24 |
| 4 | 10-A | 204 | NAP | O4D-C1D-N1N | -2.35 | 105.57 | 108.10 |
| 4 | 22-A | 204 | NAP | O2A-PA-O5B | -2.35 | 97.05 | 108.24 |
| 4 | 124-A | 204 | NAP | N3A-C2A-N1A | -2.35 | 127.03 | 128.87 |
| 4 | 39-A | 204 | NAP | O2A-PA-O5B | -2.35 | 97.06 | 108.24 |
| 4 | 154-A | 204 | NAP | O2A-PA-O3 | -2.34 | 95.22 | 105.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 129-A | 204 | NAP | O4D-C1D-N1N | -2.34 | 105.57 | 108.10 |
| 4 | 36-A | 204 | NAP | O2N-PN-O3 | -2.34 | 95.23 | 105.27 |
| 2 | 73-A | 201 | FOL | NA2-C2-N3 | -2.34 | 117.30 | 120.29 |
| 4 | 142-A | 204 | NAP | O2N-PN-O3 | -2.34 | 95.24 | 105.27 |
| 4 | 100-A | 204 | NAP | O2A-PA-O5B | -2.34 | 97.09 | 108.24 |
| 4 | 141-A | 204 | NAP | O4D-C1D-N1N | -2.34 | 105.58 | 108.10 |
| 4 | 33-A | 204 | NAP | O4D-C1D-N1N | -2.34 | 105.58 | 108.10 |
| 4 | 101-A | 204 | NAP | O2A-PA-O5B | -2.34 | 97.10 | 108.24 |
| 4 | 46-A | 204 | NAP | O2N-PN-O3 | -2.33 | 95.26 | 105.27 |
| 4 | 92-A | 204 | NAP | O2A-PA-O5B | -2.33 | 97.11 | 108.24 |
| 4 | 112-A | 204 | NAP | O4D-C1D-N1N | -2.33 | 105.58 | 108.10 |
| 4 | 92-A | 204 | NAP | O2N-PN-O3 | -2.33 | 95.27 | 105.27 |
| 4 | 139-A | 204 | NAP | O2N-PN-O3 | -2.33 | 95.27 | 105.27 |
| 2 | 164-A | 201 | FOL | CT-CA-N | -2.33 | 108.28 | 112.93 |
| 4 | 152-A | 204 | NAP | O4D-C1D-N1N | -2.33 | 105.59 | 108.10 |
| 4 | 135-A | 204 | NAP | N3A-C2A-N1A | -2.33 | 127.04 | 128.87 |
| 4 | 147-A | 204 | NAP | O4D-C1D-N1N | -2.33 | 105.59 | 108.10 |
| 4 | 101-A | 204 | NAP | O2N-PN-O3 | -2.33 | 95.30 | 105.27 |
| 4 | 20-A | 204 | NAP | O2N-PN-O3 | -2.32 | 95.30 | 105.27 |
| 4 | 26-A | 204 | NAP | O2A-PA-O5B | -2.32 | 97.16 | 108.24 |
| 4 | 69-A | 204 | NAP | O2A-PA-O5B | -2.32 | 97.16 | 108.24 |
| 4 | 135-A | 204 | NAP | O4D-C1D-N1N | -2.32 | 105.60 | 108.10 |
| 4 | 114-A | 204 | NAP | O2A-PA-O5B | -2.32 | 97.17 | 108.24 |
| 4 | 88-A | 204 | NAP | O2A-PA-O5B | -2.32 | 97.17 | 108.24 |
| 4 | 113-A | 204 | NAP | O2N-PN-O3 | -2.32 | 95.32 | 105.27 |
| 4 | 144-A | 204 | NAP | C1B-N9A-C4A | -2.32 | 124.22 | 126.81 |
| 4 | 24-A | 204 | NAP | O2A-PA-O5B | -2.32 | 97.19 | 108.24 |
| 4 | 164-A | 204 | NAP | O4D-C1D-N1N | -2.32 | 105.60 | 108.10 |
| 4 | 110-A | 204 | NAP | O2A-PA-O5B | -2.32 | 97.20 | 108.24 |
| 4 | 140-A | 204 | NAP | O2A-PA-O5B | -2.31 | 97.22 | 108.24 |
| 4 | 21-A | 204 | NAP | N3A-C2A-N1A | -2.31 | 127.06 | 128.87 |
| 2 | 1-A | 201 | FOL | C13-C14-N10 | -2.31 | 116.44 | 121.04 |
| 4 | 47-A | 204 | NAP | O4D-C1D-N1N | -2.31 | 105.61 | 108.10 |
| 2 | 32-A | 201 | FOL | CT-CA-N | -2.31 | 108.33 | 112.93 |
| 4 | 14-A | 204 | NAP | C1B-N9A-C4A | -2.31 | 124.23 | 126.81 |
| 4 | 161-A | 204 | NAP | O2A-PA-O5B | -2.31 | 97.24 | 108.24 |
| 4 | 65-A | 204 | NAP | O2A-PA-O5B | -2.31 | 97.24 | 108.24 |
| 4 | 143-A | 204 | NAP | O2A-PA-O5B | -2.31 | 97.24 | 108.24 |
| 2 | 83-A | 201 | FOL | NA2-C2-N3 | -2.31 | 117.34 | 120.29 |
| 4 | 69-A | 204 | NAP | O2N-PN-O3 | -2.31 | 95.39 | 105.27 |
| 4 | 96-A | 204 | NAP | O2A-PA-O5B | -2.30 | 97.25 | 108.24 |
| 4 | 35-A | 204 | NAP | O2A-PA-O5B | -2.30 | 97.25 | 108.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 40-A | 204 | NAP | O2A-PA-O5B | -2.30 | 97.25 | 108.24 |
| 2 | 24-A | 201 | FOL | C13-C14-N10 | -2.30 | 116.46 | 121.04 |
| 4 | 127-A | 204 | NAP | O2A-PA-O3 | -2.30 | 95.40 | 105.27 |
| 2 | 134-A | 201 | FOL | O-C-C11 | -2.30 | 117.01 | 120.95 |
| 4 | 108-A | 204 | NAP | O2B-P2B-O1X | -2.30 | 101.99 | 107.48 |
| 4 | 48-A | 204 | NAP | O2A-PA-O3 | -2.30 | 95.42 | 105.27 |
| 2 | 118-A | 201 | FOL | C15-C14-C13 | -2.30 | 115.86 | 119.06 |
| 4 | 109-A | 204 | NAP | O4D-C1D-N1N | -2.30 | 105.62 | 108.10 |
| 2 | 47-A | 201 | FOL | CT-CA-N | -2.30 | 108.35 | 112.93 |
| 4 | 143-A | 204 | NAP | C1B-N9A-C4A | -2.30 | 124.24 | 126.81 |
| 4 | 73-A | 204 | NAP | O2N-PN-O3 | -2.30 | 95.43 | 105.27 |
| 2 | 118-A | 201 | FOL | NA2-C2-N3 | -2.30 | 117.35 | 120.29 |
| 4 | 144-A | 204 | NAP | O2A-PA-O5B | -2.30 | 97.30 | 108.24 |
| 4 | 13-A | 204 | NAP | O3D-C3D-C2D | -2.29 | 104.44 | 111.86 |
| 4 | 88-A | 204 | NAP | N3A-C2A-N1A | -2.29 | 127.07 | 128.87 |
| 2 | 139-A | 201 | FOL | C16-C11-C12 | -2.29 | 115.47 | 118.61 |
| 2 | 129-A | 201 | FOL | C15-C14-C13 | -2.29 | 115.87 | 119.06 |
| 4 | 149-A | 204 | NAP | C1B-N9A-C4A | -2.29 | 124.25 | 126.81 |
| 4 | 162-A | 204 | NAP | O2N-PN-O3 | -2.29 | 95.47 | 105.27 |
| 4 | 163-A | 204 | NAP | O2A-PA-O5B | -2.29 | 97.34 | 108.24 |
| 4 | 135-A | 204 | NAP | O2A-PA-O5B | -2.29 | 97.34 | 108.24 |
| 4 | 97-A | 204 | NAP | C1B-N9A-C4A | -2.28 | 124.26 | 126.81 |
| 4 | 112-A | 204 | NAP | O2N-PN-O3 | -2.28 | 95.49 | 105.27 |
| 4 | 98-A | 204 | NAP | O2N-PN-O3 | -2.28 | 95.50 | 105.27 |
| 4 | 121-A | 204 | NAP | O2N-PN-O3 | -2.28 | 95.51 | 105.27 |
| 4 | 44-A | 204 | NAP | O2N-PN-O3 | -2.28 | 95.51 | 105.27 |
| 2 | 108-A | 201 | FOL | C13-C14-N10 | -2.28 | 116.51 | 121.04 |
| 4 | 163-A | 204 | NAP | O2N-PN-O3 | -2.27 | 95.52 | 105.27 |
| 4 | 119-A | 204 | NAP | O4D-C1D-N1N | -2.27 | 105.65 | 108.10 |
| 2 | 58-A | 201 | FOL | C13-C14-N10 | -2.27 | 116.52 | 121.04 |
| 4 | 11-A | 204 | NAP | O4D-C1D-N1N | -2.27 | 105.65 | 108.10 |
| 4 | 64-A | 204 | NAP | O2N-PN-O3 | -2.27 | 95.53 | 105.27 |
| 4 | 64-A | 204 | NAP | O2A-PA-O5B | -2.27 | 97.41 | 108.24 |
| 4 | 156-A | 204 | NAP | O2N-PN-O3 | -2.27 | 95.53 | 105.27 |
| 4 | 141-A | 204 | NAP | O2A-PA-O5B | -2.27 | 97.41 | 108.24 |
| 4 | 25-A | 204 | NAP | C1B-N9A-C4A | -2.27 | 124.27 | 126.81 |
| 4 | 110-A | 204 | NAP | O4D-C1D-N1N | -2.27 | 105.66 | 108.10 |
| 4 | 62-A | 204 | NAP | C1B-N9A-C4A | -2.27 | 124.28 | 126.81 |
| 4 | 52-A | 204 | NAP | O4D-C1D-N1N | -2.26 | 105.66 | 108.10 |
| 4 | 49-A | 204 | NAP | O2N-PN-O5D | -2.26 | 97.45 | 108.24 |
| 4 | 160-A | 204 | NAP | O2A-PA-O5B | -2.26 | 97.45 | 108.24 |
| 2 | 67-A | 201 | FOL | NA2-C2-N3 | -2.26 | 117.39 | 120.29 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 88-A | 204 | NAP | O2N-PN-O3 | -2.26 | 95.59 | 105.27 |
| 4 | 18-A | 204 | NAP | O2N-PN-O3 | -2.26 | 95.59 | 105.27 |
| 4 | 54-A | 204 | NAP | O2B-P2B-O1X | -2.26 | 102.09 | 107.48 |
| 4 | 153-A | 204 | NAP | O2A-PA-O5B | -2.26 | 97.48 | 108.24 |
| 4 | 93-A | 204 | NAP | O2N-PN-O3 | -2.25 | 95.61 | 105.27 |
| 4 | 10-A | 204 | NAP | O2A-PA-O5B | -2.25 | 97.50 | 108.24 |
| 4 | 43-A | 204 | NAP | O4D-C1D-N1N | -2.25 | 105.67 | 108.10 |
| 4 | 86-A | 204 | NAP | N3A-C2A-N1A | -2.25 | 127.10 | 128.87 |
| 4 | 2-A | 204 | NAP | O2A-PA-O5B | -2.25 | 97.51 | 108.24 |
| 2 | 98-A | 201 | FOL | CT-CA-N | -2.25 | 108.44 | 112.93 |
| 4 | 150-A | 204 | NAP | O2A-PA-O3 | -2.25 | 95.63 | 105.27 |
| 4 | 152-A | 204 | NAP | O2A-PA-O3 | -2.25 | 95.63 | 105.27 |
| 4 | 11-A | 204 | NAP | O2N-PN-O3 | -2.24 | 95.65 | 105.27 |
| 4 | 83-A | 204 | NAP | N6A-C6A-N1A | -2.24 | 114.75 | 118.52 |
| 2 | 85-A | 201 | FOL | CT-CA-N | -2.24 | 108.46 | 112.93 |
| 2 | 101-A | 201 | FOL | NA2-C2-N3 | -2.24 | 117.42 | 120.29 |
| 4 | 167-A | 204 | NAP | C1B-N9A-C4A | -2.24 | 124.31 | 126.81 |
| 4 | 47-A | 204 | NAP | O2A-PA-O5B | -2.24 | 97.56 | 108.24 |
| 4 | 165-A | 204 | NAP | O4D-C1D-N1N | -2.24 | 105.69 | 108.10 |
| 4 | 142-A | 204 | NAP | O4D-C1D-N1N | -2.24 | 105.69 | 108.10 |
| 4 | 63-A | 204 | NAP | O2N-PN-O3 | -2.24 | 95.68 | 105.27 |
| 4 | 152-A | 204 | NAP | O2A-PA-O5B | -2.24 | 97.58 | 108.24 |
| 4 | 47-A | 204 | NAP | O2N-PN-O3 | -2.24 | 95.68 | 105.27 |
| 4 | 70-A | 204 | NAP | O2A-PA-O5B | -2.24 | 97.58 | 108.24 |
| 4 | 26-A | 204 | NAP | C1B-N9A-C4A | -2.24 | 124.31 | 126.81 |
| 4 | 89-A | 204 | NAP | O2A-PA-O5B | -2.24 | 97.58 | 108.24 |
| 2 | 95-A | 201 | FOL | O-C-N | -2.23 | 118.41 | 122.45 |
| 2 | 137-A | 201 | FOL | NA2-C2-N3 | -2.23 | 117.43 | 120.29 |
| 4 | 65-A | 204 | NAP | O2N-PN-O3 | -2.23 | 95.70 | 105.27 |
| 4 | 59-A | 204 | NAP | C1B-N9A-C4A | -2.23 | 124.32 | 126.81 |
| 4 | 161-A | 204 | NAP | O2N-PN-O3 | -2.23 | 95.72 | 105.27 |
| 4 | 145-A | 204 | NAP | O2A-PA-O5B | -2.23 | 97.62 | 108.24 |
| 4 | 2-A | 204 | NAP | C1B-N9A-C4A | -2.23 | 124.32 | 126.81 |
| 4 | 90-A | 204 | NAP | O2N-PN-O3 | -2.23 | 95.72 | 105.27 |
| 4 | 39-A | 204 | NAP | N3A-C2A-N1A | -2.23 | 127.12 | 128.87 |
| 4 | 21-A | 204 | NAP | C1B-N9A-C4A | -2.23 | 124.32 | 126.81 |
| 4 | 1-A | 204 | NAP | O2A-PA-O3 | -2.22 | 95.74 | 105.27 |
| 2 | 87-A | 201 | FOL | NA2-C2-N3 | -2.22 | 117.44 | 120.29 |
| 2 | 17-A | 201 | FOL | NA2-C2-N3 | -2.22 | 117.45 | 120.29 |
| 4 | 151-A | 204 | NAP | O2A-PA-O5B | -2.22 | 97.65 | 108.24 |
| 4 | 132-A | 204 | NAP | C1B-N9A-C4A | -2.22 | 124.33 | 126.81 |
| 4 | 154-A | 204 | NAP | O4D-C1D-N1N | -2.22 | 105.71 | 108.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 25-A | 204 | NAP | N3A-C2A-N1A | -2.22 | 127.13 | 128.87 |
| 4 | 45-A | 204 | NAP | O2N-PN-O3 | -2.22 | 95.76 | 105.27 |
| 4 | 86-A | 204 | NAP | O2N-PN-O3 | -2.22 | 95.76 | 105.27 |
| 4 | 80-A | 204 | NAP | N3A-C2A-N1A | -2.22 | 127.13 | 128.87 |
| 4 | 143-A | 204 | NAP | N3A-C2A-N1A | -2.22 | 127.13 | 128.87 |
| 4 | 138-A | 204 | NAP | O4D-C1D-N1N | -2.22 | 105.71 | 108.10 |
| 2 | 10-A | 201 | FOL | O-C-N | -2.22 | 118.44 | 122.45 |
| 4 | 104-A | 204 | NAP | N3A-C2A-N1A | -2.22 | 127.13 | 128.87 |
| 4 | 72-A | 204 | NAP | O2A-PA-O5B | -2.22 | 97.68 | 108.24 |
| 2 | 103-A | 201 | FOL | CT-CA-N | -2.21 | 108.52 | 112.93 |
| 4 | 41-A | 204 | NAP | N3A-C2A-N1A | -2.21 | 127.13 | 128.87 |
| 2 | 76-A | 201 | FOL | CT-CA-N | -2.21 | 108.52 | 112.93 |
| 4 | 39-A | 204 | NAP | O3D-C3D-C2D | -2.21 | 104.71 | 111.86 |
| 4 | 57-A | 204 | NAP | C1B-N9A-C4A | -2.21 | 124.34 | 126.81 |
| 2 | 107-A | 201 | FOL | CT-CA-N | -2.21 | 108.53 | 112.93 |
| 4 | 116-A | 204 | NAP | C1B-N9A-C4A | -2.21 | 124.34 | 126.81 |
| 4 | 69-A | 204 | NAP | O2A-PA-O3 | -2.21 | 95.81 | 105.27 |
| 4 | 51-A | 204 | NAP | O2A-PA-O5B | -2.21 | 97.72 | 108.24 |
| 4 | 147-A | 204 | NAP | O2A-PA-O5B | -2.21 | 97.72 | 108.24 |
| 2 | 41-A | 201 | FOL | CT-CA-N | -2.21 | 108.53 | 112.93 |
| 4 | 122-A | 204 | NAP | O2A-PA-O3 | -2.20 | 95.82 | 105.27 |
| 4 | 107-A | 204 | NAP | O2N-PN-O3 | -2.20 | 95.82 | 105.27 |
| 2 | 146-A | 201 | FOL | CT-CA-N | -2.20 | 108.54 | 112.93 |
| 4 | 51-A | 204 | NAP | O2A-PA-O3 | -2.20 | 95.84 | 105.27 |
| 4 | 21-A | 204 | NAP | O2N-PN-O3 | -2.20 | 95.84 | 105.27 |
| 2 | 55-A | 201 | FOL | C13-C14-N10 | -2.20 | 116.67 | 121.04 |
| 4 | 120-A | 204 | NAP | O2A-PA-O5B | -2.20 | 97.76 | 108.24 |
| 4 | 162-A | 204 | NAP | O2A-PA-O5B | -2.20 | 97.77 | 108.24 |
| 4 | 83-A | 204 | NAP | O3D-C3D-C2D | -2.20 | 104.76 | 111.86 |
| 4 | 56-A | 204 | NAP | O4D-C4D-C5D | -2.19 | 101.44 | 109.29 |
| 4 | 9-A | 204 | NAP | O4D-C1D-N1N | -2.19 | 105.74 | 108.10 |
| 4 | 15-A | 204 | NAP | O4D-C1D-N1N | -2.19 | 105.74 | 108.10 |
| 2 | 58-A | 201 | FOL | NA2-C2-N3 | -2.19 | 117.49 | 120.29 |
| 4 | 46-A | 204 | NAP | C1B-N9A-C4A | -2.19 | 124.36 | 126.81 |
| 2 | 91-A | 201 | FOL | C11-C-N | -2.19 | 113.16 | 116.98 |
| 2 | 74-A | 201 | FOL | CB-CA-N | -2.19 | 106.50 | 109.92 |
| 4 | 55-A | 204 | NAP | O4D-C1D-N1N | -2.19 | 105.74 | 108.10 |
| 2 | 161-A | 201 | FOL | NA2-C2-N3 | -2.19 | 117.49 | 120.29 |
| 4 | 37-A | 204 | NAP | O2A-PA-O5B | -2.18 | 97.82 | 108.24 |
| 2 | 49-A | 201 | FOL | NA2-C2-N3 | -2.18 | 117.49 | 120.29 |
| 4 | 24-A | 204 | NAP | O2N-PN-O3 | -2.18 | 95.91 | 105.27 |
| 4 | 159-A | 204 | NAP | O2X-P2B-O2B | -2.18 | 100.09 | 106.62 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 85-A | 204 | NAP | O2N-PN-O3 | -2.18 | 95.92 | 105.27 |
| 4 | 6-A | 204 | NAP | C1B-N9A-C4A | -2.18 | 124.37 | 126.81 |
| 4 | 49-A | 204 | NAP | O2A-PA-O3 | -2.18 | 95.92 | 105.27 |
| 4 | 68-A | 204 | NAP | O2A-PA-O5B | -2.18 | 97.84 | 108.24 |
| 4 | 167-A | 204 | NAP | N3A-C2A-N1A | -2.18 | 127.16 | 128.87 |
| 4 | 94-A | 204 | NAP | O2N-PN-O3 | -2.18 | 95.94 | 105.27 |
| 4 | 51-A | 204 | NAP | O4D-C1D-N1N | -2.18 | 105.75 | 108.10 |
| 4 | 102-A | 204 | NAP | O4D-C1D-N1N | -2.18 | 105.75 | 108.10 |
| 4 | 33-A | 204 | NAP | O7N-C7N-N7N | -2.18 | 119.48 | 122.58 |
| 4 | 1-A | 204 | NAP | O2N-PN-O5D | -2.17 | 97.87 | 108.24 |
| 4 | 50-A | 204 | NAP | O2A-PA-O3 | -2.17 | 95.95 | 105.27 |
| 4 | 17-A | 204 | NAP | O2A-PA-O3 | -2.17 | 95.95 | 105.27 |
| 4 | 107-A | 204 | NAP | O2A-PA-O5B | -2.17 | 97.88 | 108.24 |
| 4 | 19-A | 204 | NAP | O2N-PN-O3 | -2.17 | 95.96 | 105.27 |
| 4 | 22-A | 204 | NAP | O7N-C7N-N7N | -2.17 | 119.49 | 122.58 |
| 4 | 75-A | 204 | NAP | O2N-PN-O3 | -2.17 | 95.97 | 105.27 |
| 4 | 74-A | 204 | NAP | N3A-C2A-N1A | -2.17 | 127.17 | 128.87 |
| 2 | 110-A | 201 | FOL | C13-C14-N10 | -2.17 | 116.73 | 121.04 |
| 2 | 142-A | 201 | FOL | NA2-C2-N3 | -2.17 | 117.52 | 120.29 |
| 4 | 115-A | 204 | NAP | C1B-N9A-C4A | -2.16 | 124.39 | 126.81 |
| 4 | 156-A | 204 | NAP | C1B-N9A-C4A | -2.16 | 124.39 | 126.81 |
| 2 | 31-A | 201 | FOL | C16-C11-C12 | -2.16 | 115.65 | 118.61 |
| 4 | 27-A | 204 | NAP | O2A-PA-O3 | -2.16 | 96.00 | 105.27 |
| 4 | 38-A | 204 | NAP | O4D-C1D-N1N | -2.16 | 105.77 | 108.10 |
| 2 | 82-A | 201 | FOL | O-C-N | -2.16 | 118.54 | 122.45 |
| 2 | 88-A | 201 | FOL | O-C-C11 | -2.16 | 117.25 | 120.95 |
| 4 | 3-A | 204 | NAP | N3A-C2A-N1A | -2.16 | 127.17 | 128.87 |
| 2 | 106-A | 201 | FOL | O-C-N | -2.15 | 118.55 | 122.45 |
| 4 | 85-A | 204 | NAP | C1B-N9A-C4A | -2.15 | 124.40 | 126.81 |
| 4 | 106-A | 204 | NAP | O2A-PA-O5B | -2.15 | 97.98 | 108.24 |
| 4 | 16-A | 204 | NAP | O2N-PN-O3 | -2.15 | 96.05 | 105.27 |
| 2 | 65-A | 201 | FOL | CB-CA-N | -2.15 | 106.56 | 109.92 |
| 4 | 105-A | 204 | NAP | O2A-PA-O5B | -2.15 | 98.00 | 108.24 |
| 4 | 148-A | 204 | NAP | O2A-PA-O3 | -2.15 | 96.07 | 105.27 |
| 4 | 99-A | 204 | NAP | O2A-PA-O3 | -2.14 | 96.08 | 105.27 |
| 2 | 136-A | 201 | FOL | C13-C14-N10 | -2.14 | 116.77 | 121.04 |
| 4 | 78-A | 204 | NAP | N3A-C2A-N1A | -2.14 | 127.19 | 128.87 |
| 4 | 102-A | 204 | NAP | O2A-PA-O5B | -2.14 | 98.02 | 108.24 |
| 4 | 93-A | 204 | NAP | N3A-C2A-N1A | -2.14 | 127.19 | 128.87 |
| 4 | 124-A | 204 | NAP | O2N-PN-O3 | -2.14 | 96.09 | 105.27 |
| 4 | 159-A | 204 | NAP | C1B-N9A-C4A | -2.14 | 124.42 | 126.81 |
| 4 | 103-A | 204 | NAP | O2A-PA-O3 | -2.14 | 96.10 | 105.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 71-A | 204 | NAP | O2A-PA-O5B | -2.14 | 98.04 | 108.24 |
| 4 | 39-A | 204 | NAP | C1B-N9A-C4A | -2.14 | 124.42 | 126.81 |
| 4 | 18-A | 204 | NAP | O2A-PA-O5B | -2.13 | 98.08 | 108.24 |
| 4 | 130-A | 204 | NAP | O2A-PA-O3 | -2.13 | 96.14 | 105.27 |
| 4 | 87-A | 204 | NAP | N3A-C2A-N1A | -2.13 | 127.20 | 128.87 |
| 2 | 116-A | 201 | FOL | C13-C14-N10 | -2.13 | 116.81 | 121.04 |
| 4 | 91-A | 204 | NAP | O4D-C1D-N1N | -2.13 | 105.81 | 108.10 |
| 4 | 38-A | 204 | NAP | O2N-PN-O3 | -2.13 | 96.15 | 105.27 |
| 4 | 165-A | 204 | NAP | O2A-PA-O3 | -2.13 | 96.16 | 105.27 |
| 4 | 16-A | 204 | NAP | C1B-N9A-C4A | -2.12 | 124.44 | 126.81 |
| 2 | 1-A | 201 | FOL | CT-CA-N | -2.12 | 108.70 | 112.93 |
| 2 | 71-A | 201 | FOL | CT-CA-N | -2.12 | 108.70 | 112.93 |
| 4 | 82-A | 204 | NAP | O2X-P2B-O2B | -2.12 | 100.28 | 106.62 |
| 4 | 148-A | 204 | NAP | O4D-C1D-N1N | -2.12 | 105.81 | 108.10 |
| 4 | 99-A | 204 | NAP | O2N-PN-O3 | -2.12 | 96.18 | 105.27 |
| 2 | 94-A | 201 | FOL | C9-C6-C7 | -2.12 | 117.66 | 121.39 |
| 4 | 161-A | 204 | NAP | O4D-C1D-N1N | -2.12 | 105.82 | 108.10 |
| 4 | 106-A | 204 | NAP | O2N-PN-O3 | -2.12 | 96.19 | 105.27 |
| 4 | 110-A | 204 | NAP | O2N-PN-O3 | -2.12 | 96.19 | 105.27 |
| 4 | 133-A | 204 | NAP | C1B-N9A-C4A | -2.12 | 124.44 | 126.81 |
| 4 | 166-A | 204 | NAP | C1B-N9A-C4A | -2.12 | 124.44 | 126.81 |
| 2 | 147-A | 201 | FOL | O-C-C11 | -2.11 | 117.33 | 120.95 |
| 4 | 16-A | 204 | NAP | O2A-PA-O3 | -2.11 | 96.22 | 105.27 |
| 2 | 34-A | 201 | FOL | C16-C11-C12 | -2.11 | 115.72 | 118.61 |
| 2 | 153-A | 201 | FOL | CB-CG-CD | -2.11 | 104.45 | 113.05 |
| 2 | 166-A | 201 | FOL | CT-CA-N | -2.11 | 108.73 | 112.93 |
| 4 | 93-A | 204 | NAP | O4D-C1D-N1N | -2.11 | 105.83 | 108.10 |
| 2 | 155-A | 201 | FOL | C16-C11-C12 | -2.10 | 115.73 | 118.61 |
| 4 | 167-A | 204 | NAP | O4D-C1D-N1N | -2.10 | 105.83 | 108.10 |
| 4 | 86-A | 204 | NAP | O3D-C3D-C2D | -2.10 | 105.06 | 111.86 |
| 4 | 51-A | 204 | NAP | C1B-N9A-C4A | -2.10 | 124.46 | 126.81 |
| 2 | 21-A | 201 | FOL | C6-N5-C4A | -2.10 | 115.80 | 118.43 |
| 4 | 80-A | 204 | NAP | O2A-PA-O3 | -2.09 | 96.29 | 105.27 |
| 2 | 32-A | 201 | FOL | C13-C14-N10 | -2.09 | 116.88 | 121.04 |
| 4 | 120-A | 204 | NAP | O3D-C3D-C2D | -2.09 | 105.09 | 111.86 |
| 4 | 56-A | 204 | NAP | C1B-N9A-C4A | -2.09 | 124.47 | 126.81 |
| 2 | 136-A | 201 | FOL | CB-CG-CD | -2.09 | 104.52 | 113.05 |
| 4 | 3-A | 204 | NAP | C1B-N9A-C4A | -2.09 | 124.47 | 126.81 |
| 2 | 15-A | 201 | FOL | C9-C6-C7 | -2.09 | 117.71 | 121.39 |
| 4 | 2-A | 204 | NAP | N3A-C2A-N1A | -2.09 | 127.23 | 128.87 |
| 2 | 150-A | 201 | FOL | CT-CA-N | -2.09 | 108.77 | 112.93 |
| 4 | 140-A | 204 | NAP | O4D-C1D-N1N | -2.09 | 105.85 | 108.10 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 38-A | 204 | NAP | O3D-C3D-C2D | -2.09 | 105.11 | 111.86 |
| 4 | 38-A | 204 | NAP | O2A-PA-O5B | -2.08 | 98.31 | 108.24 |
| 4 | 76-A | 204 | NAP | O2A-PA-O3 | -2.08 | 96.35 | 105.27 |
| 2 | 157-A | 201 | FOL | C6-N5-C4A | -2.08 | 115.83 | 118.43 |
| 2 | 92-A | 201 | FOL | CT-CA-N | -2.08 | 108.78 | 112.93 |
| 4 | 121-A | 204 | NAP | O2A-PA-O5B | -2.08 | 98.34 | 108.24 |
| 2 | 5-A | 201 | FOL | O-C-N | -2.08 | 118.69 | 122.45 |
| 2 | 6-A | 201 | FOL | C9-C6-C7 | -2.07 | 117.74 | 121.39 |
| 2 | 35-A | 201 | FOL | C13-C14-N10 | -2.07 | 116.91 | 121.04 |
| 4 | 106-A | 204 | NAP | O4D-C1D-N1N | -2.07 | 105.86 | 108.10 |
| 4 | 66-A | 204 | NAP | O2A-PA-O3 | -2.07 | 96.38 | 105.27 |
| 2 | 79-A | 201 | FOL | NA2-C2-N3 | -2.07 | 117.64 | 120.29 |
| 4 | 101-A | 204 | NAP | N3A-C2A-N1A | -2.07 | 127.25 | 128.87 |
| 4 | 15-A | 204 | NAP | N3A-C2A-N1A | -2.07 | 127.25 | 128.87 |
| 4 | 54-A | 204 | NAP | C1B-N9A-C4A | -2.07 | 124.50 | 126.81 |
| 4 | 53-A | 204 | NAP | O2A-PA-O3 | -2.07 | 96.42 | 105.27 |
| 4 | 56-A | 204 | NAP | O2X-P2B-O2B | -2.07 | 100.44 | 106.62 |
| 4 | 100-A | 204 | NAP | O2A-PA-O3 | -2.07 | 96.42 | 105.27 |
| 4 | 151-A | 204 | NAP | O2N-PN-O3 | -2.06 | 96.42 | 105.27 |
| 2 | 132-A | 201 | FOL | O-C-C11 | -2.06 | 117.41 | 120.95 |
| 4 | 126-A | 204 | NAP | O2A-PA-O3 | -2.06 | 96.43 | 105.27 |
| 4 | 117-A | 204 | NAP | O2A-PA-O3 | -2.06 | 96.43 | 105.27 |
| 4 | 14-A | 204 | NAP | O3D-C3D-C2D | -2.06 | 105.19 | 111.86 |
| 4 | 125-A | 204 | NAP | O2N-PN-O3 | -2.06 | 96.45 | 105.27 |
| 2 | 151-A | 201 | FOL | O-C-N | -2.06 | 118.73 | 122.45 |
| 4 | 15-A | 204 | NAP | O2A-PA-O3 | -2.05 | 96.47 | 105.27 |
| 4 | 146-A | 204 | NAP | O2A-PA-O5B | -2.05 | 98.45 | 108.24 |
| 2 | 40-A | 201 | FOL | CT-CA-N | -2.05 | 108.84 | 112.93 |
| 4 | 65-A | 204 | NAP | C2B-C3B-C4B | -2.05 | 96.99 | 101.85 |
| 2 | 100-A | 201 | FOL | C6-N5-C4A | -2.05 | 115.86 | 118.43 |
| 2 | 155-A | 201 | FOL | CB-CG-CD | -2.05 | 104.68 | 113.05 |
| 4 | 22-A | 204 | NAP | O2N-PN-O3 | -2.04 | 96.52 | 105.27 |
| 4 | 53-A | 204 | NAP | O4D-C1D-N1N | -2.04 | 105.90 | 108.10 |
| 4 | 155-A | 204 | NAP | C1B-N9A-C4A | -2.04 | 124.53 | 126.81 |
| 4 | 19-A | 204 | NAP | O2A-PA-O5B | -2.04 | 98.51 | 108.24 |
| 4 | 27-A | 204 | NAP | C1B-N9A-C4A | -2.04 | 124.53 | 126.81 |
| 4 | 53-A | 204 | NAP | C1B-N9A-C4A | -2.04 | 124.53 | 126.81 |
| 4 | 121-A | 204 | NAP | C1B-N9A-C4A | -2.04 | 124.53 | 126.81 |
| 4 | 97-A | 204 | NAP | O2N-PN-O3 | -2.03 | 96.55 | 105.27 |
| 2 | 143-A | 201 | FOL | C11-C-N | -2.03 | 113.43 | 116.98 |
| 4 | 110-A | 204 | NAP | O2A-PA-O3 | -2.03 | 96.56 | 105.27 |
| 2 | 79-A | 201 | FOL | C13-C14-N10 | -2.03 | 117.00 | 121.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 4 | 40-A | 204 | NAP | O4D-C1D-N1N | -2.03 | 105.92 | 108.10 |
| 4 | 55-A | 204 | NAP | O2N-PN-O3 | -2.03 | 96.58 | 105.27 |
| 4 | 116-A | 204 | NAP | O2A-PA-O3 | -2.03 | 96.59 | 105.27 |
| 4 | 142-A | 204 | NAP | O7N-C7N-C3N | -2.02 | 117.35 | 119.60 |
| 4 | 156-A | 204 | NAP | O2A-PA-O3 | -2.02 | 96.59 | 105.27 |
| 4 | 141-A | 204 | NAP | C1B-N9A-C4A | -2.02 | 124.55 | 126.81 |
| 2 | 97-A | 201 | FOL | CB-CG-CD | -2.02 | 104.80 | 113.05 |
| 4 | 89-A | 204 | NAP | N3A-C2A-N1A | -2.02 | 127.28 | 128.87 |
| 4 | 17-A | 204 | NAP | N3A-C2A-N1A | -2.02 | 127.28 | 128.87 |
| 4 | 76-A | 204 | NAP | O4D-C1D-N1N | -2.02 | 105.92 | 108.10 |
| 4 | 151-A | 204 | NAP | O2A-PA-O3 | -2.02 | 96.61 | 105.27 |
| 4 | 52-A | 204 | NAP | O2A-PA-O3 | -2.02 | 96.61 | 105.27 |
| 4 | 50-A | 204 | NAP | O4D-C1D-N1N | -2.02 | 105.92 | 108.10 |
| 2 | 132-A | 201 | FOL | CT-CA-N | -2.02 | 108.91 | 112.93 |
| 2 | 34-A | 201 | FOL | CT-CA-N | -2.02 | 108.91 | 112.93 |
| 4 | 102-A | 204 | NAP | O2A-PA-O3 | -2.02 | 96.62 | 105.27 |
| 2 | 77-A | 201 | FOL | NA2-C2-N3 | -2.02 | 117.71 | 120.29 |
| 2 | 104-A | 201 | FOL | O-C-C11 | -2.02 | 117.50 | 120.95 |
| 2 | 36-A | 201 | FOL | CT-CA-N | -2.02 | 108.91 | 112.93 |
| 4 | 146-A | 204 | NAP | C1B-N9A-C4A | -2.01 | 124.56 | 126.81 |
| 2 | 13-A | 201 | FOL | NA2-C2-N3 | -2.01 | 117.71 | 120.29 |
| 2 | 42-A | 201 | FOL | C9-C6-C7 | -2.01 | 117.85 | 121.39 |
| 4 | 166-A | 204 | NAP | O2A-PA-O3 | -2.01 | 96.64 | 105.27 |
| 4 | 126-A | 204 | NAP | C1B-N9A-C4A | -2.01 | 124.56 | 126.81 |
| 2 | 158-A | 201 | FOL | NA2-C2-N3 | -2.01 | 117.72 | 120.29 |
| 4 | 150-A | 204 | NAP | N3A-C2A-N1A | -2.01 | 127.29 | 128.87 |
| 2 | 9-A | 201 | FOL | C13-C14-N10 | -2.01 | 117.04 | 121.04 |
| 2 | 121-A | 201 | FOL | NA2-C2-N3 | -2.01 | 117.72 | 120.29 |
| 4 | 59-A | 204 | NAP | O2N-PN-O3 | -2.01 | 96.67 | 105.27 |
| 4 | 74-A | 204 | NAP | O2A-PA-O3 | -2.01 | 96.67 | 105.27 |
| 4 | 153-A | 204 | NAP | N3A-C2A-N1A | -2.01 | 127.30 | 128.87 |
| 4 | 112-A | 204 | NAP | O2B-P2B-O1X | -2.01 | 102.69 | 107.48 |
| 2 | 116-A | 201 | FOL | NA2-C2-N3 | -2.00 | 117.72 | 120.29 |
| 2 | 30-A | 201 | FOL | CB-CG-CD | -2.00 | 104.87 | 113.05 |
| 4 | 28-A | 204 | NAP | C1B-N9A-C4A | -2.00 | 124.57 | 126.81 |
| 2 | 149-A | 201 | FOL | CT-CA-N | -2.00 | 108.94 | 112.93 |
| 4 | 72-A | 204 | NAP | O7N-C7N-N7N | -2.00 | 119.73 | 122.58 |
| 4 | 162-A | 204 | NAP | C2N-C3N-C4N | 2.00 | 120.54 | 118.27 |
| 4 | 58-A | 204 | NAP | O3B-C3B-C2B | 2.00 | 116.91 | 111.13 |
| 4 | 103-A | 204 | NAP | C2N-C3N-C4N | 2.00 | 120.54 | 118.27 |
| 2 | 70-A | 201 | FOL | O-C-N | 2.01 | 126.08 | 122.45 |
| 4 | 104-A | 204 | NAP | O3B-C3B-C2B | 2.01 | 116.92 | 111.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2 | 84-A | 201 | FOL | C11-C-N | 2.01 | 120.49 | 116.98 |
| 4 | 81-A | 204 | NAP | C2D-C1D-N1N | 2.01 | 117.46 | 113.53 |
| 4 | 148-A | 204 | NAP | C2D-C1D-N1N | 2.01 | 117.46 | 113.53 |
| 4 | 9-A | 204 | NAP | O2A-PA-O1A | 2.01 | 123.00 | 112.56 |
| 4 | 114-A | 204 | NAP | C2D-C3D-C4D | 2.01 | 106.74 | 102.64 |
| 4 | 107-A | 204 | NAP | O2A-PA-O1A | 2.01 | 123.01 | 112.56 |
| 4 | 15-A | 204 | NAP | C2D-C1D-N1N | 2.01 | 117.47 | 113.53 |
| 2 | 88-A | 201 | FOL | O-C-N | 2.01 | 126.09 | 122.45 |
| 4 | 48-A | 204 | NAP | C4B-O4B-C1B | 2.01 | 111.77 | 109.64 |
| 2 | 124-A | 201 | FOL | C9-N10-C14 | 2.01 | 127.82 | 122.18 |
| 4 | 29-A | 204 | NAP | C4B-O4B-C1B | 2.01 | 111.78 | 109.64 |
| 4 | 11-A | 204 | NAP | O5B-PA-O1A | 2.01 | 117.45 | 109.21 |
| 2 | 125-A | 201 | FOL | C11-C-N | 2.01 | 120.50 | 116.98 |
| 2 | 55-A | 201 | FOL | C15-C14-N10 | 2.01 | 125.03 | 121.04 |
| 4 | 159-A | 204 | NAP | O2A-PA-O1A | 2.01 | 123.03 | 112.56 |
| 2 | 36-A | 201 | FOL | C15-C16-C11 | 2.01 | 123.13 | 120.76 |
| 4 | 51-A | 204 | NAP | C2N-C3N-C4N | 2.02 | 120.55 | 118.27 |
| 4 | 155-A | 204 | NAP | O5B-PA-O1A | 2.02 | 117.46 | 109.21 |
| 2 | 71-A | 201 | FOL | C9-C6-N5 | 2.02 | 120.13 | 116.44 |
| 2 | 10-A | 201 | FOL | C6-C9-N10 | 2.02 | 117.82 | 113.30 |
| 4 | 21-A | 204 | NAP | O2A-PA-O1A | 2.02 | 123.06 | 112.56 |
| 4 | 9-A | 204 | NAP | C2D-C1D-N1N | 2.02 | 117.49 | 113.53 |
| 4 | 86-A | 204 | NAP | O3B-C3B-C2B | 2.02 | 116.96 | 111.13 |
| 4 | 33-A | 204 | NAP | O2N-PN-O1N | 2.02 | 123.07 | 112.56 |
| 4 | 2-A | 204 | NAP | C2N-C3N-C4N | 2.02 | 120.56 | 118.27 |
| 4 | 72-A | 204 | NAP | C2N-C3N-C4N | 2.02 | 120.56 | 118.27 |
| 4 | 163-A | 204 | NAP | C2N-C3N-C4N | 2.02 | 120.56 | 118.27 |
| 4 | 23-A | 204 | NAP | C2N-C3N-C4N | 2.02 | 120.56 | 118.27 |
| 2 | 64-A | 201 | FOL | CB-CA-N | 2.02 | 113.08 | 109.92 |
| 4 | 148-A | 204 | NAP | O2X-P2B-O1X | 2.02 | 117.23 | 110.63 |
| 4 | 13-A | 204 | NAP | C2N-C3N-C4N | 2.02 | 120.56 | 118.27 |
| 4 | 33-A | 204 | NAP | O5B-PA-O1A | 2.02 | 117.50 | 109.21 |
| 4 | 55-A | 204 | NAP | O3B-C3B-C2B | 2.03 | 116.98 | 111.13 |
| 4 | 1-A | 204 | NAP | C2D-C3D-C4D | 2.03 | 106.78 | 102.64 |
| 4 | 56-A | 204 | NAP | O2X-P2B-O1X | 2.03 | 117.24 | 110.63 |
| 4 | 121-A | 204 | NAP | O2A-PA-O1A | 2.03 | 123.11 | 112.56 |
| 4 | 107-A | 204 | NAP | O2X-P2B-O1X | 2.03 | 117.24 | 110.63 |
| 2 | 141-A | 201 | FOL | C9-N10-C14 | 2.03 | 127.88 | 122.18 |
| 4 | 159-A | 204 | NAP | O5B-PA-O1A | 2.03 | 117.52 | 109.21 |
| 4 | 143-A | 204 | NAP | C2N-C3N-C4N | 2.03 | 120.57 | 118.27 |
| 4 | 21-A | 204 | NAP | O5B-PA-O1A | 2.03 | 117.53 | 109.21 |
| 4 | 130-A | 204 | NAP | C4B-O4B-C1B | 2.03 | 111.80 | 109.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2 | 84-A | 201 | FOL | CB-CG-CD | 2.03 | 121.34 | 113.05 |
| 4 | 131-A | 204 | NAP | C2N-C3N-C4N | 2.03 | 120.57 | 118.27 |
| 4 | 163-A | 204 | NAP | C2D-C1D-N1N | 2.04 | 117.52 | 113.53 |
| 4 | 105-A | 204 | NAP | C3N-C7N-N7N | 2.04 | 120.13 | 117.82 |
| 2 | 38-A | 201 | FOL | C7-N8-C8A | 2.04 | 119.55 | 116.84 |
| 4 | 68-A | 204 | NAP | O5B-PA-O1A | 2.04 | 117.56 | 109.21 |
| 4 | 49-A | 204 | NAP | O5B-C5B-C4B | 2.04 | 116.45 | 109.09 |
| 2 | 107-A | 201 | FOL | C4-C4A-N5 | 2.04 | 121.18 | 118.70 |
| 4 | 26-A | 204 | NAP | C4B-O4B-C1B | 2.04 | 111.81 | 109.64 |
| 4 | 18-A | 204 | NAP | C4B-O4B-C1B | 2.05 | 111.81 | 109.64 |
| 4 | 94-A | 204 | NAP | C2D-C1D-N1N | 2.05 | 117.54 | 113.53 |
| 4 | 100-A | 204 | NAP | C2N-C3N-C4N | 2.05 | 120.59 | 118.27 |
| 2 | 41-A | 201 | FOL | C11-C-N | 2.05 | 120.57 | 116.98 |
| 4 | 124-A | 204 | NAP | C4B-O4B-C1B | 2.05 | 111.82 | 109.64 |
| 2 | 139-A | 201 | FOL | C9-C6-N5 | 2.05 | 120.19 | 116.44 |
| 4 | 131-A | 204 | NAP | O2N-PN-O1N | 2.05 | 123.24 | 112.56 |
| 2 | 94-A | 201 | FOL | CB-CA-N | 2.06 | 113.13 | 109.92 |
| 4 | 65-A | 204 | NAP | O3B-C3B-C2B | 2.06 | 117.07 | 111.13 |
| 4 | 4-A | 204 | NAP | O3B-C3B-C2B | 2.06 | 117.07 | 111.13 |
| 4 | 4-A | 204 | NAP | C2D-C3D-C4D | 2.06 | 106.84 | 102.64 |
| 4 | 116-A | 204 | NAP | O5B-PA-O1A | 2.06 | 117.64 | 109.21 |
| 4 | 76-A | 204 | NAP | C2N-C3N-C4N | 2.06 | 120.60 | 118.27 |
| 4 | 125-A | 204 | NAP | C2N-C3N-C4N | 2.06 | 120.61 | 118.27 |
| 2 | 154-A | 201 | FOL | N1-C8A-N8 | 2.06 | 120.20 | 116.47 |
| 4 | 12-A | 204 | NAP | C2D-C3D-C4D | 2.06 | 106.86 | 102.64 |
| 4 | 134-A | 204 | NAP | O3B-C3B-C2B | 2.07 | 117.09 | 111.13 |
| 4 | 94-A | 204 | NAP | O3B-C3B-C2B | 2.07 | 117.10 | 111.13 |
| 2 | 34-A | 201 | FOL | C6-C9-N10 | 2.07 | 117.93 | 113.30 |
| 4 | 2-A | 204 | NAP | O5B-PA-O1A | 2.07 | 117.68 | 109.21 |
| 4 | 70-A | 204 | NAP | C2N-C3N-C4N | 2.07 | 120.61 | 118.27 |
| 2 | 5-A | 201 | FOL | C9-N10-C14 | 2.07 | 127.99 | 122.18 |
| 4 | 149-A | 204 | NAP | O5B-PA-O1A | 2.07 | 117.69 | 109.21 |
| 4 | 138-A | 204 | NAP | C4B-O4B-C1B | 2.07 | 111.84 | 109.64 |
| 4 | 85-A | 204 | NAP | C2D-C3D-C4D | 2.07 | 106.88 | 102.64 |
| 4 | 37-A | 204 | NAP | O5B-PA-O1A | 2.07 | 117.71 | 109.21 |
| 4 | 111-A | 204 | NAP | O2X-P2B-O1X | 2.08 | 117.40 | 110.63 |
| 4 | 71-A | 204 | NAP | O5B-PA-O1A | 2.08 | 117.72 | 109.21 |
| 4 | 41-A | 204 | NAP | O3B-C3B-C2B | 2.08 | 117.13 | 111.13 |
| 4 | 59-A | 204 | NAP | O2A-PA-O1A | 2.08 | 123.37 | 112.56 |
| 4 | 6-A | 204 | NAP | O2N-PN-O1N | 2.08 | 123.38 | 112.56 |
| 4 | 65-A | 204 | NAP | O5B-PA-O1A | 2.08 | 117.72 | 109.21 |
| 2 | 105-A | 201 | FOL | C9-N10-C14 | 2.08 | 128.02 | 122.18 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 8-A | 204 | NAP | O2N-PN-O1N | 2.08 | 123.38 | 112.56 |
| 4 | 72-A | 204 | NAP | O3B-C3B-C2B | 2.08 | 117.14 | 111.13 |
| 2 | 120-A | 201 | FOL | C15-C14-N10 | 2.08 | 125.18 | 121.04 |
| 4 | 72-A | 204 | NAP | O2A-PA-O1A | 2.08 | 123.40 | 112.56 |
| 4 | 108-A | 204 | NAP | O7N-C7N-C3N | 2.08 | 121.91 | 119.60 |
| 4 | 79-A | 204 | NAP | C4B-O4B-C1B | 2.09 | 111.85 | 109.64 |
| 4 | 21-A | 204 | NAP | C2D-C3D-C4D | 2.09 | 106.90 | 102.64 |
| 4 | 30-A | 204 | NAP | C2D-C3D-C4D | 2.09 | 106.90 | 102.64 |
| 4 | 118-A | 204 | NAP | C2N-C3N-C4N | 2.09 | 120.63 | 118.27 |
| 4 | 151-A | 204 | NAP | C2D-C3D-C4D | 2.09 | 106.91 | 102.64 |
| 4 | 106-A | 204 | NAP | O5B-PA-O1A | 2.09 | 117.75 | 109.21 |
| 4 | 78-A | 204 | NAP | C2N-C3N-C4N | 2.09 | 120.64 | 118.27 |
| 4 | 105-A | 204 | NAP | O3B-C3B-C2B | 2.09 | 117.16 | 111.13 |
| 2 | 147-A | 201 | FOL | O-C-N | 2.09 | 126.23 | 122.45 |
| 4 | 39-A | 204 | NAP | O5B-PA-O1A | 2.09 | 117.77 | 109.21 |
| 4 | 151-A | 204 | NAP | O5B-PA-O1A | 2.09 | 117.77 | 109.21 |
| 4 | 98-A | 204 | NAP | O3B-C3B-C2B | 2.09 | 117.17 | 111.13 |
| 4 | 101-A | 204 | NAP | C2D-C1D-N1N | 2.09 | 117.64 | 113.53 |
| 4 | 100-A | 204 | NAP | O5B-PA-O1A | 2.09 | 117.79 | 109.21 |
| 2 | 139-A | 201 | FOL | N1-C8A-N8 | 2.10 | 120.26 | 116.47 |
| 2 | 70-A | 201 | FOL | C4-C4A-N5 | 2.10 | 121.25 | 118.70 |
| 2 | 48-A | 201 | FOL | C6-C9-N10 | 2.10 | 118.00 | 113.30 |
| 4 | 12-A | 204 | NAP | O3X-P2B-O2X | 2.10 | 115.14 | 107.44 |
| 4 | 146-A | 204 | NAP | O2A-PA-O1A | 2.10 | 123.48 | 112.56 |
| 2 | 12-A | 201 | FOL | CB-CA-N | 2.10 | 113.20 | 109.92 |
| 4 | 157-A | 204 | NAP | C2N-C3N-C4N | 2.10 | 120.65 | 118.27 |
| 4 | 41-A | 204 | NAP | C2D-C3D-C4D | 2.10 | 106.93 | 102.64 |
| 4 | 109-A | 204 | NAP | C2D-C1D-N1N | 2.10 | 117.65 | 113.53 |
| 2 | 106-A | 201 | FOL | O-C-C11 | 2.10 | 124.56 | 120.95 |
| 4 | 34-A | 204 | NAP | O2A-PA-O1A | 2.10 | 123.50 | 112.56 |
| 2 | 122-A | 201 | FOL | C4-C4A-N5 | 2.10 | 121.26 | 118.70 |
| 4 | 83-A | 204 | NAP | O2N-PN-O1N | 2.10 | 123.51 | 112.56 |
| 4 | 85-A | 204 | NAP | O5B-PA-O1A | 2.10 | 117.83 | 109.21 |
| 2 | 112-A | 201 | FOL | C9-N10-C14 | 2.11 | 128.09 | 122.18 |
| 4 | 112-A | 204 | NAP | O2A-PA-O1A | 2.11 | 123.52 | 112.56 |
| 4 | 144-A | 204 | NAP | O2A-PA-O1A | 2.11 | 123.52 | 112.56 |
| 4 | 130-A | 204 | NAP | C2D-C1D-N1N | 2.11 | 117.66 | 113.53 |
| 4 | 48-A | 204 | NAP | O5B-PA-O1A | 2.11 | 117.84 | 109.21 |
| 2 | 129-A | 201 | FOL | N1-C8A-N8 | 2.11 | 120.29 | 116.47 |
| 4 | 125-A | 204 | NAP | O5B-PA-O1A | 2.11 | 117.86 | 109.21 |
| 4 | 149-A | 204 | NAP | C2N-C3N-C4N | 2.11 | 120.66 | 118.27 |
| 4 | 93-A | 204 | NAP | O3B-C3B-C2B | 2.11 | 117.23 | 111.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 3-A | 204 | NAP | O3B-C3B-C2B | 2.11 | 117.23 | 111.13 |
| 4 | 67-A | 204 | NAP | C2D-C1D-N1N | 2.11 | 117.67 | 113.53 |
| 4 | 29-A | 204 | NAP | C2D-C1D-N1N | 2.12 | 117.68 | 113.53 |
| 2 | 119-A | 201 | FOL | N1-C8A-N8 | 2.12 | 120.30 | 116.47 |
| 4 | 147-A | 204 | NAP | O3B-C3B-C2B | 2.12 | 117.24 | 111.13 |
| 4 | 14-A | 204 | NAP | O2X-P2B-O1X | 2.12 | 117.54 | 110.63 |
| 4 | 22-A | 204 | NAP | O3B-C3B-C2B | 2.12 | 117.25 | 111.13 |
| 4 | 150-A | 204 | NAP | C2D-C1D-N1N | 2.12 | 117.69 | 113.53 |
| 4 | 17-A | 204 | NAP | O5B-PA-O1A | 2.12 | 117.89 | 109.21 |
| 4 | 114-A | 204 | NAP | C2N-C3N-C4N | 2.12 | 120.67 | 118.27 |
| 4 | 82-A | 204 | NAP | C2N-C3N-C4N | 2.12 | 120.67 | 118.27 |
| 4 | 89-A | 204 | NAP | O2A-PA-O1A | 2.12 | 123.59 | 112.56 |
| 4 | 47-A | 204 | NAP | C2N-C3N-C4N | 2.12 | 120.67 | 118.27 |
| 4 | 12-A | 204 | NAP | C2N-C3N-C4N | 2.12 | 120.67 | 118.27 |
| 2 | 143-A | 201 | FOL | C9-N10-C14 | 2.12 | 128.14 | 122.18 |
| 4 | 103-A | 204 | NAP | C4B-O4B-C1B | 2.12 | 111.89 | 109.64 |
| 2 | 130-A | 201 | FOL | CB-CA-N | 2.12 | 113.24 | 109.92 |
| 4 | 34-A | 204 | NAP | O3B-C3B-C2B | 2.12 | 117.27 | 111.13 |
| 4 | 145-A | 204 | NAP | O2A-PA-O1A | 2.13 | 123.62 | 112.56 |
| 4 | 91-A | 204 | NAP | C2N-C3N-C4N | 2.13 | 120.68 | 118.27 |
| 2 | 94-A | 201 | FOL | C11-C-N | 2.13 | 120.70 | 116.98 |
| 4 | 73-A | 204 | NAP | O3B-C3B-C2B | 2.13 | 117.28 | 111.13 |
| 4 | 138-A | 204 | NAP | C2N-C3N-C4N | 2.13 | 120.68 | 118.27 |
| 2 | 107-A | 201 | FOL | C9-N10-C14 | 2.13 | 128.16 | 122.18 |
| 2 | 99-A | 201 | FOL | C9-N10-C14 | 2.13 | 128.16 | 122.18 |
| 4 | 155-A | 204 | NAP | O3B-C3B-C2B | 2.13 | 117.28 | 111.13 |
| 4 | 44-A | 204 | NAP | C2N-C3N-C4N | 2.13 | 120.68 | 118.27 |
| 2 | 148-A | 201 | FOL | CB-CG-CD | 2.13 | 121.73 | 113.05 |
| 4 | 154-A | 204 | NAP | C2D-C1D-N1N | 2.13 | 117.71 | 113.53 |
| 4 | 145-A | 204 | NAP | O5B-PA-O1A | 2.13 | 117.94 | 109.21 |
| 4 | 5-A | 204 | NAP | O2X-P2B-O1X | 2.13 | 117.59 | 110.63 |
| 4 | 142-A | 204 | NAP | C2N-C3N-C4N | 2.13 | 120.69 | 118.27 |
| 4 | 37-A | 204 | NAP | O2N-PN-O1N | 2.13 | 123.67 | 112.56 |
| 2 | 60-A | 201 | FOL | CB-CG-CD | 2.14 | 121.75 | 113.05 |
| 4 | 23-A | 204 | NAP | C2D-C1D-N1N | 2.14 | 117.72 | 113.53 |
| 2 | 160-A | 201 | FOL | C4-C4A-N5 | 2.14 | 121.30 | 118.70 |
| 4 | 159-A | 204 | NAP | O2X-P2B-O1X | 2.14 | 117.60 | 110.63 |
| 4 | 156-A | 204 | NAP | O2A-PA-O1A | 2.14 | 123.68 | 112.56 |
| 4 | 20-A | 204 | NAP | C2D-C1D-N1N | 2.14 | 117.72 | 113.53 |
| 4 | 71-A | 204 | NAP | O3B-C3B-C2B | 2.14 | 117.31 | 111.13 |
| 4 | 40-A | 204 | NAP | C4B-O4B-C1B | 2.14 | 111.91 | 109.64 |
| 4 | 26-A | 204 | NAP | O3B-C3B-C2B | 2.14 | 117.31 | 111.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 87-A | 204 | NAP | O3B-C3B-C2B | 2.14 | 117.31 | 111.13 |
| 4 | 95-A | 204 | NAP | C2D-C3D-C4D | 2.14 | 107.01 | 102.64 |
| 4 | 18-A | 204 | NAP | O5B-PA-O1A | 2.14 | 117.97 | 109.21 |
| 4 | 128-A | 204 | NAP | O3X-P2B-O2X | 2.14 | 115.30 | 107.44 |
| 4 | 64-A | 204 | NAP | O5B-PA-O1A | 2.14 | 117.98 | 109.21 |
| 4 | 145-A | 204 | NAP | C2N-C3N-C4N | 2.14 | 120.70 | 118.27 |
| 4 | 71-A | 204 | NAP | C2D-C3D-C4D | 2.14 | 107.02 | 102.64 |
| 2 | 124-A | 201 | FOL | N1-C8A-N8 | 2.14 | 120.35 | 116.47 |
| 4 | 71-A | 204 | NAP | O2A-PA-O1A | 2.14 | 123.71 | 112.56 |
| 4 | 76-A | 204 | NAP | C2D-C1D-N1N | 2.14 | 117.73 | 113.53 |
| 4 | 106-A | 204 | NAP | O3B-C3B-C2B | 2.14 | 117.32 | 111.13 |
| 4 | 162-A | 204 | NAP | O3B-C3B-C2B | 2.14 | 117.32 | 111.13 |
| 4 | 108-A | 204 | NAP | O2N-PN-O1N | 2.14 | 123.72 | 112.56 |
| 4 | 142-A | 204 | NAP | O3B-C3B-C2B | 2.14 | 117.33 | 111.13 |
| 2 | 152-A | 201 | FOL | N1-C8A-N8 | 2.15 | 120.35 | 116.47 |
| 2 | 61-A | 201 | FOL | CB-CA-N | 2.15 | 113.28 | 109.92 |
| 2 | 13-A | 201 | FOL | C7-N8-C8A | 2.15 | 119.69 | 116.84 |
| 2 | 57-A | 201 | FOL | C15-C16-C11 | 2.15 | 123.29 | 120.76 |
| 2 | 52-A | 201 | FOL | O-C-C11 | 2.15 | 124.63 | 120.95 |
| 2 | 37-A | 201 | FOL | C7-N8-C8A | 2.15 | 119.69 | 116.84 |
| 4 | 106-A | 204 | NAP | C2N-C3N-C4N | 2.15 | 120.70 | 118.27 |
| 2 | 96-A | 201 | FOL | C4-C4A-N5 | 2.15 | 121.31 | 118.70 |
| 2 | 46-A | 201 | FOL | C4-C4A-N5 | 2.15 | 121.31 | 118.70 |
| 2 | 129-A | 201 | FOL | C9-N10-C14 | 2.15 | 128.22 | 122.18 |
| 4 | 53-A | 204 | NAP | O5B-PA-O1A | 2.15 | 118.02 | 109.21 |
| 4 | 20-A | 204 | NAP | O2A-PA-O1A | 2.15 | 123.75 | 112.56 |
| 4 | 118-A | 204 | NAP | O3B-C3B-C2B | 2.15 | 117.34 | 111.13 |
| 4 | 30-A | 204 | NAP | O5B-PA-O1A | 2.15 | 118.02 | 109.21 |
| 2 | 29-A | 201 | FOL | C9-N10-C14 | 2.15 | 128.22 | 122.18 |
| 4 | 40-A | 204 | NAP | C2D-C3D-C4D | 2.15 | 107.04 | 102.64 |
| 4 | 11-A | 204 | NAP | O7N-C7N-C3N | 2.15 | 121.98 | 119.60 |
| 4 | 82-A | 204 | NAP | O2N-PN-O1N | 2.15 | 123.77 | 112.56 |
| 4 | 110-A | 204 | NAP | C2N-C3N-C4N | 2.16 | 120.71 | 118.27 |
| 4 | 113-A | 204 | NAP | O3B-C3B-C2B | 2.16 | 117.36 | 111.13 |
| 4 | 162-A | 204 | NAP | C2D-C1D-N1N | 2.16 | 117.76 | 113.53 |
| 2 | 33-A | 201 | FOL | C6-C9-N10 | 2.16 | 118.13 | 113.30 |
| 4 | 24-A | 204 | NAP | O2N-PN-O1N | 2.16 | 123.79 | 112.56 |
| 4 | 69-A | 204 | NAP | O5B-PA-O1A | 2.16 | 118.05 | 109.21 |
| 4 | 27-A | 204 | NAP | C4B-O4B-C1B | 2.16 | 111.93 | 109.64 |
| 4 | 52-A | 204 | NAP | O2A-PA-O1A | 2.16 | 123.80 | 112.56 |
| 4 | 14-A | 204 | NAP | C2N-C3N-C4N | 2.16 | 120.72 | 118.27 |
| 4 | 1-A | 204 | NAP | C4B-O4B-C1B | 2.16 | 111.93 | 109.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 127-A | 204 | NAP | O3B-C3B-C2B | 2.16 | 117.37 | 111.13 |
| 4 | 121-A | 204 | NAP | C2D-C1D-N1N | 2.16 | 117.77 | 113.53 |
| 4 | 88-A | 204 | NAP | O2A-PA-O1A | 2.16 | 123.81 | 112.56 |
| 4 | 4-A | 204 | NAP | C4B-O4B-C1B | 2.16 | 111.94 | 109.64 |
| 4 | 137-A | 204 | NAP | O3B-C3B-C2B | 2.16 | 117.38 | 111.13 |
| 4 | 91-A | 204 | NAP | C2D-C1D-N1N | 2.16 | 117.77 | 113.53 |
| 2 | 140-A | 201 | FOL | C9-N10-C14 | 2.16 | 128.26 | 122.18 |
| 4 | 36-A | 204 | NAP | C4B-O4B-C1B | 2.16 | 111.94 | 109.64 |
| 4 | 74-A | 204 | NAP | C2N-C3N-C4N | 2.17 | 120.72 | 118.27 |
| 2 | 24-A | 201 | FOL | C9-N10-C14 | 2.17 | 128.26 | 122.18 |
| 4 | 11-A | 204 | NAP | C2D-C3D-C4D | 2.17 | 107.07 | 102.64 |
| 2 | 31-A | 201 | FOL | CB-CA-N | 2.17 | 113.31 | 109.92 |
| 4 | 24-A | 204 | NAP | C2D-C1D-N1N | 2.17 | 117.78 | 113.53 |
| 2 | 95-A | 201 | FOL | O-C-C11 | 2.17 | 124.67 | 120.95 |
| 4 | 66-A | 204 | NAP | O5B-PA-O1A | 2.17 | 118.09 | 109.21 |
| 4 | 66-A | 204 | NAP | O3B-C3B-C2B | 2.17 | 117.40 | 111.13 |
| 4 | 70-A | 204 | NAP | O3B-C3B-C2B | 2.17 | 117.40 | 111.13 |
| 4 | 92-A | 204 | NAP | O5B-PA-O1A | 2.17 | 118.11 | 109.21 |
| 4 | 141-A | 204 | NAP | C2D-C1D-N1N | 2.17 | 117.79 | 113.53 |
| 4 | 62-A | 204 | NAP | C2N-C3N-C4N | 2.17 | 120.73 | 118.27 |
| 4 | 41-A | 204 | NAP | C4B-O4B-C1B | 2.17 | 111.95 | 109.64 |
| 2 | 147-A | 201 | FOL | CB-CA-N | 2.17 | 113.32 | 109.92 |
| 4 | 5-A | 204 | NAP | O2A-PA-O1A | 2.17 | 123.87 | 112.56 |
| 4 | 79-A | 204 | NAP | C2D-C3D-C4D | 2.17 | 107.08 | 102.64 |
| 4 | 146-A | 204 | NAP | O5B-PA-O1A | 2.18 | 118.12 | 109.21 |
| 2 | 143-A | 201 | FOL | N1-C8A-N8 | 2.18 | 120.41 | 116.47 |
| 4 | 116-A | 204 | NAP | C3N-C7N-N7N | 2.18 | 120.28 | 117.82 |
| 4 | 85-A | 204 | NAP | O3B-C3B-C2B | 2.18 | 117.42 | 111.13 |
| 4 | 39-A | 204 | NAP | O3B-C3B-C2B | 2.18 | 117.42 | 111.13 |
| 4 | 96-A | 204 | NAP | O2A-PA-O1A | 2.18 | 123.88 | 112.56 |
| 4 | 52-A | 204 | NAP | P2B-O2B-C2B | 2.18 | 127.14 | 121.56 |
| 4 | 160-A | 204 | NAP | O3B-C3B-C2B | 2.18 | 117.42 | 111.13 |
| 4 | 45-A | 204 | NAP | C2N-C3N-C4N | 2.18 | 120.74 | 118.27 |
| 4 | 72-A | 204 | NAP | O5B-PA-O1A | 2.18 | 118.13 | 109.21 |
| 4 | 118-A | 204 | NAP | O2A-PA-O1A | 2.18 | 123.90 | 112.56 |
| 2 | 133-A | 201 | FOL | N1-C8A-N8 | 2.18 | 120.42 | 116.47 |
| 4 | 24-A | 204 | NAP | O5B-PA-O1A | 2.18 | 118.15 | 109.21 |
| 4 | 77-A | 204 | NAP | C2N-C3N-C4N | 2.18 | 120.74 | 118.27 |
| 4 | 67-A | 204 | NAP | O5B-PA-O1A | 2.18 | 118.16 | 109.21 |
| 4 | 70-A | 204 | NAP | O2A-PA-O1A | 2.18 | 123.93 | 112.56 |
| 2 | 37-A | 201 | FOL | N1-C8A-N8 | 2.19 | 120.42 | 116.47 |
| 4 | 18-A | 204 | NAP | O2A-PA-O1A | 2.19 | 123.94 | 112.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2 | 19-A | 201 | FOL | N1-C8A-N8 | 2.19 | 120.43 | 116.47 |
| 4 | 91-A | 204 | NAP | O3B-C3B-C2B | 2.19 | 117.45 | 111.13 |
| 2 | 7-A | 201 | FOL | CB-CA-N | 2.19 | 113.34 | 109.92 |
| 4 | 63-A | 204 | NAP | O2A-PA-O1A | 2.19 | 123.95 | 112.56 |
| 2 | 6-A | 201 | FOL | C4-C4A-N5 | 2.19 | 121.36 | 118.70 |
| 4 | 160-A | 204 | NAP | O2A-PA-O1A | 2.19 | 123.96 | 112.56 |
| 4 | 8-A | 204 | NAP | C2N-C3N-C4N | 2.19 | 120.75 | 118.27 |
| 4 | 61-A | 204 | NAP | C2N-C3N-C4N | 2.19 | 120.75 | 118.27 |
| 4 | 43-A | 204 | NAP | O2A-PA-O1A | 2.19 | 123.97 | 112.56 |
| 4 | 46-A | 204 | NAP | O3B-C3B-C2B | 2.19 | 117.46 | 111.13 |
| 4 | 140-A | 204 | NAP | C2D-C1D-N1N | 2.19 | 117.83 | 113.53 |
| 2 | 78-A | 201 | FOL | C15-C14-N10 | 2.20 | 125.40 | 121.04 |
| 2 | 45-A | 201 | FOL | C11-C-N | 2.20 | 120.82 | 116.98 |
| 4 | 134-A | 204 | NAP | O2N-PN-O1N | 2.20 | 123.98 | 112.56 |
| 4 | 40-A | 204 | NAP | C2N-C3N-C4N | 2.20 | 120.76 | 118.27 |
| 4 | 147-A | 204 | NAP | O5B-PA-O1A | 2.20 | 118.20 | 109.21 |
| 4 | 16-A | 204 | NAP | C4B-O4B-C1B | 2.20 | 111.97 | 109.64 |
| 4 | 109-A | 204 | NAP | O3B-C3B-C2B | 2.20 | 117.48 | 111.13 |
| 2 | 154-A | 201 | FOL | C4-C4A-N5 | 2.20 | 121.37 | 118.70 |
| 4 | 101-A | 204 | NAP | O5B-PA-O1A | 2.20 | 118.22 | 109.21 |
| 4 | 111-A | 204 | NAP | O3B-C3B-C2B | 2.20 | 117.48 | 111.13 |
| 4 | 114-A | 204 | NAP | O5B-PA-O1A | 2.20 | 118.22 | 109.21 |
| 4 | 40-A | 204 | NAP | O3B-C3B-C2B | 2.20 | 117.49 | 111.13 |
| 4 | 63-A | 204 | NAP | C2N-C3N-C4N | 2.20 | 120.77 | 118.27 |
| 4 | 162-A | 204 | NAP | O2A-PA-O1A | 2.20 | 124.03 | 112.56 |
| 4 | 46-A | 204 | NAP | O5B-PA-O1A | 2.20 | 118.24 | 109.21 |
| 2 | 8-A | 201 | FOL | N1-C8A-N8 | 2.21 | 120.46 | 116.47 |
| 4 | 100-A | 204 | NAP | C2D-C1D-N1N | 2.21 | 117.85 | 113.53 |
| 4 | 139-A | 204 | NAP | O3B-C3B-C2B | 2.21 | 117.50 | 111.13 |
| 4 | 141-A | 204 | NAP | O3B-C3B-C2B | 2.21 | 117.51 | 111.13 |
| 4 | 121-A | 204 | NAP | O5B-PA-O1A | 2.21 | 118.25 | 109.21 |
| 4 | 32-A | 204 | NAP | O2X-P2B-O1X | 2.21 | 117.83 | 110.63 |
| 4 | 44-A | 204 | NAP | O2A-PA-O1A | 2.21 | 124.05 | 112.56 |
| 2 | 57-A | 201 | FOL | N1-C8A-N8 | 2.21 | 120.47 | 116.47 |
| 4 | 22-A | 204 | NAP | O2A-PA-O1A | 2.21 | 124.06 | 112.56 |
| 4 | 107-A | 204 | NAP | O2N-PN-O1N | 2.21 | 124.06 | 112.56 |
| 4 | 105-A | 204 | NAP | O5B-PA-O1A | 2.21 | 118.26 | 109.21 |
| 4 | 27-A | 204 | NAP | C2N-C3N-C4N | 2.21 | 120.78 | 118.27 |
| 4 | 9-A | 204 | NAP | C2N-C3N-C4N | 2.21 | 120.78 | 118.27 |
| 4 | 105-A | 204 | NAP | O2A-PA-O1A | 2.21 | 124.06 | 112.56 |
| 4 | 122-A | 204 | NAP | O3B-C3B-C2B | 2.21 | 117.53 | 111.13 |
| 4 | 47-A | 204 | NAP | O2A-PA-O1A | 2.21 | 124.08 | 112.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 2-A | 204 | NAP | O3B-C3B-C2B | 2.21 | 117.53 | 111.13 |
| 4 | 166-A | 204 | NAP | O3B-C3B-C2B | 2.22 | 117.53 | 111.13 |
| 4 | 70-A | 204 | NAP | O5B-PA-O1A | 2.22 | 118.28 | 109.21 |
| 4 | 84-A | 204 | NAP | O2A-PA-O1A | 2.22 | 124.09 | 112.56 |
| 4 | 140-A | 204 | NAP | O2A-PA-O1A | 2.22 | 124.11 | 112.56 |
| 2 | 53-A | 201 | FOL | N1-C8A-N8 | 2.22 | 120.49 | 116.47 |
| 4 | 109-A | 204 | NAP | O2N-PN-O1N | 2.22 | 124.11 | 112.56 |
| 4 | 102-A | 204 | NAP | O3B-C3B-C2B | 2.22 | 117.54 | 111.13 |
| 4 | 107-A | 204 | NAP | C2N-C3N-C4N | 2.22 | 120.79 | 118.27 |
| 4 | 134-A | 204 | NAP | N6A-C6A-N1A | 2.22 | 122.24 | 118.52 |
| 4 | 145-A | 204 | NAP | C2D-C1D-N1N | 2.22 | 117.89 | 113.53 |
| 4 | 55-A | 204 | NAP | C2N-C3N-C4N | 2.23 | 120.79 | 118.27 |
| 4 | 115-A | 204 | NAP | C2D-C3D-C4D | 2.23 | 107.19 | 102.64 |
| 4 | 146-A | 204 | NAP | O3B-C3B-C2B | 2.23 | 117.56 | 111.13 |
| 2 | 26-A | 201 | FOL | N1-C8A-N8 | 2.23 | 120.50 | 116.47 |
| 2 | 121-A | 201 | FOL | N1-C8A-N8 | 2.23 | 120.50 | 116.47 |
| 2 | 63-A | 201 | FOL | C11-C-N | 2.23 | 120.88 | 116.98 |
| 4 | 90-A | 204 | NAP | O2A-PA-O1A | 2.23 | 124.16 | 112.56 |
| 4 | 16-A | 204 | NAP | O5B-PA-O1A | 2.23 | 118.35 | 109.21 |
| 4 | 7-A | 204 | NAP | O3B-C3B-C2B | 2.23 | 117.58 | 111.13 |
| 2 | 118-A | 201 | FOL | O-C-C11 | 2.23 | 124.78 | 120.95 |
| 2 | 136-A | 201 | FOL | C9-N10-C14 | 2.24 | 128.46 | 122.18 |
| 4 | 164-A | 204 | NAP | O3B-C3B-C2B | 2.24 | 117.59 | 111.13 |
| 4 | 62-A | 204 | NAP | O2A-PA-O1A | 2.24 | 124.19 | 112.56 |
| 4 | 66-A | 204 | NAP | C2N-C3N-C4N | 2.24 | 120.80 | 118.27 |
| 4 | 88-A | 204 | NAP | O3B-C3B-C2B | 2.24 | 117.59 | 111.13 |
| 2 | 48-A | 201 | FOL | C9-C6-N5 | 2.24 | 120.53 | 116.44 |
| 2 | 4-A | 201 | FOL | C9-N10-C14 | 2.24 | 128.47 | 122.18 |
| 2 | 102-A | 201 | FOL | C11-C-N | 2.24 | 120.90 | 116.98 |
| 4 | 38-A | 204 | NAP | C2D-C3D-C4D | 2.24 | 107.22 | 102.64 |
| 4 | 144-A | 204 | NAP | O5B-PA-O1A | 2.24 | 118.38 | 109.21 |
| 2 | 86-A | 201 | FOL | CB-CA-N | 2.24 | 113.42 | 109.92 |
| 4 | 97-A | 204 | NAP | C2N-C3N-C4N | 2.24 | 120.81 | 118.27 |
| 4 | 153-A | 204 | NAP | O5B-PA-O1A | 2.24 | 118.39 | 109.21 |
| 4 | 161-A | 204 | NAP | O3B-C3B-C2B | 2.24 | 117.61 | 111.13 |
| 4 | 141-A | 204 | NAP | O2A-PA-O1A | 2.25 | 124.25 | 112.56 |
| 4 | 120-A | 204 | NAP | O5B-PA-O1A | 2.25 | 118.41 | 109.21 |
| 4 | 121-A | 204 | NAP | O3B-C3B-C2B | 2.25 | 117.62 | 111.13 |
| 4 | 10-A | 204 | NAP | O2A-PA-O1A | 2.25 | 124.26 | 112.56 |
| 4 | 92-A | 204 | NAP | C2N-C3N-C4N | 2.25 | 120.82 | 118.27 |
| 4 | 149-A | 204 | NAP | O2X-P2B-O1X | 2.25 | 117.97 | 110.63 |
| 4 | 148-A | 204 | NAP | O5B-PA-O1A | 2.25 | 118.43 | 109.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 123-A | 204 | NAP | O3B-C3B-C2B | 2.25 | 117.63 | 111.13 |
| 4 | 19-A | 204 | NAP | C2N-C3N-C4N | 2.25 | 120.82 | 118.27 |
| 4 | 156-A | 204 | NAP | O3B-C3B-C2B | 2.25 | 117.64 | 111.13 |
| 2 | 69-A | 201 | FOL | C11-C-N | 2.25 | 120.92 | 116.98 |
| 4 | 147-A | 204 | NAP | O2A-PA-O1A | 2.25 | 124.28 | 112.56 |
| 4 | 124-A | 204 | NAP | C2N-C3N-C4N | 2.25 | 120.82 | 118.27 |
| 2 | 127-A | 201 | FOL | C4-C4A-N5 | 2.25 | 121.44 | 118.70 |
| 4 | 86-A | 204 | NAP | O3X-P2B-O2X | 2.25 | 115.72 | 107.44 |
| 2 | 62-A | 201 | FOL | C9-N10-C14 | 2.26 | 128.51 | 122.18 |
| 4 | 45-A | 204 | NAP | C2D-C1D-N1N | 2.26 | 117.95 | 113.53 |
| 2 | 79-A | 201 | FOL | C9-N10-C14 | 2.26 | 128.52 | 122.18 |
| 4 | 159-A | 204 | NAP | C2N-C3N-C4N | 2.26 | 120.83 | 118.27 |
| 4 | 26-A | 204 | NAP | O2A-PA-O1A | 2.26 | 124.31 | 112.56 |
| 4 | 117-A | 204 | NAP | O3B-C3B-C2B | 2.26 | 117.66 | 111.13 |
| 4 | 45-A | 204 | NAP | O3B-C3B-C2B | 2.26 | 117.66 | 111.13 |
| 4 | 91-A | 204 | NAP | O5B-PA-O1A | 2.26 | 118.46 | 109.21 |
| 4 | 20-A | 204 | NAP | C2N-C3N-C4N | 2.26 | 120.83 | 118.27 |
| 2 | 117-A | 201 | FOL | N1-C8A-N8 | 2.26 | 120.56 | 116.47 |
| 2 | 130-A | 201 | FOL | C9-N10-C14 | 2.26 | 128.53 | 122.18 |
| 4 | 153-A | 204 | NAP | C2D-C1D-N1N | 2.26 | 117.97 | 113.53 |
| 4 | 90-A | 204 | NAP | C4B-O4B-C1B | 2.26 | 112.04 | 109.64 |
| 4 | 109-A | 204 | NAP | O2A-PA-O1A | 2.27 | 124.34 | 112.56 |
| 4 | 152-A | 204 | NAP | O5B-PA-O1A | 2.27 | 118.49 | 109.21 |
| 4 | 143-A | 204 | NAP | O5B-PA-O1A | 2.27 | 118.49 | 109.21 |
| 4 | 115-A | 204 | NAP | O5B-PA-O1A | 2.27 | 118.49 | 109.21 |
| 4 | 19-A | 204 | NAP | O2A-PA-O1A | 2.27 | 124.35 | 112.56 |
| 4 | 101-A | 204 | NAP | C2N-C3N-C4N | 2.27 | 120.84 | 118.27 |
| 2 | 83-A | 201 | FOL | C15-C16-C11 | 2.27 | 123.43 | 120.76 |
| 4 | 69-A | 204 | NAP | C2D-C1D-N1N | 2.27 | 117.98 | 113.53 |
| 4 | 74-A | 204 | NAP | O5B-PA-O1A | 2.27 | 118.51 | 109.21 |
| 4 | 105-A | 204 | NAP | O2N-PN-O1N | 2.27 | 124.38 | 112.56 |
| 4 | 44-A | 204 | NAP | O2N-PN-O1N | 2.27 | 124.38 | 112.56 |
| 4 | 114-A | 204 | NAP | O2A-PA-O1A | 2.27 | 124.39 | 112.56 |
| 2 | 28-A | 201 | FOL | C4-C4A-N5 | 2.27 | 121.46 | 118.70 |
| 4 | 4-A | 204 | NAP | C2N-C3N-C4N | 2.27 | 120.84 | 118.27 |
| 4 | 17-A | 204 | NAP | O3B-C3B-C2B | 2.27 | 117.70 | 111.13 |
| 4 | 127-A | 204 | NAP | C4B-O4B-C1B | 2.27 | 112.05 | 109.64 |
| 2 | 24-A | 201 | FOL | C15-C14-N10 | 2.27 | 125.56 | 121.04 |
| 4 | 112-A | 204 | NAP | C2N-C3N-C4N | 2.27 | 120.85 | 118.27 |
| 2 | 116-A | 201 | FOL | CB-CA-N | 2.28 | 113.48 | 109.92 |
| 2 | 107-A | 201 | FOL | N1-C8A-N8 | 2.28 | 120.59 | 116.47 |
| 4 | 151-A | 204 | NAP | O3B-C3B-C2B | 2.28 | 117.70 | 111.13 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 106-A | 204 | NAP | O2N-PN-O1N | 2.28 | 124.41 | 112.56 |
| 4 | 135-A | 204 | NAP | C2D-C1D-N1N | 2.28 | 118.00 | 113.53 |
| 4 | 25-A | 204 | NAP | O5B-PA-O1A | 2.28 | 118.54 | 109.21 |
| 4 | 157-A | 204 | NAP | O3B-C3B-C2B | 2.28 | 117.71 | 111.13 |
| 4 | 111-A | 204 | NAP | C2N-C3N-C4N | 2.28 | 120.85 | 118.27 |
| 4 | 1-A | 204 | NAP | O5B-PA-O1A | 2.28 | 118.55 | 109.21 |
| 4 | 47-A | 204 | NAP | O5B-PA-O1A | 2.28 | 118.55 | 109.21 |
| 4 | 98-A | 204 | NAP | C2N-C3N-C4N | 2.28 | 120.86 | 118.27 |
| 2 | 25-A | 201 | FOL | C4-C4A-N5 | 2.28 | 121.47 | 118.70 |
| 4 | 161-A | 204 | NAP | C2D-C1D-N1N | 2.28 | 118.01 | 113.53 |
| 4 | 111-A | 204 | NAP | C2D-C1D-N1N | 2.28 | 118.01 | 113.53 |
| 4 | 9-A | 204 | NAP | O2N-PN-O1N | 2.29 | 124.45 | 112.56 |
| 4 | 67-A | 204 | NAP | C4B-O4B-C1B | 2.29 | 112.07 | 109.64 |
| 4 | 77-A | 204 | NAP | O5B-PA-O1A | 2.29 | 118.59 | 109.21 |
| 4 | 142-A | 204 | NAP | O2A-PA-O1A | 2.29 | 124.48 | 112.56 |
| 4 | 163-A | 204 | NAP | O2A-PA-O1A | 2.29 | 124.48 | 112.56 |
| 4 | 143-A | 204 | NAP | O2A-PA-O1A | 2.29 | 124.49 | 112.56 |
| 4 | 46-A | 204 | NAP | O2A-PA-O1A | 2.29 | 124.49 | 112.56 |
| 4 | 41-A | 204 | NAP | O5B-PA-O1A | 2.29 | 118.60 | 109.21 |
| 4 | 50-A | 204 | NAP | C2N-C3N-C4N | 2.29 | 120.87 | 118.27 |
| 4 | 13-A | 204 | NAP | O2A-PA-O1A | 2.29 | 124.50 | 112.56 |
| 4 | 126-A | 204 | NAP | C2D-C1D-N1N | 2.29 | 118.03 | 113.53 |
| 4 | 97-A | 204 | NAP | O2A-PA-O1A | 2.29 | 124.50 | 112.56 |
| 4 | 95-A | 204 | NAP | O2N-PN-O1N | 2.30 | 124.50 | 112.56 |
| 4 | 150-A | 204 | NAP | O3B-C3B-C2B | 2.30 | 117.76 | 111.13 |
| 2 | 134-A | 201 | FOL | CT-CA-N | 2.30 | 117.52 | 112.93 |
| 4 | 45-A | 204 | NAP | O2A-PA-O1A | 2.30 | 124.52 | 112.56 |
| 4 | 95-A | 204 | NAP | C2D-C1D-N1N | 2.30 | 118.04 | 113.53 |
| 2 | 78-A | 201 | FOL | C9-N10-C14 | 2.30 | 128.64 | 122.18 |
| 4 | 54-A | 204 | NAP | C4B-O4B-C1B | 2.30 | 112.08 | 109.64 |
| 4 | 135-A | 204 | NAP | O3B-C3B-C2B | 2.30 | 117.78 | 111.13 |
| 4 | 115-A | 204 | NAP | O3B-C3B-C2B | 2.30 | 117.78 | 111.13 |
| 2 | 42-A | 201 | FOL | N1-C8A-N8 | 2.30 | 120.64 | 116.47 |
| 4 | 142-A | 204 | NAP | O3X-P2B-O2X | 2.30 | 115.90 | 107.44 |
| 4 | 11-A | 204 | NAP | O2A-PA-O1A | 2.30 | 124.55 | 112.56 |
| 2 | 111-A | 201 | FOL | C4-C4A-N5 | 2.30 | 121.50 | 118.70 |
| 4 | 81-A | 204 | NAP | O2N-PN-O1N | 2.30 | 124.55 | 112.56 |
| 4 | 55-A | 204 | NAP | O2A-PA-O1A | 2.31 | 124.55 | 112.56 |
| 4 | 124-A | 204 | NAP | O3B-C3B-C2B | 2.31 | 117.79 | 111.13 |
| 4 | 22-A | 204 | NAP | O2N-PN-O1N | 2.31 | 124.56 | 112.56 |
| 4 | 23-A | 204 | NAP | O5B-PA-O1A | 2.31 | 118.65 | 109.21 |
| 4 | 87-A | 204 | NAP | O2A-PA-O1A | 2.31 | 124.56 | 112.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 90-A | 204 | NAP | C2D-C1D-N1N | 2.31 | 118.05 | 113.53 |
| 4 | 36-A | 204 | NAP | O5B-PA-O1A | 2.31 | 118.65 | 109.21 |
| 4 | 115-A | 204 | NAP | O2A-PA-O1A | 2.31 | 124.56 | 112.56 |
| 4 | 70-A | 204 | NAP | C2D-C3D-C4D | 2.31 | 107.35 | 102.64 |
| 4 | 110-A | 204 | NAP | C2D-C1D-N1N | 2.31 | 118.05 | 113.53 |
| 4 | 62-A | 204 | NAP | C4B-O4B-C1B | 2.31 | 112.09 | 109.64 |
| 4 | 124-A | 204 | NAP | O5B-PA-O1A | 2.31 | 118.65 | 109.21 |
| 4 | 34-A | 204 | NAP | O2N-PN-O1N | 2.31 | 124.56 | 112.56 |
| 4 | 143-A | 204 | NAP | O3B-C3B-C2B | 2.31 | 117.80 | 111.13 |
| 4 | 126-A | 204 | NAP | O5B-PA-O1A | 2.31 | 118.67 | 109.21 |
| 2 | 2-A | 201 | FOL | CB-CA-N | 2.31 | 113.53 | 109.92 |
| 4 | 76-A | 204 | NAP | O5B-PA-O1A | 2.31 | 118.67 | 109.21 |
| 4 | 116-A | 204 | NAP | O3B-C3B-C2B | 2.31 | 117.81 | 111.13 |
| 4 | 107-A | 204 | NAP | O5B-PA-O1A | 2.31 | 118.68 | 109.21 |
| 4 | 111-A | 204 | NAP | O2A-PA-O1A | 2.31 | 124.59 | 112.56 |
| 4 | 18-A | 204 | NAP | O3B-C3B-C2B | 2.31 | 117.81 | 111.13 |
| 4 | 35-A | 204 | NAP | O5B-PA-O1A | 2.32 | 118.69 | 109.21 |
| 4 | 12-A | 204 | NAP | O5B-PA-O1A | 2.32 | 118.69 | 109.21 |
| 4 | 91-A | 204 | NAP | O2N-PN-O1N | 2.32 | 124.61 | 112.56 |
| 4 | 18-A | 204 | NAP | C2D-C1D-N1N | 2.32 | 118.07 | 113.53 |
| 4 | 100-A | 204 | NAP | O3B-C3B-C2B | 2.32 | 117.83 | 111.13 |
| 4 | 14-A | 204 | NAP | O2A-PA-O1A | 2.32 | 124.63 | 112.56 |
| 4 | 102-A | 204 | NAP | C2N-C3N-C4N | 2.32 | 120.90 | 118.27 |
| 4 | 96-A | 204 | NAP | C2D-C1D-N1N | 2.32 | 118.08 | 113.53 |
| 4 | 90-A | 204 | NAP | O2N-PN-O1N | 2.32 | 124.64 | 112.56 |
| 4 | 36-A | 204 | NAP | O2A-PA-O1A | 2.32 | 124.64 | 112.56 |
| 2 | 57-A | 201 | FOL | C9-N10-C14 | 2.32 | 128.70 | 122.18 |
| 4 | 158-A | 204 | NAP | O3B-C3B-C2B | 2.32 | 117.84 | 111.13 |
| 4 | 141-A | 204 | NAP | O5B-PA-O1A | 2.32 | 118.73 | 109.21 |
| 4 | 96-A | 204 | NAP | O5B-PA-O1A | 2.32 | 118.73 | 109.21 |
| 4 | 87-A | 204 | NAP | O2N-PN-O1N | 2.33 | 124.66 | 112.56 |
| 4 | 164-A | 204 | NAP | O5B-PA-O1A | 2.33 | 118.73 | 109.21 |
| 4 | 49-A | 204 | NAP | O2A-PA-O1A | 2.33 | 124.66 | 112.56 |
| 4 | 161-A | 204 | NAP | O2A-PA-O1A | 2.33 | 124.66 | 112.56 |
| 2 | 128-A | 201 | FOL | C11-C-N | 2.33 | 121.05 | 116.98 |
| 2 | 74-A | 201 | FOL | N1-C8A-N8 | 2.33 | 120.68 | 116.47 |
| 4 | 35-A | 204 | NAP | O2A-PA-O1A | 2.33 | 124.67 | 112.56 |
| 4 | 61-A | 204 | NAP | O2A-PA-O1A | 2.33 | 124.67 | 112.56 |
| 4 | 55-A | 204 | NAP | O5B-PA-O1A | 2.33 | 118.75 | 109.21 |
| 4 | 12-A | 204 | NAP | O2A-PA-O1A | 2.33 | 124.68 | 112.56 |
| 4 | 113-A | 204 | NAP | C2N-C3N-C4N | 2.33 | 120.91 | 118.27 |
| 4 | 22-A | 204 | NAP | O5B-PA-O1A | 2.33 | 118.76 | 109.21 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 141-A | 204 | NAP | O2N-PN-O1N | 2.33 | 124.70 | 112.56 |
| 4 | 161-A | 204 | NAP | O2N-PN-O1N | 2.33 | 124.70 | 112.56 |
| 4 | 135-A | 204 | NAP | O2A-PA-O1A | 2.33 | 124.70 | 112.56 |
| 4 | 113-A | 204 | NAP | O2N-PN-O1N | 2.34 | 124.71 | 112.56 |
| 2 | 118-A | 201 | FOL | C12-C13-C14 | 2.34 | 122.92 | 120.30 |
| 4 | 39-A | 204 | NAP | C2N-C3N-C4N | 2.34 | 120.92 | 118.27 |
| 4 | 81-A | 204 | NAP | O3B-C3B-C2B | 2.34 | 117.89 | 111.13 |
| 4 | 95-A | 204 | NAP | O2A-PA-O1A | 2.34 | 124.74 | 112.56 |
| 4 | 86-A | 204 | NAP | O5B-PA-O1A | 2.34 | 118.80 | 109.21 |
| 4 | 150-A | 204 | NAP | O5B-PA-O1A | 2.34 | 118.80 | 109.21 |
| 4 | 55-A | 204 | NAP | O2N-PN-O1N | 2.34 | 124.76 | 112.56 |
| 4 | 132-A | 204 | NAP | C2D-C1D-N1N | 2.34 | 118.13 | 113.53 |
| 4 | 9-A | 204 | NAP | O3B-C3B-C2B | 2.35 | 117.90 | 111.13 |
| 4 | 21-A | 204 | NAP | O3B-C3B-C2B | 2.35 | 117.91 | 111.13 |
| 4 | 60-A | 204 | NAP | O3B-C3B-C2B | 2.35 | 117.91 | 111.13 |
| 4 | 40-A | 204 | NAP | O2A-PA-O1A | 2.35 | 124.78 | 112.56 |
| 4 | 37-A | 204 | NAP | O2A-PA-O1A | 2.35 | 124.78 | 112.56 |
| 4 | 38-A | 204 | NAP | O3B-C3B-C2B | 2.35 | 117.92 | 111.13 |
| 4 | 89-A | 204 | NAP | O3B-C3B-C2B | 2.35 | 117.92 | 111.13 |
| 4 | 96-A | 204 | NAP | O2N-PN-O1N | 2.35 | 124.79 | 112.56 |
| 2 | 20-A | 201 | FOL | CB-CA-N | 2.35 | 113.60 | 109.92 |
| 4 | 136-A | 204 | NAP | O3B-C3B-C2B | 2.35 | 117.92 | 111.13 |
| 4 | 19-A | 204 | NAP | O3X-P2B-O2X | 2.35 | 116.08 | 107.44 |
| 4 | 110-A | 204 | NAP | O5B-PA-O1A | 2.35 | 118.84 | 109.21 |
| 4 | 60-A | 204 | NAP | C2N-C3N-C4N | 2.35 | 120.94 | 118.27 |
| 4 | 84-A | 204 | NAP | O3B-C3B-C2B | 2.35 | 117.93 | 111.13 |
| 4 | 38-A | 204 | NAP | O2N-PN-O1N | 2.35 | 124.81 | 112.56 |
| 4 | 66-A | 204 | NAP | C2D-C1D-N1N | 2.35 | 118.15 | 113.53 |
| 4 | 15-A | 204 | NAP | O5B-PA-O1A | 2.35 | 118.85 | 109.21 |
| 4 | 106-A | 204 | NAP | C2D-C1D-N1N | 2.36 | 118.15 | 113.53 |
| 4 | 136-A | 204 | NAP | O3X-P2B-O2X | 2.36 | 116.09 | 107.44 |
| 4 | 103-A | 204 | NAP | C2D-C1D-N1N | 2.36 | 118.15 | 113.53 |
| 4 | 11-A | 204 | NAP | O3B-C3B-C2B | 2.36 | 117.94 | 111.13 |
| 4 | 35-A | 204 | NAP | O3B-C3B-C2B | 2.36 | 117.94 | 111.13 |
| 2 | 136-A | 201 | FOL | C15-C14-N10 | 2.36 | 125.72 | 121.04 |
| 4 | 37-A | 204 | NAP | O3B-C3B-C2B | 2.36 | 117.94 | 111.13 |
| 4 | 142-A | 204 | NAP | C2D-C1D-N1N | 2.36 | 118.16 | 113.53 |
| 4 | 60-A | 204 | NAP | O2A-PA-O1A | 2.36 | 124.84 | 112.56 |
| 2 | 66-A | 201 | FOL | N1-C8A-N8 | 2.36 | 120.74 | 116.47 |
| 4 | 142-A | 204 | NAP | O2N-PN-O1N | 2.36 | 124.85 | 112.56 |
| 4 | 136-A | 204 | NAP | O5B-PA-O1A | 2.36 | 118.88 | 109.21 |
| 4 | 64-A | 204 | NAP | O2A-PA-O1A | 2.36 | 124.85 | 112.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 155-A | 204 | NAP | O2N-PN-O1N | 2.37 | 124.86 | 112.56 |
| 4 | 110-A | 204 | NAP | O2N-PN-O1N | 2.37 | 124.87 | 112.56 |
| 4 | 44-A | 204 | NAP | O3B-C3B-C2B | 2.37 | 117.96 | 111.13 |
| 4 | 75-A | 204 | NAP | C2N-C3N-C4N | 2.37 | 120.95 | 118.27 |
| 4 | 68-A | 204 | NAP | O2A-PA-O1A | 2.37 | 124.88 | 112.56 |
| 4 | 50-A | 204 | NAP | O5B-PA-O1A | 2.37 | 118.91 | 109.21 |
| 4 | 155-A | 204 | NAP | C2N-C3N-C4N | 2.37 | 120.95 | 118.27 |
| 2 | 66-A | 201 | FOL | C4-C4A-N5 | 2.37 | 121.58 | 118.70 |
| 4 | 83-A | 204 | NAP | C2D-C3D-C4D | 2.37 | 107.49 | 102.64 |
| 2 | 9-A | 201 | FOL | CB-CA-N | 2.37 | 113.63 | 109.92 |
| 4 | 113-A | 204 | NAP | O2A-PA-O1A | 2.37 | 124.90 | 112.56 |
| 4 | 73-A | 204 | NAP | C2N-C3N-C4N | 2.37 | 120.96 | 118.27 |
| 4 | 38-A | 204 | NAP | O2A-PA-O1A | 2.37 | 124.91 | 112.56 |
| 4 | 37-A | 204 | NAP | C2N-C3N-C4N | 2.37 | 120.96 | 118.27 |
| 2 | 30-A | 201 | FOL | N1-C8A-N8 | 2.37 | 120.77 | 116.47 |
| 2 | 134-A | 201 | FOL | N1-C8A-N8 | 2.37 | 120.77 | 116.47 |
| 4 | 94-A | 204 | NAP | O2A-PA-O1A | 2.37 | 124.92 | 112.56 |
| 4 | 137-A | 204 | NAP | O2A-PA-O1A | 2.38 | 124.92 | 112.56 |
| 2 | 90-A | 201 | FOL | CB-CA-N | 2.38 | 113.63 | 109.92 |
| 4 | 75-A | 204 | NAP | O3B-C3B-C2B | 2.38 | 117.99 | 111.13 |
| 4 | 73-A | 204 | NAP | O5B-PA-O1A | 2.38 | 118.94 | 109.21 |
| 4 | 114-A | 204 | NAP | O3B-C3B-C2B | 2.38 | 118.00 | 111.13 |
| 4 | 8-A | 204 | NAP | C2D-C1D-N1N | 2.38 | 118.19 | 113.53 |
| 4 | 80-A | 204 | NAP | O2A-PA-O1A | 2.38 | 124.94 | 112.56 |
| 4 | 97-A | 204 | NAP | O2N-PN-O1N | 2.38 | 124.94 | 112.56 |
| 4 | 84-A | 204 | NAP | O2N-PN-O1N | 2.38 | 124.94 | 112.56 |
| 4 | 55-A | 204 | NAP | C2D-C1D-N1N | 2.38 | 118.20 | 113.53 |
| 4 | 45-A | 204 | NAP | O5B-PA-O1A | 2.38 | 118.96 | 109.21 |
| 4 | 144-A | 204 | NAP | C2D-C1D-N1N | 2.38 | 118.20 | 113.53 |
| 4 | 153-A | 204 | NAP | O2A-PA-O1A | 2.38 | 124.96 | 112.56 |
| 4 | 34-A | 204 | NAP | C2D-C1D-N1N | 2.38 | 118.20 | 113.53 |
| 4 | 109-A | 204 | NAP | C2D-C3D-C4D | 2.38 | 107.51 | 102.64 |
| 4 | 80-A | 204 | NAP | O3B-C3B-C2B | 2.38 | 118.02 | 111.13 |
| 4 | 98-A | 204 | NAP | O2N-PN-O1N | 2.38 | 124.97 | 112.56 |
| 2 | 152-A | 201 | FOL | C15-C16-C11 | 2.38 | 123.57 | 120.76 |
| 2 | 100-A | 201 | FOL | N1-C8A-N8 | 2.39 | 120.79 | 116.47 |
| 4 | 117-A | 204 | NAP | C2N-C3N-C4N | 2.39 | 120.97 | 118.27 |
| 4 | 125-A | 204 | NAP | O2N-PN-O1N | 2.39 | 124.98 | 112.56 |
| 4 | 14-A | 204 | NAP | O3B-C3B-C2B | 2.39 | 118.02 | 111.13 |
| 4 | 105-A | 204 | NAP | C2N-C3N-C4N | 2.39 | 120.97 | 118.27 |
| 4 | 59-A | 204 | NAP | C2D-C3D-C4D | 2.39 | 107.53 | 102.64 |
| 4 | 73-A | 204 | NAP | O2A-PA-O1A | 2.39 | 125.00 | 112.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2 | 58-A | 201 | FOL | C9-N10-C14 | 2.39 | 128.90 | 122.18 |
| 4 | 163-A | 204 | NAP | O5B-PA-O1A | 2.39 | 119.01 | 109.21 |
| 4 | 36-A | 204 | NAP | C2D-C1D-N1N | 2.39 | 118.22 | 113.53 |
| 2 | 157-A | 201 | FOL | C9-N10-C14 | 2.40 | 128.91 | 122.18 |
| 4 | 60-A | 204 | NAP | O5B-PA-O1A | 2.40 | 119.02 | 109.21 |
| 4 | 167-A | 204 | NAP | O3B-C3B-C2B | 2.40 | 118.05 | 111.13 |
| 4 | 151-A | 204 | NAP | O2N-PN-O1N | 2.40 | 125.03 | 112.56 |
| 4 | 161-A | 204 | NAP | C2D-C3D-C4D | 2.40 | 107.54 | 102.64 |
| 4 | 76-A | 204 | NAP | N6A-C6A-N1A | 2.40 | 122.54 | 118.52 |
| 2 | 99-A | 201 | FOL | O-C-C11 | 2.40 | 125.07 | 120.95 |
| 4 | 12-A | 204 | NAP | C4B-O4B-C1B | 2.40 | 112.19 | 109.64 |
| 2 | 15-A | 201 | FOL | C4-C4A-N5 | 2.40 | 121.62 | 118.70 |
| 4 | 129-A | 204 | NAP | C4B-O4B-C1B | 2.40 | 112.19 | 109.64 |
| 2 | 12-A | 201 | FOL | C4-C4A-N5 | 2.40 | 121.62 | 118.70 |
| 4 | 14-A | 204 | NAP | O5B-PA-O1A | 2.40 | 119.05 | 109.21 |
| 4 | 104-A | 204 | NAP | C2N-C3N-C4N | 2.40 | 120.99 | 118.27 |
| 4 | 167-A | 204 | NAP | O2A-PA-O1A | 2.40 | 125.07 | 112.56 |
| 4 | 28-A | 204 | NAP | C4B-O4B-C1B | 2.40 | 112.19 | 109.64 |
| 4 | 118-A | 204 | NAP | C4B-O4B-C1B | 2.40 | 112.19 | 109.64 |
| 4 | 151-A | 204 | NAP | O2A-PA-O1A | 2.41 | 125.08 | 112.56 |
| 4 | 147-A | 204 | NAP | O2N-PN-O1N | 2.41 | 125.08 | 112.56 |
| 4 | 48-A | 204 | NAP | O3B-C3B-C2B | 2.41 | 118.09 | 111.13 |
| 4 | 6-A | 204 | NAP | O2X-P2B-O1X | 2.41 | 118.49 | 110.63 |
| 4 | 78-A | 204 | NAP | O5B-PA-O1A | 2.41 | 119.08 | 109.21 |
| 4 | 25-A | 204 | NAP | C4B-O4B-C1B | 2.41 | 112.20 | 109.64 |
| 2 | 40-A | 201 | FOL | C4-C4A-N5 | 2.41 | 121.63 | 118.70 |
| 4 | 50-A | 204 | NAP | O2A-PA-O1A | 2.41 | 125.12 | 112.56 |
| 4 | 126-A | 204 | NAP | O2A-PA-O1A | 2.41 | 125.12 | 112.56 |
| 4 | 160-A | 204 | NAP | O2N-PN-O1N | 2.42 | 125.13 | 112.56 |
| 4 | 160-A | 204 | NAP | O5B-PA-O1A | 2.42 | 119.11 | 109.21 |
| 4 | 1-A | 204 | NAP | O2A-PA-O1A | 2.42 | 125.14 | 112.56 |
| 4 | 140-A | 204 | NAP | O5B-PA-O1A | 2.42 | 119.11 | 109.21 |
| 4 | 23-A | 204 | NAP | O3B-C3B-C2B | 2.42 | 118.12 | 111.13 |
| 4 | 160-A | 204 | NAP | C2D-C1D-N1N | 2.42 | 118.27 | 113.53 |
| 4 | 138-A | 204 | NAP | O2A-PA-O1A | 2.42 | 125.15 | 112.56 |
| 4 | 136-A | 204 | NAP | O2A-PA-O1A | 2.42 | 125.16 | 112.56 |
| 2 | 108-A | 201 | FOL | C9-N10-C14 | 2.42 | 128.98 | 122.18 |
| 4 | 51-A | 204 | NAP | O2A-PA-O1A | 2.42 | 125.16 | 112.56 |
| 2 | 123-A | 201 | FOL | N1-C8A-N8 | 2.42 | 120.85 | 116.47 |
| 4 | 16-A | 204 | NAP | C2N-C3N-C4N | 2.42 | 121.02 | 118.27 |
| 4 | 144-A | 204 | NAP | O3B-C3B-C2B | 2.42 | 118.13 | 111.13 |
| 4 | 94-A | 204 | NAP | O2N-PN-O1N | 2.42 | 125.17 | 112.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 3-A | 204 | NAP | C4B-O4B-C1B | 2.42 | 112.21 | 109.64 |
| 4 | 102-A | 204 | NAP | C4B-O4B-C1B | 2.42 | 112.21 | 109.64 |
| 4 | 149-A | 204 | NAP | O2A-PA-O1A | 2.42 | 125.17 | 112.56 |
| 2 | 119-A | 201 | FOL | C4-C4A-N5 | 2.42 | 121.65 | 118.70 |
| 4 | 139-A | 204 | NAP | O2N-PN-O1N | 2.43 | 125.18 | 112.56 |
| 4 | 5-A | 204 | NAP | O3B-C3B-C2B | 2.43 | 118.14 | 111.13 |
| 4 | 39-A | 204 | NAP | C2D-C3D-C4D | 2.43 | 107.60 | 102.64 |
| 4 | 139-A | 204 | NAP | O5B-PA-O1A | 2.43 | 119.15 | 109.21 |
| 4 | 110-A | 204 | NAP | O3B-C3B-C2B | 2.43 | 118.14 | 111.13 |
| 2 | 5-A | 201 | FOL | CB-CA-N | 2.43 | 113.72 | 109.92 |
| 2 | 6-A | 201 | FOL | C9-C6-N5 | 2.43 | 120.88 | 116.44 |
| 4 | 117-A | 204 | NAP | O2A-PA-O1A | 2.43 | 125.22 | 112.56 |
| 4 | 167-A | 204 | NAP | O5B-PA-O1A | 2.43 | 119.17 | 109.21 |
| 4 | 27-A | 204 | NAP | O2A-PA-O1A | 2.43 | 125.23 | 112.56 |
| 2 | 48-A | 201 | FOL | C4-C4A-N5 | 2.43 | 121.66 | 118.70 |
| 4 | 65-A | 204 | NAP | O2A-PA-O1A | 2.43 | 125.23 | 112.56 |
| 4 | 69-A | 204 | NAP | O2N-PN-O1N | 2.43 | 125.23 | 112.56 |
| 4 | 133-A | 204 | NAP | O3B-C3B-C2B | 2.44 | 118.17 | 111.13 |
| 4 | 129-A | 204 | NAP | C2D-C1D-N1N | 2.44 | 118.31 | 113.53 |
| 4 | 162-A | 204 | NAP | O2N-PN-O1N | 2.44 | 125.24 | 112.56 |
| 4 | 8-A | 204 | NAP | O3B-C3B-C2B | 2.44 | 118.17 | 111.13 |
| 4 | 39-A | 204 | NAP | O2A-PA-O1A | 2.44 | 125.24 | 112.56 |
| 4 | 162-A | 204 | NAP | O5B-PA-O1A | 2.44 | 119.20 | 109.21 |
| 2 | 27-A | 201 | FOL | C4-C4A-N5 | 2.44 | 121.67 | 118.70 |
| 4 | 148-A | 204 | NAP | O2N-PN-O1N | 2.44 | 125.27 | 112.56 |
| 4 | 51-A | 204 | NAP | C2D-C1D-N1N | 2.44 | 118.32 | 113.53 |
| 4 | 16-A | 204 | NAP | O2N-PN-O1N | 2.44 | 125.27 | 112.56 |
| 2 | 76-A | 201 | FOL | C9-C6-N5 | 2.44 | 120.91 | 116.44 |
| 2 | 136-A | 201 | FOL | N1-C8A-N8 | 2.44 | 120.89 | 116.47 |
| 4 | 145-A | 204 | NAP | O3B-C3B-C2B | 2.44 | 118.19 | 111.13 |
| 4 | 107-A | 204 | NAP | C2D-C1D-N1N | 2.45 | 118.33 | 113.53 |
| 4 | 146-A | 204 | NAP | C2D-C1D-N1N | 2.45 | 118.33 | 113.53 |
| 2 | 158-A | 201 | FOL | N1-C8A-N8 | 2.45 | 120.90 | 116.47 |
| 2 | 18-A | 201 | FOL | CB-CA-N | 2.45 | 113.75 | 109.92 |
| 4 | 98-A | 204 | NAP | O5B-PA-O1A | 2.45 | 119.24 | 109.21 |
| 4 | 117-A | 204 | NAP | O5B-PA-O1A | 2.45 | 119.24 | 109.21 |
| 4 | 50-A | 204 | NAP | C2D-C1D-N1N | 2.45 | 118.33 | 113.53 |
| 4 | 40-A | 204 | NAP | O2N-PN-O1N | 2.45 | 125.31 | 112.56 |
| 4 | 142-A | 204 | NAP | O5B-PA-O1A | 2.45 | 119.25 | 109.21 |
| 2 | 57-A | 201 | FOL | C9-C6-N5 | 2.45 | 120.93 | 116.44 |
| 4 | 139-A | 204 | NAP | C2D-C1D-N1N | 2.45 | 118.34 | 113.53 |
| 2 | 50-A | 201 | FOL | N1-C8A-N8 | 2.46 | 120.91 | 116.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 158-A | 204 | NAP | C2N-C3N-C4N | 2.46 | 121.05 | 118.27 |
| 4 | 124-A | 204 | NAP | O2N-PN-O1N | 2.46 | 125.34 | 112.56 |
| 4 | 36-A | 204 | NAP | C2N-C3N-C4N | 2.46 | 121.05 | 118.27 |
| 4 | 63-A | 204 | NAP | O3B-C3B-C2B | 2.46 | 118.22 | 111.13 |
| 4 | 43-A | 204 | NAP | O5B-PA-O1A | 2.46 | 119.27 | 109.21 |
| 4 | 139-A | 204 | NAP | O2A-PA-O1A | 2.46 | 125.35 | 112.56 |
| 4 | 15-A | 204 | NAP | O3B-C3B-C2B | 2.46 | 118.23 | 111.13 |
| 4 | 52-A | 204 | NAP | O3B-C3B-C2B | 2.46 | 118.23 | 111.13 |
| 4 | 26-A | 204 | NAP | O5B-PA-O1A | 2.46 | 119.28 | 109.21 |
| 4 | 97-A | 204 | NAP | O5B-PA-O1A | 2.46 | 119.29 | 109.21 |
| 4 | 166-A | 204 | NAP | O2A-PA-O1A | 2.46 | 125.37 | 112.56 |
| 2 | 1-A | 201 | FOL | O-C-N | 2.46 | 126.91 | 122.45 |
| 4 | 132-A | 204 | NAP | O3B-C3B-C2B | 2.46 | 118.25 | 111.13 |
| 4 | 43-A | 204 | NAP | O3B-C3B-C2B | 2.47 | 118.26 | 111.13 |
| 4 | 130-A | 204 | NAP | O3B-C3B-C2B | 2.47 | 118.27 | 111.13 |
| 4 | 42-A | 204 | NAP | C2N-C3N-C4N | 2.47 | 121.07 | 118.27 |
| 4 | 138-A | 204 | NAP | O3B-C3B-C2B | 2.47 | 118.27 | 111.13 |
| 2 | 66-A | 201 | FOL | CB-CA-N | 2.47 | 113.79 | 109.92 |
| 4 | 119-A | 204 | NAP | O5B-PA-O1A | 2.48 | 119.35 | 109.21 |
| 4 | 3-A | 204 | NAP | C2D-C1D-N1N | 2.48 | 118.39 | 113.53 |
| 4 | 86-A | 204 | NAP | O2A-PA-O1A | 2.48 | 125.45 | 112.56 |
| 4 | 24-A | 204 | NAP | C4B-O4B-C1B | 2.48 | 112.27 | 109.64 |
| 2 | 138-A | 201 | FOL | CB-CA-N | 2.48 | 113.79 | 109.92 |
| 4 | 44-A | 204 | NAP | C2D-C1D-N1N | 2.48 | 118.39 | 113.53 |
| 4 | 68-A | 204 | NAP | O2N-PN-O1N | 2.48 | 125.46 | 112.56 |
| 2 | 110-A | 201 | FOL | N1-C8A-N8 | 2.48 | 120.96 | 116.47 |
| 4 | 23-A | 204 | NAP | O2A-PA-O1A | 2.48 | 125.47 | 112.56 |
| 4 | 11-A | 204 | NAP | C2D-C1D-N1N | 2.48 | 118.39 | 113.53 |
| 4 | 26-A | 204 | NAP | C2N-C3N-C4N | 2.48 | 121.08 | 118.27 |
| 4 | 13-A | 204 | NAP | O2N-PN-O1N | 2.48 | 125.47 | 112.56 |
| 4 | 135-A | 204 | NAP | O2N-PN-O1N | 2.48 | 125.48 | 112.56 |
| 4 | 105-A | 204 | NAP | C2D-C1D-N1N | 2.48 | 118.40 | 113.53 |
| 4 | 122-A | 204 | NAP | C2D-C1D-N1N | 2.48 | 118.40 | 113.53 |
| 4 | 93-A | 204 | NAP | O2N-PN-O1N | 2.48 | 125.49 | 112.56 |
| 4 | 146-A | 204 | NAP | O2N-PN-O1N | 2.48 | 125.49 | 112.56 |
| 4 | 144-A | 204 | NAP | O2N-PN-O1N | 2.48 | 125.49 | 112.56 |
| 4 | 160-A | 204 | NAP | C2N-C3N-C4N | 2.49 | 121.09 | 118.27 |
| 4 | 163-A | 204 | NAP | O2N-PN-O1N | 2.49 | 125.49 | 112.56 |
| 4 | 21-A | 204 | NAP | C4B-O4B-C1B | 2.49 | 112.28 | 109.64 |
| 4 | 10-A | 204 | NAP | C2N-C3N-C4N | 2.49 | 121.09 | 118.27 |
| 2 | 144-A | 201 | FOL | C15-C14-N10 | 2.49 | 125.98 | 121.04 |
| 4 | 126-A | 204 | NAP | O2N-PN-O1N | 2.49 | 125.51 | 112.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 161-A | 204 | NAP | O5B-PA-O1A | 2.49 | 119.40 | 109.21 |
| 4 | 102-A | 204 | NAP | C2D-C1D-N1N | 2.49 | 118.41 | 113.53 |
| 4 | 24-A | 204 | NAP | C2N-C3N-C4N | 2.49 | 121.09 | 118.27 |
| 4 | 144-A | 204 | NAP | C2N-C3N-C4N | 2.49 | 121.09 | 118.27 |
| 4 | 92-A | 204 | NAP | C2D-C1D-N1N | 2.49 | 118.42 | 113.53 |
| 2 | 65-A | 201 | FOL | C4-C4A-N5 | 2.49 | 121.73 | 118.70 |
| 4 | 20-A | 204 | NAP | C4B-O4B-C1B | 2.49 | 112.29 | 109.64 |
| 4 | 16-A | 204 | NAP | C2D-C1D-N1N | 2.49 | 118.42 | 113.53 |
| 4 | 98-A | 204 | NAP | O2A-PA-O1A | 2.49 | 125.54 | 112.56 |
| 4 | 88-A | 204 | NAP | O2N-PN-O1N | 2.50 | 125.55 | 112.56 |
| 4 | 90-A | 204 | NAP | O5B-PA-O1A | 2.50 | 119.43 | 109.21 |
| 2 | 80-A | 201 | FOL | O-C-C11 | 2.50 | 125.23 | 120.95 |
| 4 | 30-A | 204 | NAP | C2N-C3N-C4N | 2.50 | 121.10 | 118.27 |
| 4 | 92-A | 204 | NAP | O2N-PN-O1N | 2.50 | 125.55 | 112.56 |
| 4 | 30-A | 204 | NAP | O2A-PA-O1A | 2.50 | 125.55 | 112.56 |
| 2 | 141-A | 201 | FOL | N1-C8A-N8 | 2.50 | 120.99 | 116.47 |
| 2 | 21-A | 201 | FOL | C11-C-N | 2.50 | 121.35 | 116.98 |
| 4 | 13-A | 204 | NAP | O5B-PA-O1A | 2.50 | 119.45 | 109.21 |
| 4 | 130-A | 204 | NAP | O2A-PA-O1A | 2.50 | 125.57 | 112.56 |
| 4 | 89-A | 204 | NAP | O5B-PA-O1A | 2.50 | 119.46 | 109.21 |
| 4 | 165-A | 204 | NAP | O5B-PA-O1A | 2.50 | 119.46 | 109.21 |
| 2 | 96-A | 201 | FOL | CB-CA-N | 2.51 | 113.84 | 109.92 |
| 4 | 16-A | 204 | NAP | O3B-C3B-C2B | 2.51 | 118.37 | 111.13 |
| 4 | 159-A | 204 | NAP | O3B-C3B-C2B | 2.51 | 118.37 | 111.13 |
| 4 | 85-A | 204 | NAP | O2N-PN-O1N | 2.51 | 125.60 | 112.56 |
| 4 | 138-A | 204 | NAP | O5B-PA-O1A | 2.51 | 119.47 | 109.21 |
| 4 | 145-A | 204 | NAP | O2N-PN-O1N | 2.51 | 125.60 | 112.56 |
| 4 | 148-A | 204 | NAP | O3B-C3B-C2B | 2.51 | 118.37 | 111.13 |
| 4 | 24-A | 204 | NAP | O2A-PA-O1A | 2.51 | 125.61 | 112.56 |
| 4 | 33-A | 204 | NAP | O3B-C3B-C2B | 2.51 | 118.37 | 111.13 |
| 4 | 85-A | 204 | NAP | O2A-PA-O1A | 2.51 | 125.61 | 112.56 |
| 4 | 16-A | 204 | NAP | O2A-PA-O1A | 2.51 | 125.62 | 112.56 |
| 4 | 51-A | 204 | NAP | O3B-C3B-C2B | 2.51 | 118.38 | 111.13 |
| 2 | 80-A | 201 | FOL | C6-C9-N10 | 2.51 | 118.92 | 113.30 |
| 2 | 96-A | 201 | FOL | N1-C8A-N8 | 2.51 | 121.02 | 116.47 |
| 4 | 88-A | 204 | NAP | O5B-PA-O1A | 2.51 | 119.50 | 109.21 |
| 4 | 54-A | 204 | NAP | O2N-PN-O1N | 2.51 | 125.64 | 112.56 |
| 2 | 29-A | 201 | FOL | C11-C-N | 2.52 | 121.38 | 116.98 |
| 4 | 25-A | 204 | NAP | O2N-PN-O1N | 2.52 | 125.66 | 112.56 |
| 2 | 151-A | 201 | FOL | CB-CA-N | 2.52 | 113.86 | 109.92 |
| 4 | 95-A | 204 | NAP | O5B-PA-O1A | 2.52 | 119.52 | 109.21 |
| 4 | 61-A | 204 | NAP | C2D-C1D-N1N | 2.52 | 118.47 | 113.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2 | 130-A | 201 | FOL | N1-C8A-N8 | 2.52 | 121.03 | 116.47 |
| 2 | 94-A | 201 | FOL | N1-C8A-N8 | 2.52 | 121.03 | 116.47 |
| 4 | 39-A | 204 | NAP | O2N-PN-O1N | 2.52 | 125.68 | 112.56 |
| 4 | 12-A | 204 | NAP | O2N-PN-O1N | 2.52 | 125.68 | 112.56 |
| 4 | 137-A | 204 | NAP | O5B-PA-O1A | 2.53 | 119.55 | 109.21 |
| 4 | 111-A | 204 | NAP | O5B-PA-O1A | 2.53 | 119.55 | 109.21 |
| 4 | 17-A | 204 | NAP | O2A-PA-O1A | 2.53 | 125.71 | 112.56 |
| 4 | 52-A | 204 | NAP | C2D-C1D-N1N | 2.53 | 118.49 | 113.53 |
| 2 | 63-A | 201 | FOL | C9-C6-N5 | 2.53 | 121.06 | 116.44 |
| 4 | 41-A | 204 | NAP | O2A-PA-O1A | 2.53 | 125.72 | 112.56 |
| 4 | 147-A | 204 | NAP | C2D-C1D-N1N | 2.53 | 118.49 | 113.53 |
| 2 | 141-A | 201 | FOL | C11-C-N | 2.53 | 121.41 | 116.98 |
| 4 | 11-A | 204 | NAP | O2N-PN-O1N | 2.53 | 125.73 | 112.56 |
| 4 | 159-A | 204 | NAP | C2D-C1D-N1N | 2.53 | 118.50 | 113.53 |
| 4 | 143-A | 204 | NAP | O2N-PN-O1N | 2.53 | 125.75 | 112.56 |
| 4 | 150-A | 204 | NAP | O2N-PN-O1N | 2.54 | 125.75 | 112.56 |
| 4 | 165-A | 204 | NAP | O2N-PN-O1N | 2.54 | 125.75 | 112.56 |
| 4 | 167-A | 204 | NAP | O2N-PN-O1N | 2.54 | 125.76 | 112.56 |
| 4 | 113-A | 204 | NAP | O5B-PA-O1A | 2.54 | 119.60 | 109.21 |
| 4 | 116-A | 204 | NAP | O2N-PN-O1N | 2.54 | 125.76 | 112.56 |
| 2 | 118-A | 201 | FOL | C15-C14-N10 | 2.54 | 126.08 | 121.04 |
| 2 | 4-A | 201 | FOL | N1-C8A-N8 | 2.54 | 121.06 | 116.47 |
| 4 | 21-A | 204 | NAP | C2D-C1D-N1N | 2.54 | 118.51 | 113.53 |
| 4 | 127-A | 204 | NAP | O2A-PA-O1A | 2.54 | 125.78 | 112.56 |
| 4 | 17-A | 204 | NAP | O2N-PN-O1N | 2.54 | 125.78 | 112.56 |
| 4 | 104-A | 204 | NAP | O2A-PA-O1A | 2.54 | 125.78 | 112.56 |
| 2 | 13-A | 201 | FOL | N1-C8A-N8 | 2.54 | 121.07 | 116.47 |
| 4 | 12-A | 204 | NAP | O3B-C3B-C2B | 2.54 | 118.47 | 111.13 |
| 4 | 157-A | 204 | NAP | C2D-C1D-N1N | 2.54 | 118.51 | 113.53 |
| 4 | 7-A | 204 | NAP | C2N-C3N-C4N | 2.54 | 121.15 | 118.27 |
| 4 | 164-A | 204 | NAP | O2A-PA-O1A | 2.54 | 125.78 | 112.56 |
| 4 | 69-A | 204 | NAP | O2A-PA-O1A | 2.54 | 125.79 | 112.56 |
| 4 | 101-A | 204 | NAP | O2A-PA-O1A | 2.55 | 125.80 | 112.56 |
| 4 | 23-A | 204 | NAP | C4B-O4B-C1B | 2.55 | 112.34 | 109.64 |
| 4 | 80-A | 204 | NAP | C4B-O4B-C1B | 2.55 | 112.34 | 109.64 |
| 4 | 152-A | 204 | NAP | O2A-PA-O1A | 2.55 | 125.82 | 112.56 |
| 4 | 61-A | 204 | NAP | O5B-PA-O1A | 2.55 | 119.65 | 109.21 |
| 4 | 99-A | 204 | NAP | O5B-PA-O1A | 2.55 | 119.66 | 109.21 |
| 2 | 85-A | 201 | FOL | N1-C8A-N8 | 2.55 | 121.09 | 116.47 |
| 2 | 129-A | 201 | FOL | C4-C4A-N5 | 2.55 | 121.80 | 118.70 |
| 4 | 66-A | 204 | NAP | O2N-PN-O1N | 2.55 | 125.84 | 112.56 |
| 4 | 45-A | 204 | NAP | O2N-PN-O1N | 2.55 | 125.84 | 112.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 2-A | 204 | NAP | O2A-PA-O1A | 2.56 | 125.85 | 112.56 |
| 4 | 61-A | 204 | NAP | O3B-C3B-C2B | 2.56 | 118.51 | 111.13 |
| 4 | 86-A | 204 | NAP | O2N-PN-O1N | 2.56 | 125.86 | 112.56 |
| 4 | 91-A | 204 | NAP | O2A-PA-O1A | 2.56 | 125.88 | 112.56 |
| 2 | 124-A | 201 | FOL | O-C-N | 2.56 | 127.09 | 122.45 |
| 4 | 76-A | 204 | NAP | O2A-PA-O1A | 2.56 | 125.88 | 112.56 |
| 4 | 111-A | 204 | NAP | O2N-PN-O1N | 2.56 | 125.89 | 112.56 |
| 4 | 102-A | 204 | NAP | O2A-PA-O1A | 2.56 | 125.89 | 112.56 |
| 4 | 112-A | 204 | NAP | O5B-PA-O1A | 2.56 | 119.70 | 109.21 |
| 4 | 41-A | 204 | NAP | O2N-PN-O1N | 2.56 | 125.90 | 112.56 |
| 2 | 74-A | 201 | FOL | C15-C16-C11 | 2.56 | 123.78 | 120.76 |
| 4 | 148-A | 204 | NAP | O2A-PA-O1A | 2.56 | 125.90 | 112.56 |
| 4 | 117-A | 204 | NAP | C3N-C7N-N7N | 2.56 | 120.72 | 117.82 |
| 4 | 122-A | 204 | NAP | O2A-PA-O1A | 2.56 | 125.90 | 112.56 |
| 4 | 108-A | 204 | NAP | O2X-P2B-O1X | 2.57 | 119.01 | 110.63 |
| 2 | 142-A | 201 | FOL | CB-CA-N | 2.57 | 113.93 | 109.92 |
| 4 | 64-A | 204 | NAP | O3B-C3B-C2B | 2.57 | 118.55 | 111.13 |
| 4 | 110-A | 204 | NAP | O2A-PA-O1A | 2.57 | 125.94 | 112.56 |
| 4 | 75-A | 204 | NAP | O5B-PA-O1A | 2.57 | 119.74 | 109.21 |
| 4 | 46-A | 204 | NAP | C2N-C3N-C4N | 2.57 | 121.18 | 118.27 |
| 4 | 43-A | 204 | NAP | O2N-PN-O1N | 2.57 | 125.94 | 112.56 |
| 4 | 132-A | 204 | NAP | C2N-C3N-C4N | 2.57 | 121.19 | 118.27 |
| 4 | 36-A | 204 | NAP | O2N-PN-O1N | 2.57 | 125.95 | 112.56 |
| 4 | 123-A | 204 | NAP | C2D-C1D-N1N | 2.57 | 118.58 | 113.53 |
| 4 | 42-A | 204 | NAP | O2N-PN-O1N | 2.57 | 125.95 | 112.56 |
| 4 | 92-A | 204 | NAP | O2A-PA-O1A | 2.58 | 125.97 | 112.56 |
| 4 | 42-A | 204 | NAP | C2D-C1D-N1N | 2.58 | 118.58 | 113.53 |
| 4 | 74-A | 204 | NAP | C2D-C1D-N1N | 2.58 | 118.58 | 113.53 |
| 4 | 63-A | 204 | NAP | O5B-PA-O1A | 2.58 | 119.77 | 109.21 |
| 4 | 56-A | 204 | NAP | C2N-C3N-C4N | 2.58 | 121.19 | 118.27 |
| 4 | 41-A | 204 | NAP | C2D-C1D-N1N | 2.58 | 118.59 | 113.53 |
| 4 | 75-A | 204 | NAP | O2A-PA-O1A | 2.58 | 125.98 | 112.56 |
| 4 | 101-A | 204 | NAP | O3B-C3B-C2B | 2.58 | 118.59 | 111.13 |
| 4 | 57-A | 204 | NAP | C2D-C1D-N1N | 2.58 | 118.59 | 113.53 |
| 4 | 25-A | 204 | NAP | O2A-PA-O1A | 2.58 | 126.00 | 112.56 |
| 4 | 67-A | 204 | NAP | O2A-PA-O1A | 2.58 | 126.00 | 112.56 |
| 4 | 48-A | 204 | NAP | O2A-PA-O1A | 2.58 | 126.00 | 112.56 |
| 4 | 49-A | 204 | NAP | O3B-C3B-C2B | 2.58 | 118.59 | 111.13 |
| 4 | 112-A | 204 | NAP | O2N-PN-O1N | 2.59 | 126.01 | 112.56 |
| 4 | 37-A | 204 | NAP | C2D-C1D-N1N | 2.59 | 118.60 | 113.53 |
| 4 | 131-A | 204 | NAP | O3B-C3B-C2B | 2.59 | 118.60 | 111.13 |
| 4 | 10-A | 204 | NAP | O2N-PN-O1N | 2.59 | 126.02 | 112.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 125-A | 204 | NAP | O3B-C3B-C2B | 2.59 | 118.61 | 111.13 |
| 4 | 62-A | 204 | NAP | O5B-PA-O1A | 2.59 | 119.81 | 109.21 |
| 4 | 122-A | 204 | NAP | N6A-C6A-N1A | 2.59 | 122.86 | 118.52 |
| 4 | 153-A | 204 | NAP | O2N-PN-O1N | 2.59 | 126.04 | 112.56 |
| 4 | 66-A | 204 | NAP | O2A-PA-O1A | 2.59 | 126.04 | 112.56 |
| 4 | 130-A | 204 | NAP | O5B-PA-O1A | 2.59 | 119.83 | 109.21 |
| 4 | 67-A | 204 | NAP | O2N-PN-O1N | 2.59 | 126.06 | 112.56 |
| 2 | 115-A | 201 | FOL | C9-N10-C14 | 2.60 | 129.47 | 122.18 |
| 4 | 35-A | 204 | NAP | O2N-PN-O1N | 2.60 | 126.07 | 112.56 |
| 2 | 55-A | 201 | FOL | CB-CA-N | 2.60 | 113.98 | 109.92 |
| 4 | 90-A | 204 | NAP | O3B-C3B-C2B | 2.60 | 118.63 | 111.13 |
| 4 | 33-A | 204 | NAP | C4B-O4B-C1B | 2.60 | 112.40 | 109.64 |
| 4 | 71-A | 204 | NAP | C2N-C3N-C4N | 2.60 | 121.21 | 118.27 |
| 4 | 62-A | 204 | NAP | O2N-PN-O1N | 2.60 | 126.08 | 112.56 |
| 4 | 53-A | 204 | NAP | O2A-PA-O1A | 2.60 | 126.08 | 112.56 |
| 4 | 127-A | 204 | NAP | O2N-PN-O1N | 2.60 | 126.08 | 112.56 |
| 2 | 131-A | 201 | FOL | CB-CG-CD | 2.60 | 123.64 | 113.05 |
| 4 | 127-A | 204 | NAP | C2D-C1D-N1N | 2.60 | 118.63 | 113.53 |
| 4 | 143-A | 204 | NAP | C2D-C1D-N1N | 2.60 | 118.63 | 113.53 |
| 4 | 99-A | 204 | NAP | O2N-PN-O1N | 2.60 | 126.09 | 112.56 |
| 4 | 1-A | 204 | NAP | O3B-C3B-C2B | 2.60 | 118.64 | 111.13 |
| 2 | 98-A | 201 | FOL | C4-C4A-N5 | 2.60 | 121.86 | 118.70 |
| 4 | 66-A | 204 | NAP | C4B-O4B-C1B | 2.60 | 112.40 | 109.64 |
| 4 | 44-A | 204 | NAP | O5B-PA-O1A | 2.61 | 119.88 | 109.21 |
| 4 | 73-A | 204 | NAP | O2N-PN-O1N | 2.61 | 126.13 | 112.56 |
| 4 | 118-A | 204 | NAP | C2D-C1D-N1N | 2.61 | 118.65 | 113.53 |
| 4 | 20-A | 204 | NAP | O3B-C3B-C2B | 2.61 | 118.67 | 111.13 |
| 4 | 38-A | 204 | NAP | C2D-C1D-N1N | 2.61 | 118.66 | 113.53 |
| 4 | 152-A | 204 | NAP | O2N-PN-O1N | 2.62 | 126.19 | 112.56 |
| 4 | 27-A | 204 | NAP | C2D-C1D-N1N | 2.62 | 118.67 | 113.53 |
| 4 | 149-A | 204 | NAP | O2N-PN-O1N | 2.62 | 126.20 | 112.56 |
| 4 | 15-A | 204 | NAP | O2A-PA-O1A | 2.62 | 126.20 | 112.56 |
| 4 | 1-A | 204 | NAP | C2D-C1D-N1N | 2.62 | 118.68 | 113.53 |
| 2 | 91-A | 201 | FOL | O-C-C11 | 2.62 | 125.45 | 120.95 |
| 4 | 36-A | 204 | NAP | O3B-C3B-C2B | 2.63 | 118.71 | 111.13 |
| 4 | 47-A | 204 | NAP | O2N-PN-O1N | 2.63 | 126.22 | 112.56 |
| 4 | 4-A | 204 | NAP | O2A-PA-O1A | 2.63 | 126.22 | 112.56 |
| 4 | 21-A | 204 | NAP | O2N-PN-O1N | 2.63 | 126.23 | 112.56 |
| 4 | 75-A | 204 | NAP | O2N-PN-O1N | 2.63 | 126.23 | 112.56 |
| 4 | 134-A | 204 | NAP | C2D-C1D-N1N | 2.63 | 118.68 | 113.53 |
| 4 | 32-A | 204 | NAP | C2N-C3N-C4N | 2.63 | 121.25 | 118.27 |
| 4 | 102-A | 204 | NAP | O2N-PN-O1N | 2.63 | 126.26 | 112.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 88-A | 204 | NAP | C2D-C1D-N1N | 2.63 | 118.69 | 113.53 |
| 4 | 32-A | 204 | NAP | C2D-C1D-N1N | 2.64 | 118.70 | 113.53 |
| 4 | 63-A | 204 | NAP | O2N-PN-O1N | 2.64 | 126.28 | 112.56 |
| 4 | 13-A | 204 | NAP | O3B-C3B-C2B | 2.64 | 118.75 | 111.13 |
| 4 | 99-A | 204 | NAP | O3B-C3B-C2B | 2.64 | 118.75 | 111.13 |
| 4 | 26-A | 204 | NAP | C2D-C1D-N1N | 2.64 | 118.70 | 113.53 |
| 4 | 5-A | 204 | NAP | C2D-C1D-N1N | 2.64 | 118.70 | 113.53 |
| 4 | 166-A | 204 | NAP | O2N-PN-O1N | 2.64 | 126.29 | 112.56 |
| 2 | 42-A | 201 | FOL | C4-C4A-N5 | 2.64 | 121.91 | 118.70 |
| 4 | 23-A | 204 | NAP | O5D-PN-O1N | 2.64 | 120.02 | 109.21 |
| 4 | 30-A | 204 | NAP | O2N-PN-O1N | 2.64 | 126.31 | 112.56 |
| 4 | 6-A | 204 | NAP | O3B-C3B-C2B | 2.65 | 118.77 | 111.13 |
| 2 | 137-A | 201 | FOL | N1-C8A-N8 | 2.65 | 121.26 | 116.47 |
| 2 | 138-A | 201 | FOL | C15-C14-N10 | 2.65 | 126.30 | 121.04 |
| 4 | 164-A | 204 | NAP | O7N-C7N-C3N | 2.65 | 122.53 | 119.60 |
| 4 | 61-A | 204 | NAP | O2N-PN-O1N | 2.65 | 126.36 | 112.56 |
| 2 | 64-A | 201 | FOL | C15-C14-N10 | 2.65 | 126.31 | 121.04 |
| 2 | 89-A | 201 | FOL | N1-C8A-N8 | 2.65 | 121.27 | 116.47 |
| 4 | 19-A | 204 | NAP | O2N-PN-O1N | 2.66 | 126.38 | 112.56 |
| 2 | 13-A | 201 | FOL | C4-C4A-N5 | 2.66 | 121.93 | 118.70 |
| 4 | 136-A | 204 | NAP | O2N-PN-O1N | 2.66 | 126.39 | 112.56 |
| 4 | 42-A | 204 | NAP | O2A-PA-O1A | 2.66 | 126.39 | 112.56 |
| 2 | 19-A | 201 | FOL | CB-CA-N | 2.66 | 114.08 | 109.92 |
| 2 | 128-A | 201 | FOL | CB-CA-N | 2.66 | 114.08 | 109.92 |
| 4 | 5-A | 204 | NAP | C2N-C3N-C4N | 2.66 | 121.28 | 118.27 |
| 4 | 5-A | 204 | NAP | O5B-PA-O1A | 2.66 | 120.11 | 109.21 |
| 2 | 129-A | 201 | FOL | C15-C16-C11 | 2.66 | 123.90 | 120.76 |
| 4 | 140-A | 204 | NAP | O3B-C3B-C2B | 2.66 | 118.82 | 111.13 |
| 4 | 156-A | 204 | NAP | O5B-PA-O1A | 2.66 | 120.12 | 109.21 |
| 4 | 17-A | 204 | NAP | C2N-C3N-C4N | 2.66 | 121.29 | 118.27 |
| 4 | 166-A | 204 | NAP | O5B-PA-O1A | 2.67 | 120.12 | 109.21 |
| 4 | 122-A | 204 | NAP | O5B-PA-O1A | 2.67 | 120.13 | 109.21 |
| 4 | 150-A | 204 | NAP | O7N-C7N-C3N | 2.67 | 122.55 | 119.60 |
| 4 | 100-A | 204 | NAP | O2A-PA-O1A | 2.67 | 126.44 | 112.56 |
| 4 | 26-A | 204 | NAP | O2N-PN-O1N | 2.67 | 126.47 | 112.56 |
| 4 | 166-A | 204 | NAP | C2D-C1D-N1N | 2.67 | 118.77 | 113.53 |
| 4 | 116-A | 204 | NAP | O2A-PA-O1A | 2.67 | 126.48 | 112.56 |
| 4 | 103-A | 204 | NAP | O2A-PA-O1A | 2.68 | 126.48 | 112.56 |
| 4 | 3-A | 204 | NAP | O5B-PA-O1A | 2.68 | 120.17 | 109.21 |
| 4 | 93-A | 204 | NAP | O2A-PA-O1A | 2.68 | 126.48 | 112.56 |
| 4 | 5-A | 204 | NAP | O2N-PN-O1N | 2.68 | 126.49 | 112.56 |
| 4 | 18-A | 204 | NAP | O2N-PN-O1N | 2.68 | 126.50 | 112.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 126-A | 204 | NAP | O3B-C3B-C2B | 2.68 | 118.87 | 111.13 |
| 2 | 167-A | 201 | FOL | C15-C14-N10 | 2.68 | 126.36 | 121.04 |
| 4 | 74-A | 204 | NAP | O2N-PN-O1N | 2.68 | 126.51 | 112.56 |
| 4 | 123-A | 204 | NAP | O5B-PA-O1A | 2.68 | 120.19 | 109.21 |
| 4 | 27-A | 204 | NAP | O2N-PN-O1N | 2.68 | 126.53 | 112.56 |
| 4 | 62-A | 204 | NAP | O3B-C3B-C2B | 2.69 | 118.89 | 111.13 |
| 4 | 130-A | 204 | NAP | C2N-C3N-C4N | 2.69 | 121.31 | 118.27 |
| 4 | 140-A | 204 | NAP | O2N-PN-O1N | 2.69 | 126.53 | 112.56 |
| 4 | 80-A | 204 | NAP | C2D-C1D-N1N | 2.69 | 118.80 | 113.53 |
| 4 | 165-A | 204 | NAP | O2A-PA-O1A | 2.69 | 126.55 | 112.56 |
| 4 | 65-A | 204 | NAP | O2N-PN-O1N | 2.69 | 126.55 | 112.56 |
| 2 | 146-A | 201 | FOL | N1-C8A-N8 | 2.69 | 121.34 | 116.47 |
| 4 | 59-A | 204 | NAP | O2N-PN-O1N | 2.69 | 126.56 | 112.56 |
| 4 | 25-A | 204 | NAP | O3B-C3B-C2B | 2.69 | 118.90 | 111.13 |
| 4 | 115-A | 204 | NAP | O2N-PN-O1N | 2.69 | 126.56 | 112.56 |
| 4 | 154-A | 204 | NAP | O5B-PA-O1A | 2.70 | 120.25 | 109.21 |
| 4 | 54-A | 204 | NAP | C2D-C1D-N1N | 2.70 | 118.81 | 113.53 |
| 2 | 7-A | 201 | FOL | N1-C8A-N8 | 2.70 | 121.35 | 116.47 |
| 4 | 79-A | 204 | NAP | O5B-PA-O1A | 2.70 | 120.28 | 109.21 |
| 2 | 48-A | 201 | FOL | C11-C-N | 2.70 | 121.71 | 116.98 |
| 4 | 50-A | 204 | NAP | O2N-PN-O1N | 2.70 | 126.63 | 112.56 |
| 2 | 56-A | 201 | FOL | N1-C8A-N8 | 2.70 | 121.36 | 116.47 |
| 4 | 49-A | 204 | NAP | O5B-PA-O1A | 2.71 | 120.29 | 109.21 |
| 4 | 24-A | 204 | NAP | O3B-C3B-C2B | 2.71 | 118.95 | 111.13 |
| 2 | 9-A | 201 | FOL | N1-C8A-N8 | 2.71 | 121.37 | 116.47 |
| 2 | 115-A | 201 | FOL | N1-C8A-N8 | 2.71 | 121.37 | 116.47 |
| 4 | 152-A | 204 | NAP | C2D-C1D-N1N | 2.71 | 118.84 | 113.53 |
| 4 | 14-A | 204 | NAP | O2N-PN-O1N | 2.71 | 126.67 | 112.56 |
| 2 | 34-A | 201 | FOL | C15-C16-C11 | 2.71 | 123.96 | 120.76 |
| 4 | 137-A | 204 | NAP | O2N-PN-O1N | 2.71 | 126.68 | 112.56 |
| 4 | 43-A | 204 | NAP | C2D-C1D-N1N | 2.72 | 118.86 | 113.53 |
| 2 | 118-A | 201 | FOL | C9-N10-C14 | 2.72 | 129.81 | 122.18 |
| 4 | 164-A | 204 | NAP | O2N-PN-O1N | 2.72 | 126.70 | 112.56 |
| 2 | 113-A | 201 | FOL | N1-C8A-N8 | 2.72 | 121.39 | 116.47 |
| 4 | 29-A | 204 | NAP | O5B-PA-O1A | 2.72 | 120.35 | 109.21 |
| 2 | 26-A | 201 | FOL | C4-C4A-N5 | 2.72 | 122.01 | 118.70 |
| 2 | 108-A | 201 | FOL | C15-C14-N10 | 2.72 | 126.45 | 121.04 |
| 4 | 114-A | 204 | NAP | O2N-PN-O1N | 2.72 | 126.72 | 112.56 |
| 4 | 123-A | 204 | NAP | O2N-PN-O1N | 2.72 | 126.72 | 112.56 |
| 4 | 19-A | 204 | NAP | O3B-C3B-C2B | 2.72 | 118.99 | 111.13 |
| 4 | 123-A | 204 | NAP | O2A-PA-O1A | 2.72 | 126.73 | 112.56 |
| 4 | 79-A | 204 | NAP | O2A-PA-O1A | 2.73 | 126.75 | 112.56 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 87-A | 204 | NAP | O5B-PA-O1A | 2.73 | 120.39 | 109.21 |
| 4 | 59-A | 204 | NAP | O3B-C3B-C2B | 2.73 | 119.02 | 111.13 |
| 4 | 12-A | 204 | NAP | C2D-C1D-N1N | 2.73 | 118.89 | 113.53 |
| 4 | 104-A | 204 | NAP | O5B-PA-O1A | 2.74 | 120.41 | 109.21 |
| 4 | 77-A | 204 | NAP | O2A-PA-O1A | 2.74 | 126.80 | 112.56 |
| 4 | 99-A | 204 | NAP | O2A-PA-O1A | 2.74 | 126.82 | 112.56 |
| 4 | 35-A | 204 | NAP | O7N-C7N-C3N | 2.75 | 122.64 | 119.60 |
| 4 | 56-A | 204 | NAP | O5D-PN-O1N | 2.75 | 120.46 | 109.21 |
| 2 | 71-A | 201 | FOL | N1-C8A-N8 | 2.75 | 121.44 | 116.47 |
| 4 | 49-A | 204 | NAP | C2D-C1D-N1N | 2.75 | 118.92 | 113.53 |
| 2 | 2-A | 201 | FOL | N1-C8A-N8 | 2.75 | 121.45 | 116.47 |
| 4 | 128-A | 204 | NAP | C2D-C1D-N1N | 2.75 | 118.92 | 113.53 |
| 4 | 75-A | 204 | NAP | C2D-C1D-N1N | 2.75 | 118.93 | 113.53 |
| 4 | 74-A | 204 | NAP | O2A-PA-O1A | 2.76 | 126.89 | 112.56 |
| 4 | 89-A | 204 | NAP | O2N-PN-O1N | 2.76 | 126.90 | 112.56 |
| 2 | 51-A | 201 | FOL | N1-C8A-N8 | 2.76 | 121.46 | 116.47 |
| 2 | 70-A | 201 | FOL | N1-C8A-N8 | 2.76 | 121.46 | 116.47 |
| 4 | 23-A | 204 | NAP | O2N-PN-O1N | 2.76 | 126.90 | 112.56 |
| 4 | 33-A | 204 | NAP | C2D-C1D-N1N | 2.76 | 118.94 | 113.53 |
| 4 | 118-A | 204 | NAP | O5B-PA-O1A | 2.76 | 120.50 | 109.21 |
| 4 | 3-A | 204 | NAP | O2N-PN-O1N | 2.76 | 126.92 | 112.56 |
| 2 | 26-A | 201 | FOL | C11-C-N | 2.76 | 121.81 | 116.98 |
| 4 | 4-A | 204 | NAP | O2N-PN-O1N | 2.76 | 126.94 | 112.56 |
| 2 | 126-A | 201 | FOL | CB-CA-N | 2.77 | 114.24 | 109.92 |
| 2 | 126-A | 201 | FOL | C9-C6-N5 | 2.77 | 121.50 | 116.44 |
| 4 | 28-A | 204 | NAP | O5B-PA-O1A | 2.77 | 120.53 | 109.21 |
| 4 | 70-A | 204 | NAP | O2N-PN-O1N | 2.77 | 126.96 | 112.56 |
| 2 | 23-A | 201 | FOL | C4-N3-C2 | 2.77 | 119.60 | 116.02 |
| 4 | 149-A | 204 | NAP | O3B-C3B-C2B | 2.77 | 119.13 | 111.13 |
| 4 | 42-A | 204 | NAP | O5B-PA-O1A | 2.77 | 120.56 | 109.21 |
| 4 | 167-A | 204 | NAP | C2D-C1D-N1N | 2.77 | 118.96 | 113.53 |
| 2 | 21-A | 201 | FOL | C9-C6-N5 | 2.77 | 121.51 | 116.44 |
| 4 | 104-A | 204 | NAP | O2N-PN-O1N | 2.77 | 126.99 | 112.56 |
| 4 | 28-A | 204 | NAP | C2D-C1D-N1N | 2.77 | 118.97 | 113.53 |
| 2 | 155-A | 201 | FOL | N1-C8A-N8 | 2.77 | 121.49 | 116.47 |
| 4 | 137-A | 204 | NAP | C2D-C1D-N1N | 2.77 | 118.97 | 113.53 |
| 4 | 158-A | 204 | NAP | C2D-C1D-N1N | 2.77 | 118.97 | 113.53 |
| 2 | 58-A | 201 | FOL | C12-C13-C14 | 2.78 | 123.41 | 120.30 |
| 4 | 15-A | 204 | NAP | C2N-C3N-C4N | 2.78 | 121.42 | 118.27 |
| 4 | 3-A | 204 | NAP | O2A-PA-O1A | 2.78 | 127.04 | 112.56 |
| 4 | 136-A | 204 | NAP | C2D-C1D-N1N | 2.79 | 118.99 | 113.53 |
| 4 | 71-A | 204 | NAP | C2D-C1D-N1N | 2.79 | 118.99 | 113.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 71-A | 204 | NAP | O2N-PN-O1N | 2.79 | 127.07 | 112.56 |
| 2 | 94-A | 201 | FOL | C9-C6-N5 | 2.79 | 121.54 | 116.44 |
| 4 | 103-A | 204 | NAP | O5B-PA-O1A | 2.79 | 120.63 | 109.21 |
| 4 | 90-A | 204 | NAP | O7N-C7N-C3N | 2.79 | 122.69 | 119.60 |
| 2 | 52-A | 201 | FOL | C15-C14-N10 | 2.79 | 126.58 | 121.04 |
| 4 | 156-A | 204 | NAP | O2N-PN-O1N | 2.79 | 127.09 | 112.56 |
| 4 | 154-A | 204 | NAP | O2A-PA-O1A | 2.80 | 127.11 | 112.56 |
| 4 | 40-A | 204 | NAP | C2D-C1D-N1N | 2.80 | 119.01 | 113.53 |
| 4 | 64-A | 204 | NAP | O2N-PN-O1N | 2.80 | 127.11 | 112.56 |
| 4 | 48-A | 204 | NAP | C2D-C1D-N1N | 2.80 | 119.01 | 113.53 |
| 4 | 124-A | 204 | NAP | O2A-PA-O1A | 2.80 | 127.12 | 112.56 |
| 4 | 20-A | 204 | NAP | O2N-PN-O1N | 2.80 | 127.13 | 112.56 |
| 4 | 155-A | 204 | NAP | C2D-C1D-N1N | 2.80 | 119.02 | 113.53 |
| 4 | 138-A | 204 | NAP | C2D-C1D-N1N | 2.80 | 119.03 | 113.53 |
| 4 | 130-A | 204 | NAP | O2N-PN-O1N | 2.80 | 127.14 | 112.56 |
| 2 | 127-A | 201 | FOL | C11-C-N | 2.80 | 121.88 | 116.98 |
| 2 | 122-A | 201 | FOL | N1-C8A-N8 | 2.81 | 121.55 | 116.47 |
| 4 | 70-A | 204 | NAP | C2D-C1D-N1N | 2.81 | 119.04 | 113.53 |
| 4 | 60-A | 204 | NAP | O2N-PN-O1N | 2.81 | 127.19 | 112.56 |
| 4 | 72-A | 204 | NAP | O2N-PN-O1N | 2.81 | 127.19 | 112.56 |
| 4 | 29-A | 204 | NAP | O2N-PN-O1N | 2.81 | 127.20 | 112.56 |
| 4 | 80-A | 204 | NAP | O5B-PA-O1A | 2.81 | 120.73 | 109.21 |
| 2 | 153-A | 201 | FOL | CB-CA-N | 2.82 | 114.32 | 109.92 |
| 4 | 80-A | 204 | NAP | O2N-PN-O1N | 2.82 | 127.22 | 112.56 |
| 2 | 25-A | 201 | FOL | N1-C8A-N8 | 2.82 | 121.57 | 116.47 |
| 4 | 50-A | 204 | NAP | O3B-C3B-C2B | 2.82 | 119.27 | 111.13 |
| 4 | 76-A | 204 | NAP | O2N-PN-O1N | 2.82 | 127.23 | 112.56 |
| 2 | 132-A | 201 | FOL | N1-C8A-N8 | 2.82 | 121.58 | 116.47 |
| 4 | 94-A | 204 | NAP | O5B-PA-O1A | 2.82 | 120.76 | 109.21 |
| 2 | 59-A | 201 | FOL | CB-CA-N | 2.82 | 114.33 | 109.92 |
| 2 | 104-A | 201 | FOL | CB-CA-N | 2.82 | 114.33 | 109.92 |
| 2 | 68-A | 201 | FOL | N1-C8A-N8 | 2.83 | 121.59 | 116.47 |
| 2 | 155-A | 201 | FOL | C9-N10-C14 | 2.83 | 130.14 | 122.18 |
| 4 | 28-A | 204 | NAP | O2N-PN-O1N | 2.84 | 127.32 | 112.56 |
| 4 | 78-A | 204 | NAP | O2A-PA-O1A | 2.84 | 127.34 | 112.56 |
| 4 | 165-A | 204 | NAP | C2D-C1D-N1N | 2.84 | 119.10 | 113.53 |
| 2 | 166-A | 201 | FOL | N1-C8A-N8 | 2.84 | 121.62 | 116.47 |
| 2 | 105-A | 201 | FOL | N1-C8A-N8 | 2.85 | 121.62 | 116.47 |
| 4 | 93-A | 204 | NAP | O5B-PA-O1A | 2.85 | 120.86 | 109.21 |
| 2 | 47-A | 201 | FOL | C4-C4A-N5 | 2.85 | 122.16 | 118.70 |
| 4 | 127-A | 204 | NAP | O5B-PA-O1A | 2.85 | 120.87 | 109.21 |
| 2 | 118-A | 201 | FOL | N1-C8A-N8 | 2.85 | 121.63 | 116.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 107-A | 204 | NAP | C2D-C3D-C4D | 2.85 | 108.47 | 102.64 |
| 4 | 46-A | 204 | NAP | O2N-PN-O1N | 2.85 | 127.40 | 112.56 |
| 4 | 128-A | 204 | NAP | O2A-PA-O1A | 2.85 | 127.41 | 112.56 |
| 4 | 121-A | 204 | NAP | O2N-PN-O1N | 2.85 | 127.41 | 112.56 |
| 2 | 125-A | 201 | FOL | N1-C8A-N8 | 2.86 | 121.65 | 116.47 |
| 4 | 122-A | 204 | NAP | O2N-PN-O1N | 2.87 | 127.47 | 112.56 |
| 2 | 34-A | 201 | FOL | O-C-C11 | 2.87 | 125.87 | 120.95 |
| 4 | 154-A | 204 | NAP | O2N-PN-O1N | 2.87 | 127.50 | 112.56 |
| 2 | 100-A | 201 | FOL | C9-C6-N5 | 2.87 | 121.69 | 116.44 |
| 4 | 138-A | 204 | NAP | O2N-PN-O1N | 2.87 | 127.51 | 112.56 |
| 4 | 2-A | 204 | NAP | O2N-PN-O1N | 2.87 | 127.52 | 112.56 |
| 4 | 150-A | 204 | NAP | O2A-PA-O1A | 2.88 | 127.52 | 112.56 |
| 4 | 47-A | 204 | NAP | C2D-C1D-N1N | 2.88 | 119.17 | 113.53 |
| 4 | 125-A | 204 | NAP | O2A-PA-O1A | 2.88 | 127.53 | 112.56 |
| 4 | 58-A | 204 | NAP | O2N-PN-O1N | 2.88 | 127.53 | 112.56 |
| 2 | 64-A | 201 | FOL | O-C-N | 2.88 | 127.67 | 122.45 |
| 4 | 54-A | 204 | NAP | O2A-PA-O1A | 2.88 | 127.56 | 112.56 |
| 4 | 51-A | 204 | NAP | O2N-PN-O1N | 2.88 | 127.56 | 112.56 |
| 4 | 54-A | 204 | NAP | O5B-PA-O1A | 2.88 | 121.02 | 109.21 |
| 2 | 54-A | 201 | FOL | C15-C14-N10 | 2.89 | 126.78 | 121.04 |
| 2 | 34-A | 201 | FOL | C9-N10-C14 | 2.89 | 130.29 | 122.18 |
| 4 | 27-A | 204 | NAP | O5B-PA-O1A | 2.89 | 121.04 | 109.21 |
| 2 | 138-A | 201 | FOL | C9-N10-C14 | 2.90 | 130.31 | 122.18 |
| 4 | 29-A | 204 | NAP | O2A-PA-O1A | 2.90 | 127.63 | 112.56 |
| 4 | 4-A | 204 | NAP | O5B-PA-O1A | 2.91 | 121.12 | 109.21 |
| 4 | 53-A | 204 | NAP | O2N-PN-O1N | 2.91 | 127.69 | 112.56 |
| 4 | 50-A | 204 | NAP | C4B-O4B-C1B | 2.91 | 112.73 | 109.64 |
| 4 | 129-A | 204 | NAP | O2N-PN-O1N | 2.91 | 127.72 | 112.56 |
| 2 | 26-A | 201 | FOL | C9-C6-N5 | 2.92 | 121.78 | 116.44 |
| 4 | 17-A | 204 | NAP | C2D-C1D-N1N | 2.93 | 119.27 | 113.53 |
| 4 | 93-A | 204 | NAP | C2D-C1D-N1N | 2.93 | 119.27 | 113.53 |
| 2 | 139-A | 201 | FOL | C4-C4A-N5 | 2.93 | 122.26 | 118.70 |
| 4 | 15-A | 204 | NAP | O2N-PN-O1N | 2.94 | 127.83 | 112.56 |
| 2 | 146-A | 201 | FOL | CB-CA-N | 2.94 | 114.51 | 109.92 |
| 2 | 18-A | 201 | FOL | N1-C8A-N8 | 2.94 | 121.79 | 116.47 |
| 2 | 42-A | 201 | FOL | C9-C6-N5 | 2.94 | 121.82 | 116.44 |
| 2 | 24-A | 201 | FOL | N1-C8A-N8 | 2.95 | 121.80 | 116.47 |
| 4 | 42-A | 204 | NAP | C4B-O4B-C1B | 2.95 | 112.77 | 109.64 |
| 4 | 115-A | 204 | NAP | O7N-C7N-C3N | 2.95 | 122.86 | 119.60 |
| 4 | 109-A | 204 | NAP | O2X-P2B-O1X | 2.95 | 120.26 | 110.63 |
| 4 | 128-A | 204 | NAP | O2N-PN-O1N | 2.95 | 127.92 | 112.56 |
| 2 | 92-A | 201 | FOL | N1-C8A-N8 | 2.95 | 121.82 | 116.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 4 | 19-A | 204 | NAP | C4B-O4B-C1B | 2.96 | 112.78 | 109.64 |
| 2 | 87-A | 201 | FOL | N1-C8A-N8 | 2.96 | 121.83 | 116.47 |
| 2 | 125-A | 201 | FOL | CB-CA-N | 2.96 | 114.55 | 109.92 |
| 2 | 37-A | 201 | FOL | C9-C6-N5 | 2.97 | 121.86 | 116.44 |
| 4 | 100-A | 204 | NAP | O2N-PN-O1N | 2.97 | 128.02 | 112.56 |
| 4 | 28-A | 204 | NAP | O2A-PA-O1A | 2.97 | 128.03 | 112.56 |
| 4 | 131-A | 204 | NAP | C2D-C1D-N1N | 2.97 | 119.36 | 113.53 |
| 2 | 82-A | 201 | FOL | C11-C-N | 2.98 | 122.19 | 116.98 |
| 2 | 65-A | 201 | FOL | C9-C6-N5 | 2.98 | 121.89 | 116.44 |
| 4 | 101-A | 204 | NAP | O2N-PN-O1N | 2.98 | 128.06 | 112.56 |
| 2 | 157-A | 201 | FOL | C4-N3-C2 | 2.98 | 119.87 | 116.02 |
| 4 | 79-A | 204 | NAP | C2D-C1D-N1N | 2.99 | 119.39 | 113.53 |
| 2 | 114-A | 201 | FOL | N1-C8A-N8 | 2.99 | 121.88 | 116.47 |
| 4 | 84-A | 204 | NAP | C2D-C1D-N1N | 2.99 | 119.40 | 113.53 |
| 2 | 40-A | 201 | FOL | N1-C8A-N8 | 3.00 | 121.89 | 116.47 |
| 4 | 77-A | 204 | NAP | O2N-PN-O1N | 3.00 | 128.16 | 112.56 |
| 2 | 140-A | 201 | FOL | CB-CA-N | 3.00 | 114.61 | 109.92 |
| 4 | 98-A | 204 | NAP | C2D-C1D-N1N | 3.01 | 119.43 | 113.53 |
| 2 | 84-A | 201 | FOL | N1-C8A-N8 | 3.01 | 121.91 | 116.47 |
| 2 | 162-A | 201 | FOL | N1-C8A-N8 | 3.01 | 121.91 | 116.47 |
| 4 | 79-A | 204 | NAP | O2N-PN-O1N | 3.01 | 128.22 | 112.56 |
| 4 | 1-A | 204 | NAP | O2N-PN-O1N | 3.01 | 128.23 | 112.56 |
| 2 | 14-A | 201 | FOL | CB-CG-CD | 3.02 | 125.36 | 113.05 |
| 2 | 153-A | 201 | FOL | C4-N3-C2 | 3.02 | 119.92 | 116.02 |
| 2 | 58-A | 201 | FOL | C15-C14-N10 | 3.02 | 127.04 | 121.04 |
| 2 | 14-A | 201 | FOL | N1-C8A-N8 | 3.03 | 121.94 | 116.47 |
| 4 | 129-A | 204 | NAP | O2A-PA-O1A | 3.03 | 128.31 | 112.56 |
| 2 | 32-A | 201 | FOL | N1-C8A-N8 | 3.03 | 121.95 | 116.47 |
| 4 | 99-A | 204 | NAP | C2D-C1D-N1N | 3.03 | 119.47 | 113.53 |
| 4 | 103-A | 204 | NAP | O2N-PN-O1N | 3.04 | 128.36 | 112.56 |
| 2 | 131-A | 201 | FOL | C4-N3-C2 | 3.04 | 119.94 | 116.02 |
| 4 | 164-A | 204 | NAP | C2D-C1D-N1N | 3.04 | 119.49 | 113.53 |
| 4 | 117-A | 204 | NAP | C2D-C1D-N1N | 3.04 | 119.49 | 113.53 |
| 2 | 17-A | 201 | FOL | N1-C8A-N8 | 3.04 | 121.97 | 116.47 |
| 4 | 52-A | 204 | NAP | O2N-PN-O1N | 3.04 | 128.39 | 112.56 |
| 4 | 48-A | 204 | NAP | O2N-PN-O1N | 3.06 | 128.47 | 112.56 |
| 2 | 11-A | 201 | FOL | N1-C8A-N8 | 3.06 | 122.00 | 116.47 |
| 4 | 119-A | 204 | NAP | C2D-C1D-N1N | 3.06 | 119.54 | 113.53 |
| 2 | 86-A | 201 | FOL | N1-C8A-N8 | 3.07 | 122.02 | 116.47 |
| 4 | 63-A | 204 | NAP | C2D-C1D-N1N | 3.07 | 119.54 | 113.53 |
| 2 | 36-A | 201 | FOL | N1-C8A-N8 | 3.07 | 122.02 | 116.47 |
| 2 | 44-A | 201 | FOL | N1-C8A-N8 | 3.07 | 122.03 | 116.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2 | 69-A | 201 | FOL | N1-C8A-N8 | 3.07 | 122.03 | 116.47 |
| 2 | 72-A | 201 | FOL | N1-C8A-N8 | 3.07 | 122.03 | 116.47 |
| 2 | 55-A | 201 | FOL | N1-C8A-N8 | 3.08 | 122.04 | 116.47 |
| 2 | 156-A | 201 | FOL | N1-C8A-N8 | 3.08 | 122.04 | 116.47 |
| 2 | 33-A | 201 | FOL | N1-C8A-N8 | 3.08 | 122.05 | 116.47 |
| 2 | 22-A | 201 | FOL | N1-C8A-N8 | 3.09 | 122.06 | 116.47 |
| 4 | 49-A | 204 | NAP | O2N-PN-O1N | 3.09 | 128.63 | 112.56 |
| 2 | 126-A | 201 | FOL | CT-CA-N | 3.10 | 119.11 | 112.93 |
| 2 | 150-A | 201 | FOL | N1-C8A-N8 | 3.10 | 122.08 | 116.47 |
| 2 | 37-A | 201 | FOL | C4-C4A-N5 | 3.10 | 122.47 | 118.70 |
| 4 | 4-A | 204 | NAP | C2D-C1D-N1N | 3.11 | 119.63 | 113.53 |
| 4 | 128-A | 204 | NAP | O5B-PA-O1A | 3.11 | 121.96 | 109.21 |
| 2 | 1-A | 201 | FOL | N1-C8A-N8 | 3.12 | 122.11 | 116.47 |
| 2 | 158-A | 201 | FOL | C4-N3-C2 | 3.13 | 120.06 | 116.02 |
| 2 | 119-A | 201 | FOL | CB-CA-N | 3.13 | 114.81 | 109.92 |
| 2 | 135-A | 201 | FOL | N1-C8A-N8 | 3.14 | 122.16 | 116.47 |
| 2 | 103-A | 201 | FOL | CB-CA-N | 3.15 | 114.84 | 109.92 |
| 4 | 129-A | 204 | NAP | O5B-PA-O1A | 3.15 | 122.12 | 109.21 |
| 4 | 78-A | 204 | NAP | O2N-PN-O1N | 3.15 | 128.97 | 112.56 |
| 2 | 21-A | 201 | FOL | C4-C4A-N5 | 3.16 | 122.54 | 118.70 |
| 2 | 140-A | 201 | FOL | N1-C8A-N8 | 3.16 | 122.19 | 116.47 |
| 2 | 109-A | 201 | FOL | N1-C8A-N8 | 3.17 | 122.20 | 116.47 |
| 4 | 25-A | 204 | NAP | C2D-C1D-N1N | 3.18 | 119.76 | 113.53 |
| 4 | 120-A | 204 | NAP | O2N-PN-O1N | 3.18 | 129.09 | 112.56 |
| 4 | 85-A | 204 | NAP | C2D-C1D-N1N | 3.18 | 119.76 | 113.53 |
| 2 | 3-A | 201 | FOL | N1-C8A-N8 | 3.19 | 122.25 | 116.47 |
| 2 | 45-A | 201 | FOL | N1-C8A-N8 | 3.20 | 122.25 | 116.47 |
| 2 | 79-A | 201 | FOL | N1-C8A-N8 | 3.20 | 122.25 | 116.47 |
| 2 | 145-A | 201 | FOL | N1-C8A-N8 | 3.20 | 122.26 | 116.47 |
| 4 | 156-A | 204 | NAP | C2D-C1D-N1N | 3.20 | 119.81 | 113.53 |
| 2 | 61-A | 201 | FOL | N1-C8A-N8 | 3.21 | 122.27 | 116.47 |
| 2 | 63-A | 201 | FOL | N1-C8A-N8 | 3.21 | 122.28 | 116.47 |
| 2 | 82-A | 201 | FOL | N1-C8A-N8 | 3.23 | 122.31 | 116.47 |
| 2 | 59-A | 201 | FOL | CB-CG-CD | 3.23 | 126.23 | 113.05 |
| 2 | 113-A | 201 | FOL | CB-CA-N | 3.24 | 114.98 | 109.92 |
| 2 | 88-A | 201 | FOL | N1-C8A-N8 | 3.24 | 122.33 | 116.47 |
| 4 | 155-A | 204 | NAP | O3X-P2B-O2X | 3.25 | 119.38 | 107.44 |
| 4 | 104-A | 204 | NAP | C2D-C3D-C4D | 3.27 | 109.32 | 102.64 |
| 4 | 104-A | 204 | NAP | C2D-C1D-N1N | 3.28 | 119.96 | 113.53 |
| 2 | 162-A | 201 | FOL | C4-N3-C2 | 3.28 | 120.26 | 116.02 |
| 2 | 126-A | 201 | FOL | C11-C-N | 3.28 | 122.72 | 116.98 |
| 2 | 157-A | 201 | FOL | N1-C8A-N8 | 3.29 | 122.42 | 116.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2 | 165-A | 201 | FOL | C4-N3-C2 | 3.29 | 120.27 | 116.02 |
| 2 | 20-A | 201 | FOL | C4-N3-C2 | 3.29 | 120.27 | 116.02 |
| 2 | 147-A | 201 | FOL | N1-C8A-N8 | 3.29 | 122.42 | 116.47 |
| 4 | 30-A | 204 | NAP | C2D-C1D-N1N | 3.29 | 119.99 | 113.53 |
| 4 | 56-A | 204 | NAP | C2D-C1D-N1N | 3.30 | 119.99 | 113.53 |
| 2 | 13-A | 201 | FOL | CB-CG-CD | 3.30 | 126.48 | 113.05 |
| 2 | 90-A | 201 | FOL | N1-C8A-N8 | 3.31 | 122.45 | 116.47 |
| 2 | 39-A | 201 | FOL | N1-C8A-N8 | 3.32 | 122.48 | 116.47 |
| 2 | 77-A | 201 | FOL | N1-C8A-N8 | 3.33 | 122.49 | 116.47 |
| 2 | 67-A | 201 | FOL | N1-C8A-N8 | 3.33 | 122.50 | 116.47 |
| 2 | 62-A | 201 | FOL | N1-C8A-N8 | 3.33 | 122.50 | 116.47 |
| 2 | 9-A | 201 | FOL | C4-N3-C2 | 3.33 | 120.33 | 116.02 |
| 4 | 59-A | 204 | NAP | C2D-C1D-N1N | 3.34 | 120.07 | 113.53 |
| 2 | 59-A | 201 | FOL | C4-N3-C2 | 3.35 | 120.35 | 116.02 |
| 2 | 31-A | 201 | FOL | N1-C8A-N8 | 3.35 | 122.54 | 116.47 |
| 2 | 46-A | 201 | FOL | CB-CA-N | 3.37 | 115.19 | 109.92 |
| 2 | 34-A | 201 | FOL | N1-C8A-N8 | 3.37 | 122.57 | 116.47 |
| 2 | 66-A | 201 | FOL | C15-C14-N10 | 3.37 | 127.74 | 121.04 |
| 2 | 159-A | 201 | FOL | N1-C8A-N8 | 3.38 | 122.58 | 116.47 |
| 2 | 48-A | 201 | FOL | CB-CG-CD | 3.38 | 126.84 | 113.05 |
| 2 | 34-A | 201 | FOL | C15-C14-N10 | 3.39 | 127.77 | 121.04 |
| 4 | 31-A | 204 | NAP | O3X-P2B-O2B | 3.39 | 116.77 | 106.62 |
| 2 | 64-A | 201 | FOL | N1-C8A-N8 | 3.40 | 122.61 | 116.47 |
| 2 | 34-A | 201 | FOL | C4-N3-C2 | 3.40 | 120.41 | 116.02 |
| 4 | 31-A | 204 | NAP | C2D-C1D-N1N | 3.41 | 120.21 | 113.53 |
| 2 | 60-A | 201 | FOL | N1-C8A-N8 | 3.41 | 122.64 | 116.47 |
| 2 | 153-A | 201 | FOL | N1-C8A-N8 | 3.41 | 122.65 | 116.47 |
| 2 | 97-A | 201 | FOL | N1-C8A-N8 | 3.41 | 122.65 | 116.47 |
| 2 | 148-A | 201 | FOL | N1-C8A-N8 | 3.42 | 122.65 | 116.47 |
| 2 | 99-A | 201 | FOL | N1-C8A-N8 | 3.42 | 122.66 | 116.47 |
| 2 | 149-A | 201 | FOL | CB-CG-CD | 3.42 | 127.01 | 113.05 |
| 2 | 109-A | 201 | FOL | CB-CA-N | 3.43 | 115.28 | 109.92 |
| 2 | 144-A | 201 | FOL | CB-CA-N | 3.43 | 115.28 | 109.92 |
| 4 | 89-A | 204 | NAP | C2D-C1D-N1N | 3.44 | 120.27 | 113.53 |
| 2 | 54-A | 201 | FOL | N1-C8A-N8 | 3.45 | 122.70 | 116.47 |
| 2 | 127-A | 201 | FOL | N1-C8A-N8 | 3.45 | 122.72 | 116.47 |
| 2 | 163-A | 201 | FOL | N1-C8A-N8 | 3.47 | 122.75 | 116.47 |
| 4 | 151-A | 204 | NAP | C2D-C1D-N1N | 3.47 | 120.34 | 113.53 |
| 4 | 49-A | 204 | NAP | O7N-C7N-C3N | 3.47 | 123.45 | 119.60 |
| 2 | 153-A | 201 | FOL | C11-C-N | 3.48 | 123.07 | 116.98 |
| 2 | 120-A | 201 | FOL | N1-C8A-N8 | 3.50 | 122.80 | 116.47 |
| 2 | 149-A | 201 | FOL | C4-N3-C2 | 3.50 | 120.54 | 116.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2 | 73-A | 201 | FOL | C4-N3-C2 | 3.50 | 120.54 | 116.02 |
| 2 | 116-A | 201 | FOL | N1-C8A-N8 | 3.50 | 122.80 | 116.47 |
| 2 | 117-A | 201 | FOL | C4-N3-C2 | 3.51 | 120.56 | 116.02 |
| 2 | 16-A | 201 | FOL | C4-N3-C2 | 3.52 | 120.56 | 116.02 |
| 2 | 46-A | 201 | FOL | N1-C8A-N8 | 3.52 | 122.84 | 116.47 |
| 4 | 139-A | 204 | NAP | O7N-C7N-C3N | 3.52 | 123.50 | 119.60 |
| 2 | 89-A | 201 | FOL | C4-N3-C2 | 3.52 | 120.57 | 116.02 |
| 2 | 4-A | 201 | FOL | CB-CA-N | 3.53 | 115.44 | 109.92 |
| 4 | 35-A | 204 | NAP | C2D-C1D-N1N | 3.54 | 120.46 | 113.53 |
| 2 | 159-A | 201 | FOL | C4-N3-C2 | 3.54 | 120.59 | 116.02 |
| 2 | 149-A | 201 | FOL | N1-C8A-N8 | 3.55 | 122.90 | 116.47 |
| 2 | 112-A | 201 | FOL | N1-C8A-N8 | 3.58 | 122.94 | 116.47 |
| 4 | 119-A | 204 | NAP | C4B-O4B-C1B | 3.58 | 113.44 | 109.64 |
| 2 | 76-A | 201 | FOL | C4-C4A-N5 | 3.58 | 123.06 | 118.70 |
| 2 | 33-A | 201 | FOL | CB-CG-CD | 3.58 | 127.67 | 113.05 |
| 2 | 95-A | 201 | FOL | N1-C8A-N8 | 3.59 | 122.97 | 116.47 |
| 2 | 129-A | 201 | FOL | CB-CA-N | 3.60 | 115.55 | 109.92 |
| 2 | 147-A | 201 | FOL | C4-N3-C2 | 3.61 | 120.69 | 116.02 |
| 2 | 144-A | 201 | FOL | N1-C8A-N8 | 3.64 | 123.05 | 116.47 |
| 2 | 101-A | 201 | FOL | C4-N3-C2 | 3.64 | 120.72 | 116.02 |
| 2 | 20-A | 201 | FOL | N1-C8A-N8 | 3.65 | 123.08 | 116.47 |
| 2 | 35-A | 201 | FOL | N1-C8A-N8 | 3.65 | 123.08 | 116.47 |
| 2 | 43-A | 201 | FOL | C4-N3-C2 | 3.66 | 120.75 | 116.02 |
| 2 | 165-A | 201 | FOL | N1-C8A-N8 | 3.66 | 123.09 | 116.47 |
| 2 | 73-A | 201 | FOL | N1-C8A-N8 | 3.68 | 123.12 | 116.47 |
| 2 | 145-A | 201 | FOL | CB-CA-N | 3.69 | 115.68 | 109.92 |
| 2 | 138-A | 201 | FOL | N1-C8A-N8 | 3.70 | 123.16 | 116.47 |
| 2 | 126-A | 201 | FOL | C4-C4A-N5 | 3.70 | 123.19 | 118.70 |
| 2 | 59-A | 201 | FOL | N1-C8A-N8 | 3.71 | 123.18 | 116.47 |
| 2 | 161-A | 201 | FOL | N1-C8A-N8 | 3.72 | 123.20 | 116.47 |
| 2 | 81-A | 201 | FOL | N1-C8A-N8 | 3.72 | 123.20 | 116.47 |
| 4 | 83-A | 204 | NAP | C2D-C1D-N1N | 3.72 | 120.83 | 113.53 |
| 4 | 108-A | 204 | NAP | O3D-C3D-C4D | 3.73 | 122.16 | 111.01 |
| 2 | 93-A | 201 | FOL | N1-C8A-N8 | 3.74 | 123.23 | 116.47 |
| 2 | 166-A | 201 | FOL | C4-N3-C2 | 3.74 | 120.86 | 116.02 |
| 2 | 78-A | 201 | FOL | N1-C8A-N8 | 3.75 | 123.25 | 116.47 |
| 2 | 67-A | 201 | FOL | CB-CA-N | 3.75 | 115.78 | 109.92 |
| 2 | 10-A | 201 | FOL | C4-N3-C2 | 3.75 | 120.87 | 116.02 |
| 4 | 33-A | 204 | NAP | O7N-C7N-C3N | 3.76 | 123.77 | 119.60 |
| 2 | 30-A | 201 | FOL | C4-C4A-N5 | 3.77 | 123.28 | 118.70 |
| 2 | 127-A | 201 | FOL | CB-CA-N | 3.78 | 115.83 | 109.92 |
| 2 | 23-A | 201 | FOL | N1-C8A-N8 | 3.78 | 123.31 | 116.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2 | 89-A | 201 | FOL | CB-CA-N | 3.78 | 115.83 | 109.92 |
| 2 | 5-A | 201 | FOL | C4-N3-C2 | 3.79 | 120.91 | 116.02 |
| 2 | 114-A | 201 | FOL | C4-N3-C2 | 3.79 | 120.91 | 116.02 |
| 2 | 35-A | 201 | FOL | C4-N3-C2 | 3.79 | 120.92 | 116.02 |
| 2 | 5-A | 201 | FOL | N1-C8A-N8 | 3.81 | 123.36 | 116.47 |
| 2 | 52-A | 201 | FOL | N1-C8A-N8 | 3.82 | 123.38 | 116.47 |
| 2 | 101-A | 201 | FOL | N1-C8A-N8 | 3.82 | 123.38 | 116.47 |
| 2 | 48-A | 201 | FOL | C4-N3-C2 | 3.82 | 120.96 | 116.02 |
| 2 | 106-A | 201 | FOL | N1-C8A-N8 | 3.83 | 123.40 | 116.47 |
| 2 | 52-A | 201 | FOL | C4-N3-C2 | 3.83 | 120.97 | 116.02 |
| 2 | 58-A | 201 | FOL | N1-C8A-N8 | 3.84 | 123.42 | 116.47 |
| 2 | 91-A | 201 | FOL | N1-C8A-N8 | 3.85 | 123.44 | 116.47 |
| 2 | 144-A | 201 | FOL | C4-N3-C2 | 3.87 | 121.02 | 116.02 |
| 2 | 33-A | 201 | FOL | C4-N3-C2 | 3.88 | 121.03 | 116.02 |
| 2 | 108-A | 201 | FOL | C4-N3-C2 | 3.88 | 121.04 | 116.02 |
| 2 | 80-A | 201 | FOL | N1-C8A-N8 | 3.89 | 123.51 | 116.47 |
| 2 | 90-A | 201 | FOL | C4-N3-C2 | 3.90 | 121.05 | 116.02 |
| 2 | 120-A | 201 | FOL | C4-N3-C2 | 3.90 | 121.06 | 116.02 |
| 2 | 102-A | 201 | FOL | C4-N3-C2 | 3.91 | 121.07 | 116.02 |
| 2 | 103-A | 201 | FOL | N1-C8A-N8 | 3.92 | 123.56 | 116.47 |
| 2 | 108-A | 201 | FOL | N1-C8A-N8 | 3.92 | 123.56 | 116.47 |
| 2 | 92-A | 201 | FOL | C4-N3-C2 | 3.92 | 121.08 | 116.02 |
| 4 | 18-A | 204 | NAP | O7N-C7N-C3N | 3.93 | 123.95 | 119.60 |
| 2 | 162-A | 201 | FOL | CB-CA-N | 3.93 | 116.06 | 109.92 |
| 2 | 32-A | 201 | FOL | C4-N3-C2 | 3.94 | 121.11 | 116.02 |
| 2 | 48-A | 201 | FOL | N1-C8A-N8 | 3.96 | 123.64 | 116.47 |
| 2 | 29-A | 201 | FOL | N1-C8A-N8 | 3.96 | 123.64 | 116.47 |
| 2 | 16-A | 201 | FOL | N1-C8A-N8 | 3.97 | 123.64 | 116.47 |
| 2 | 39-A | 201 | FOL | C4-N3-C2 | 4.01 | 121.20 | 116.02 |
| 2 | 111-A | 201 | FOL | CB-CA-N | 4.03 | 116.22 | 109.92 |
| 2 | 93-A | 201 | FOL | CB-CA-N | 4.04 | 116.23 | 109.92 |
| 2 | 56-A | 201 | FOL | CB-CA-N | 4.05 | 116.25 | 109.92 |
| 2 | 17-A | 201 | FOL | C4-N3-C2 | 4.06 | 121.26 | 116.02 |
| 2 | 75-A | 201 | FOL | N1-C8A-N8 | 4.07 | 123.83 | 116.47 |
| 2 | 142-A | 201 | FOL | C4-N3-C2 | 4.07 | 121.28 | 116.02 |
| 2 | 49-A | 201 | FOL | N1-C8A-N8 | 4.08 | 123.86 | 116.47 |
| 2 | 1-A | 201 | FOL | CB-CA-N | 4.09 | 116.31 | 109.92 |
| 2 | 128-A | 201 | FOL | N1-C8A-N8 | 4.09 | 123.86 | 116.47 |
| 2 | 12-A | 201 | FOL | C4-N3-C2 | 4.09 | 121.30 | 116.02 |
| 2 | 142-A | 201 | FOL | N1-C8A-N8 | 4.09 | 123.87 | 116.47 |
| 2 | 152-A | 201 | FOL | C4-N3-C2 | 4.10 | 121.31 | 116.02 |
| 2 | 40-A | 201 | FOL | CB-CA-N | 4.11 | 116.34 | 109.92 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 2 | 86-A | 201 | FOL | C4-N3-C2 | 4.12 | 121.34 | 116.02 |
| 2 | 45-A | 201 | FOL | C4-N3-C2 | 4.13 | 121.36 | 116.02 |
| 2 | 118-A | 201 | FOL | CB-CA-N | 4.13 | 116.38 | 109.92 |
| 2 | 87-A | 201 | FOL | C4-N3-C2 | 4.13 | 121.36 | 116.02 |
| 2 | 44-A | 201 | FOL | CB-CA-N | 4.14 | 116.40 | 109.92 |
| 2 | 109-A | 201 | FOL | C4-N3-C2 | 4.16 | 121.39 | 116.02 |
| 2 | 94-A | 201 | FOL | C4-N3-C2 | 4.16 | 121.39 | 116.02 |
| 2 | 57-A | 201 | FOL | CB-CA-N | 4.16 | 116.42 | 109.92 |
| 2 | 40-A | 201 | FOL | C4-N3-C2 | 4.16 | 121.40 | 116.02 |
| 2 | 80-A | 201 | FOL | CB-CA-N | 4.18 | 116.45 | 109.92 |
| 2 | 95-A | 201 | FOL | C4-N3-C2 | 4.18 | 121.42 | 116.02 |
| 2 | 2-A | 201 | FOL | C4-N3-C2 | 4.19 | 121.44 | 116.02 |
| 2 | 41-A | 201 | FOL | N1-C8A-N8 | 4.20 | 124.07 | 116.47 |
| 2 | 103-A | 201 | FOL | C4-N3-C2 | 4.21 | 121.46 | 116.02 |
| 2 | 102-A | 201 | FOL | N1-C8A-N8 | 4.23 | 124.12 | 116.47 |
| 2 | 112-A | 201 | FOL | C4-N3-C2 | 4.23 | 121.48 | 116.02 |
| 2 | 108-A | 201 | FOL | CB-CA-N | 4.23 | 116.53 | 109.92 |
| 2 | 104-A | 201 | FOL | N1-C8A-N8 | 4.25 | 124.15 | 116.47 |
| 2 | 10-A | 201 | FOL | N1-C8A-N8 | 4.25 | 124.17 | 116.47 |
| 2 | 41-A | 201 | FOL | C4-N3-C2 | 4.28 | 121.55 | 116.02 |
| 2 | 91-A | 201 | FOL | C4-N3-C2 | 4.30 | 121.57 | 116.02 |
| 2 | 38-A | 201 | FOL | N1-C8A-N8 | 4.30 | 124.25 | 116.47 |
| 2 | 134-A | 201 | FOL | C11-C-N | 4.30 | 124.50 | 116.98 |
| 2 | 96-A | 201 | FOL | C4-N3-C2 | 4.30 | 121.58 | 116.02 |
| 2 | 80-A | 201 | FOL | C4-N3-C2 | 4.31 | 121.58 | 116.02 |
| 2 | 124-A | 201 | FOL | C4-N3-C2 | 4.31 | 121.59 | 116.02 |
| 2 | 160-A | 201 | FOL | CB-CA-N | 4.31 | 116.66 | 109.92 |
| 2 | 124-A | 201 | FOL | CB-CA-N | 4.32 | 116.67 | 109.92 |
| 2 | 135-A | 201 | FOL | C4-N3-C2 | 4.32 | 121.61 | 116.02 |
| 2 | 140-A | 201 | FOL | C4-N3-C2 | 4.33 | 121.61 | 116.02 |
| 2 | 64-A | 201 | FOL | C4-N3-C2 | 4.35 | 121.64 | 116.02 |
| 2 | 93-A | 201 | FOL | C4-N3-C2 | 4.35 | 121.64 | 116.02 |
| 2 | 62-A | 201 | FOL | C4-N3-C2 | 4.35 | 121.64 | 116.02 |
| 2 | 60-A | 201 | FOL | C4-N3-C2 | 4.36 | 121.65 | 116.02 |
| 2 | 85-A | 201 | FOL | C4-N3-C2 | 4.36 | 121.66 | 116.02 |
| 2 | 131-A | 201 | FOL | N1-C8A-N8 | 4.37 | 124.37 | 116.47 |
| 2 | 43-A | 201 | FOL | N1-C8A-N8 | 4.37 | 124.37 | 116.47 |
| 4 | 117-A | 204 | NAP | O2N-PN-O1N | 4.39 | 135.38 | 112.56 |
| 2 | 137-A | 201 | FOL | C4-N3-C2 | 4.39 | 121.69 | 116.02 |
| 2 | 116-A | 201 | FOL | C4-N3-C2 | 4.39 | 121.69 | 116.02 |
| 2 | 54-A | 201 | FOL | C4-N3-C2 | 4.41 | 121.71 | 116.02 |
| 2 | 81-A | 201 | FOL | C4-N3-C2 | 4.41 | 121.72 | 116.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2 | 30-A | 201 | FOL | C4-N3-C2 | 4.42 | 121.73 | 116.02 |
| 2 | 24-A | 201 | FOL | CB-CA-N | 4.43 | 116.83 | 109.92 |
| 2 | 55-A | 201 | FOL | C4-N3-C2 | 4.46 | 121.78 | 116.02 |
| 2 | 148-A | 201 | FOL | C4-N3-C2 | 4.46 | 121.78 | 116.02 |
| 2 | 129-A | 201 | FOL | C4-N3-C2 | 4.47 | 121.80 | 116.02 |
| 2 | 127-A | 201 | FOL | C4-N3-C2 | 4.50 | 121.83 | 116.02 |
| 2 | 156-A | 201 | FOL | C4-N3-C2 | 4.50 | 121.83 | 116.02 |
| 2 | 165-A | 201 | FOL | CB-CA-N | 4.51 | 116.96 | 109.92 |
| 2 | 138-A | 201 | FOL | C4-N3-C2 | 4.51 | 121.84 | 116.02 |
| 2 | 24-A | 201 | FOL | C4-N3-C2 | 4.51 | 121.85 | 116.02 |
| 2 | 47-A | 201 | FOL | C4-N3-C2 | 4.52 | 121.86 | 116.02 |
| 2 | 150-A | 201 | FOL | C4-N3-C2 | 4.54 | 121.89 | 116.02 |
| 2 | 36-A | 201 | FOL | C4-N3-C2 | 4.54 | 121.89 | 116.02 |
| 2 | 31-A | 201 | FOL | C4-N3-C2 | 4.55 | 121.89 | 116.02 |
| 2 | 3-A | 201 | FOL | C4-N3-C2 | 4.55 | 121.90 | 116.02 |
| 2 | 115-A | 201 | FOL | C4-N3-C2 | 4.56 | 121.91 | 116.02 |
| 2 | 99-A | 201 | FOL | C4-N3-C2 | 4.57 | 121.92 | 116.02 |
| 2 | 84-A | 201 | FOL | C4-N3-C2 | 4.57 | 121.92 | 116.02 |
| 2 | 42-A | 201 | FOL | C4-N3-C2 | 4.57 | 121.93 | 116.02 |
| 2 | 7-A | 201 | FOL | C4-N3-C2 | 4.58 | 121.93 | 116.02 |
| 2 | 34-A | 201 | FOL | C12-C13-C14 | 4.58 | 125.44 | 120.30 |
| 2 | 158-A | 201 | FOL | CB-CA-N | 4.61 | 117.12 | 109.92 |
| 2 | 10-A | 201 | FOL | CB-CA-N | 4.61 | 117.13 | 109.92 |
| 2 | 29-A | 201 | FOL | C4-N3-C2 | 4.62 | 121.98 | 116.02 |
| 2 | 132-A | 201 | FOL | C4-N3-C2 | 4.62 | 121.98 | 116.02 |
| 2 | 141-A | 201 | FOL | C4-N3-C2 | 4.63 | 122.00 | 116.02 |
| 2 | 83-A | 201 | FOL | C4-N3-C2 | 4.63 | 122.00 | 116.02 |
| 2 | 118-A | 201 | FOL | C4-N3-C2 | 4.64 | 122.01 | 116.02 |
| 2 | 15-A | 201 | FOL | C4-N3-C2 | 4.64 | 122.02 | 116.02 |
| 2 | 87-A | 201 | FOL | CB-CA-N | 4.65 | 117.19 | 109.92 |
| 2 | 1-A | 201 | FOL | C4-N3-C2 | 4.65 | 122.03 | 116.02 |
| 2 | 68-A | 201 | FOL | C4-N3-C2 | 4.65 | 122.03 | 116.02 |
| 2 | 58-A | 201 | FOL | C4-N3-C2 | 4.65 | 122.03 | 116.02 |
| 2 | 161-A | 201 | FOL | C4-N3-C2 | 4.66 | 122.04 | 116.02 |
| 2 | 23-A | 201 | FOL | CB-CA-N | 4.67 | 117.21 | 109.92 |
| 2 | 21-A | 201 | FOL | C4-N3-C2 | 4.67 | 122.06 | 116.02 |
| 2 | 146-A | 201 | FOL | C4-N3-C2 | 4.68 | 122.07 | 116.02 |
| 2 | 81-A | 201 | FOL | CB-CA-N | 4.68 | 117.24 | 109.92 |
| 2 | 50-A | 201 | FOL | C4-N3-C2 | 4.69 | 122.08 | 116.02 |
| 2 | 122-A | 201 | FOL | C4-N3-C2 | 4.71 | 122.10 | 116.02 |
| 2 | 60-A | 201 | FOL | CB-CA-N | 4.73 | 117.30 | 109.92 |
| 2 | 74-A | 201 | FOL | C4-N3-C2 | 4.74 | 122.14 | 116.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2 | 69-A | 201 | FOL | CB-CA-N | 4.74 | 117.33 | 109.92 |
| 2 | 38-A | 201 | FOL | C4-N3-C2 | 4.75 | 122.15 | 116.02 |
| 2 | 130-A | 201 | FOL | C4-N3-C2 | 4.75 | 122.15 | 116.02 |
| 2 | 11-A | 201 | FOL | CB-CA-N | 4.75 | 117.34 | 109.92 |
| 2 | 82-A | 201 | FOL | CB-CA-N | 4.76 | 117.36 | 109.92 |
| 2 | 44-A | 201 | FOL | C4-N3-C2 | 4.79 | 122.20 | 116.02 |
| 2 | 78-A | 201 | FOL | C4-N3-C2 | 4.80 | 122.22 | 116.02 |
| 2 | 145-A | 201 | FOL | C4-N3-C2 | 4.80 | 122.22 | 116.02 |
| 2 | 155-A | 201 | FOL | C4-N3-C2 | 4.82 | 122.25 | 116.02 |
| 2 | 104-A | 201 | FOL | C4-N3-C2 | 4.82 | 122.25 | 116.02 |
| 2 | 70-A | 201 | FOL | C4-N3-C2 | 4.84 | 122.28 | 116.02 |
| 2 | 113-A | 201 | FOL | C4-N3-C2 | 4.84 | 122.28 | 116.02 |
| 2 | 63-A | 201 | FOL | CB-CA-N | 4.86 | 117.51 | 109.92 |
| 2 | 49-A | 201 | FOL | C4-N3-C2 | 4.86 | 122.30 | 116.02 |
| 2 | 79-A | 201 | FOL | C4-N3-C2 | 4.86 | 122.30 | 116.02 |
| 2 | 82-A | 201 | FOL | C4-N3-C2 | 4.89 | 122.34 | 116.02 |
| 2 | 26-A | 201 | FOL | C4-N3-C2 | 4.90 | 122.36 | 116.02 |
| 2 | 75-A | 201 | FOL | C4-N3-C2 | 4.91 | 122.36 | 116.02 |
| 2 | 121-A | 201 | FOL | C4-N3-C2 | 4.92 | 122.37 | 116.02 |
| 2 | 4-A | 201 | FOL | C4-N3-C2 | 4.92 | 122.38 | 116.02 |
| 2 | 65-A | 201 | FOL | C4-N3-C2 | 4.94 | 122.40 | 116.02 |
| 2 | 62-A | 201 | FOL | CB-CA-N | 4.95 | 117.65 | 109.92 |
| 2 | 11-A | 201 | FOL | C4-N3-C2 | 4.95 | 122.42 | 116.02 |
| 2 | 46-A | 201 | FOL | C4-N3-C2 | 4.95 | 122.42 | 116.02 |
| 2 | 100-A | 201 | FOL | C4-N3-C2 | 4.95 | 122.42 | 116.02 |
| 2 | 67-A | 201 | FOL | C4-N3-C2 | 4.96 | 122.42 | 116.02 |
| 2 | 119-A | 201 | FOL | C4-N3-C2 | 4.97 | 122.44 | 116.02 |
| 2 | 88-A | 201 | FOL | C4-N3-C2 | 4.97 | 122.44 | 116.02 |
| 2 | 163-A | 201 | FOL | C4-N3-C2 | 5.00 | 122.47 | 116.02 |
| 2 | 6-A | 201 | FOL | C4-N3-C2 | 5.00 | 122.48 | 116.02 |
| 2 | 97-A | 201 | FOL | C4-N3-C2 | 5.01 | 122.49 | 116.02 |
| 2 | 139-A | 201 | FOL | C4-N3-C2 | 5.01 | 122.49 | 116.02 |
| 2 | 105-A | 201 | FOL | C4-N3-C2 | 5.01 | 122.50 | 116.02 |
| 2 | 106-A | 201 | FOL | C4-N3-C2 | 5.02 | 122.51 | 116.02 |
| 2 | 71-A | 201 | FOL | C4-N3-C2 | 5.03 | 122.51 | 116.02 |
| 2 | 28-A | 201 | FOL | C4-N3-C2 | 5.04 | 122.53 | 116.02 |
| 2 | 51-A | 201 | FOL | C4-N3-C2 | 5.08 | 122.58 | 116.02 |
| 2 | 57-A | 201 | FOL | C4-N3-C2 | 5.09 | 122.59 | 116.02 |
| 2 | 61-A | 201 | FOL | C4-N3-C2 | 5.09 | 122.59 | 116.02 |
| 2 | 77-A | 201 | FOL | C4-N3-C2 | 5.09 | 122.60 | 116.02 |
| 2 | 19-A | 201 | FOL | C4-N3-C2 | 5.09 | 122.60 | 116.02 |
| 2 | 18-A | 201 | FOL | C4-N3-C2 | 5.10 | 122.61 | 116.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 2 | 37-A | 201 | FOL | C4-N3-C2 | 5.12 | 122.64 | 116.02 |
| 2 | 128-A | 201 | FOL | C4-N3-C2 | 5.13 | 122.64 | 116.02 |
| 2 | 70-A | 201 | FOL | CB-CA-N | 5.14 | 117.96 | 109.92 |
| 2 | 69-A | 201 | FOL | C4-N3-C2 | 5.15 | 122.68 | 116.02 |
| 2 | 143-A | 201 | FOL | C4-N3-C2 | 5.16 | 122.68 | 116.02 |
| 2 | 123-A | 201 | FOL | C4-N3-C2 | 5.20 | 122.74 | 116.02 |
| 2 | 151-A | 201 | FOL | C4-N3-C2 | 5.22 | 122.76 | 116.02 |
| 2 | 160-A | 201 | FOL | C4-N3-C2 | 5.24 | 122.79 | 116.02 |
| 2 | 22-A | 201 | FOL | C4-N3-C2 | 5.24 | 122.79 | 116.02 |
| 2 | 125-A | 201 | FOL | C4-N3-C2 | 5.27 | 122.83 | 116.02 |
| 2 | 110-A | 201 | FOL | C4-N3-C2 | 5.29 | 122.85 | 116.02 |
| 2 | 154-A | 201 | FOL | C4-N3-C2 | 5.35 | 122.93 | 116.02 |
| 2 | 63-A | 201 | FOL | C4-N3-C2 | 5.43 | 123.04 | 116.02 |
| 2 | 66-A | 201 | FOL | C4-N3-C2 | 5.47 | 123.09 | 116.02 |
| 2 | 26-A | 201 | FOL | CB-CA-N | 5.48 | 118.47 | 109.92 |
| 2 | 56-A | 201 | FOL | C4-N3-C2 | 5.57 | 123.22 | 116.02 |
| 2 | 134-A | 201 | FOL | C4-N3-C2 | 5.59 | 123.24 | 116.02 |
| 2 | 107-A | 201 | FOL | C4-N3-C2 | 5.61 | 123.27 | 116.02 |
| 2 | 164-A | 201 | FOL | C4-N3-C2 | 5.61 | 123.27 | 116.02 |
| 2 | 27-A | 201 | FOL | C4-N3-C2 | 5.63 | 123.29 | 116.02 |
| 2 | 25-A | 201 | FOL | C4-N3-C2 | 5.64 | 123.30 | 116.02 |
| 2 | 139-A | 201 | FOL | CB-CA-N | 5.65 | 118.74 | 109.92 |
| 2 | 43-A | 201 | FOL | CB-CA-N | 5.66 | 118.76 | 109.92 |
| 2 | 53-A | 201 | FOL | C4-N3-C2 | 5.67 | 123.35 | 116.02 |
| 2 | 111-A | 201 | FOL | C4-N3-C2 | 5.69 | 123.37 | 116.02 |
| 2 | 92-A | 201 | FOL | CB-CA-N | 5.71 | 118.84 | 109.92 |
| 2 | 136-A | 201 | FOL | C4-N3-C2 | 5.72 | 123.41 | 116.02 |
| 2 | 84-A | 201 | FOL | CB-CA-N | 5.72 | 118.86 | 109.92 |
| 2 | 14-A | 201 | FOL | C4-N3-C2 | 5.85 | 123.58 | 116.02 |
| 2 | 72-A | 201 | FOL | C4-N3-C2 | 5.95 | 123.70 | 116.02 |
| 2 | 8-A | 201 | FOL | C4-N3-C2 | 5.96 | 123.72 | 116.02 |
| 2 | 167-A | 201 | FOL | C4-N3-C2 | 6.14 | 123.95 | 116.02 |
| 2 | 85-A | 201 | FOL | CB-CA-N | 6.28 | 119.73 | 109.92 |
| 2 | 13-A | 201 | FOL | CB-CA-N | 6.30 | 119.76 | 109.92 |
| 2 | 14-A | 201 | FOL | CB-CA-N | 6.34 | 119.83 | 109.92 |
| 2 | 126-A | 201 | FOL | C4-N3-C2 | 6.37 | 124.25 | 116.02 |
| 4 | 119-A | 204 | NAP | O2N-PN-O1N | 6.57 | 146.73 | 112.56 |
| 2 | 25-A | 201 | FOL | CB-CA-N | 6.59 | 120.22 | 109.92 |
| 2 | 98-A | 201 | FOL | C4-N3-C2 | 6.61 | 124.57 | 116.02 |
| 2 | 83-A | 201 | FOL | CB-CA-N | 6.62 | 120.27 | 109.92 |
| 2 | 76-A | 201 | FOL | C4-N3-C2 | 6.90 | 124.94 | 116.02 |
| 2 | 133-A | 201 | FOL | C4-N3-C2 | 7.11 | 125.20 | 116.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^{\circ}$) | Ideal($^{\circ}$) |
|-----|-------|-----|------|------------|-------|------------------------|---------------------|
| 2 | 13-A | 201 | FOL | C4-N3-C2 | 7.16 | 125.27 | 116.02 |
| 2 | 39-A | 201 | FOL | CB-CA-N | 7.22 | 121.19 | 109.92 |
| 2 | 112-A | 201 | FOL | CB-CA-N | 7.34 | 121.38 | 109.92 |
| 2 | 110-A | 201 | FOL | CB-CA-N | 7.91 | 122.27 | 109.92 |
| 2 | 115-A | 201 | FOL | CB-CA-N | 8.03 | 122.46 | 109.92 |
| 2 | 114-A | 201 | FOL | CB-CA-N | 8.14 | 122.64 | 109.92 |
| 4 | 56-A | 204 | NAP | O2N-PN-O1N | 8.40 | 156.26 | 112.56 |
| 4 | 118-A | 204 | NAP | O2N-PN-O1N | 10.51 | 167.26 | 112.56 |
| 4 | 57-A | 204 | NAP | O2N-PN-O1N | 11.69 | 173.38 | 112.56 |

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section will therefore be empty.