



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 09:22 AM BST

PDB ID : 4P3R
Title : Cryogenic WT DHFR, time-averaged ensemble
Authors : Keedy, D.A.; van den Bedem, H.; Fraser, J.S.
Deposited on : 2014-03-10
Resolution : 1.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

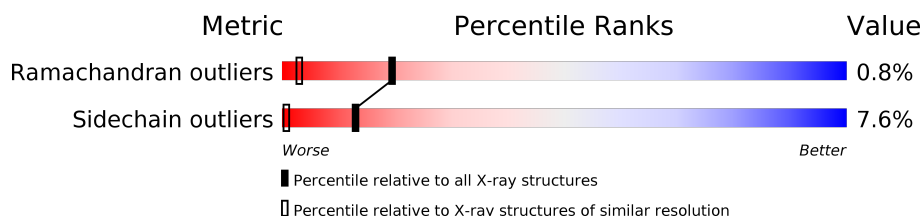
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.15 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 | 138981 | 1483 (1.18-1.10) |
| Sidechain outliers | 138945 | 1480 (1.18-1.10) |















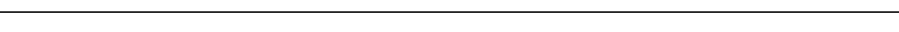

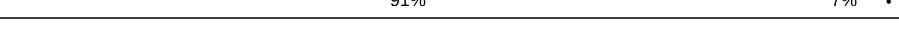

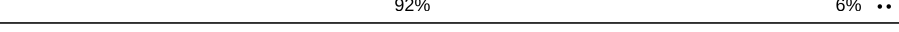






The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | 1-A | 159 | 92% 5% . . |
| 1 | 10-A | 159 | 92% 6% . |
| 1 | 100-A | 159 | 92% 7% . |
| 1 | 101-A | 159 | 90% 8% . . |
| 1 | 102-A | 159 | 89% 9% . |
| 1 | 103-A | 159 | 87% 12% . |
| 1 | 104-A | 159 | 89% 9% . |
| 1 | 105-A | 159 | 91% 9% |
| 1 | 106-A | 159 | 92% 6% . |















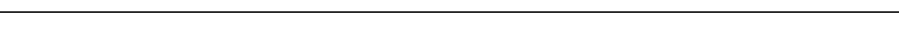

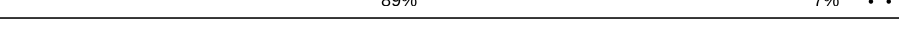

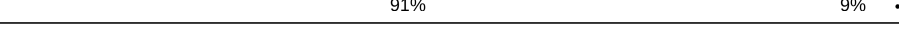
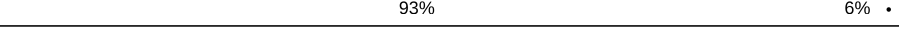
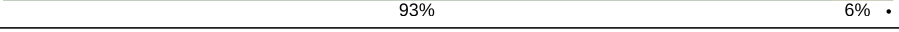




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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 107-A | 159 |  91% 8% . |
| 1 | 108-A | 159 |  91% 8% . |
| 1 | 109-A | 159 |  89% 9% .. |
| 1 | 11-A | 159 |  93% 6% . |
| 1 | 110-A | 159 |  88% 10% . |
| 1 | 111-A | 159 |  88% 11% . |
| 1 | 112-A | 159 |  90% 9% . |
| 1 | 113-A | 159 |  89% 11% . |
| 1 | 114-A | 159 |  92% 8% . |
| 1 | 115-A | 159 |  92% 5% .. |
| 1 | 116-A | 159 |  95% . . |
| 1 | 117-A | 159 |  93% 7% |
| 1 | 118-A | 159 |  94% 6% . |
| 1 | 119-A | 159 |  94% 5% . |
| 1 | 12-A | 159 |  91% 9% |
| 1 | 120-A | 159 |  91% 7% . |
| 1 | 121-A | 159 |  88% 9% .. |
| 1 | 122-A | 159 |  92% 6% .. |
| 1 | 123-A | 159 |  91% 7% . |
| 1 | 124-A | 159 |  89% 9% . |
| 1 | 125-A | 159 |  92% 7% .. |
| 1 | 126-A | 159 |  91% 8% . |
| 1 | 127-A | 159 |  91% 6% .. |
| 1 | 128-A | 159 |  92% 5% .. |
| 1 | 129-A | 159 |  88% 12% |

















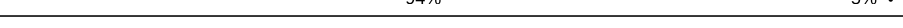
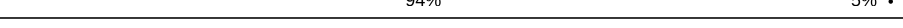

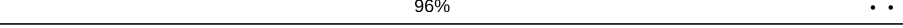





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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | 13-A | 159 |  89% 9% .. |
| 1 | 130-A | 159 |  91% 8% . |
| 1 | 131-A | 159 |  89% 8% .. |
| 1 | 132-A | 159 |  87% 10% .. |
| 1 | 133-A | 159 |  91% 6% .. |
| 1 | 134-A | 159 |  93% 5% .. |
| 1 | 135-A | 159 |  92% 6% . |
| 1 | 136-A | 159 |  89% 10% .. |
| 1 | 137-A | 159 |  89% 8% .. |
| 1 | 138-A | 159 |  91% 9% . |
| 1 | 139-A | 159 |  92% 6% . |
| 1 | 14-A | 159 |  92% 6% . |
| 1 | 140-A | 159 |  87% 10% .. |
| 1 | 141-A | 159 |  89% 9% .. |
| 1 | 142-A | 159 |  88% 9% .. |
| 1 | 143-A | 159 |  89% 7% .. |
| 1 | 144-A | 159 |  89% 8% .. |
| 1 | 145-A | 159 |  91% 9% . |
| 1 | 146-A | 159 |  93% 6% . |
| 1 | 147-A | 159 |  93% 6% . |
| 1 | 148-A | 159 |  93% 5% .. |
| 1 | 149-A | 159 |  89% 9% .. |
| 1 | 15-A | 159 |  93% 6% . |
| 1 | 150-A | 159 |  90% 9% . |
| 1 | 151-A | 159 |  91% 6% .. |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 152-A | 159 |  91% 9% . |
| 1 | 153-A | 159 |  89% 9% . |
| 1 | 154-A | 159 |  88% 11% . |
| 1 | 155-A | 159 |  92% 6% . |
| 1 | 156-A | 159 |  91% 7% . |
| 1 | 157-A | 159 |  90% 9% . |
| 1 | 158-A | 159 |  94% 5% .. |
| 1 | 159-A | 159 |  94% 6% . |
| 1 | 16-A | 159 |  94% 6% . |
| 1 | 160-A | 159 |  89% 9% . |
| 1 | 161-A | 159 |  94% 5% . |
| 1 | 162-A | 159 |  91% 9% . |
| 1 | 163-A | 159 |  89% 10% . |
| 1 | 164-A | 159 |  91% 8% . |
| 1 | 165-A | 159 |  92% 6% . |
| 1 | 166-A | 159 |  94% 5% . |
| 1 | 167-A | 159 |  94% 5% . |
| 1 | 168-A | 159 |  89% 9% . |
| 1 | 169-A | 159 |  96% .. |
| 1 | 17-A | 159 |  92% 8% |
| 1 | 170-A | 159 |  93% 6% . |
| 1 | 171-A | 159 |  92% 6% . |
| 1 | 172-A | 159 |  89% 9% . |
| 1 | 173-A | 159 |  89% 9% . |
| 1 | 174-A | 159 |  90% 8% . |







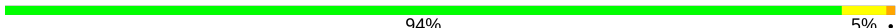


















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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | 175-A | 159 |  90% 8% . |
| 1 | 176-A | 159 |  92% 8% . |
| 1 | 177-A | 159 |  94% . . |
| 1 | 178-A | 159 |  91% 6% . |
| 1 | 179-A | 159 |  92% 6% . |
| 1 | 18-A | 159 |  91% 8% . |
| 1 | 180-A | 159 |  91% 9% . |
| 1 | 181-A | 159 |  90% 8% . |
| 1 | 182-A | 159 |  91% 8% . |
| 1 | 183-A | 159 |  89% 9% . |
| 1 | 184-A | 159 |  90% 8% . |
| 1 | 185-A | 159 |  89% 10% . |
| 1 | 186-A | 159 |  92% 6% . |
| 1 | 187-A | 159 |  89% 8% . |
| 1 | 188-A | 159 |  89% 10% . |
| 1 | 189-A | 159 |  92% 7% . |
| 1 | 19-A | 159 |  89% 9% . |
| 1 | 190-A | 159 |  90% 6% . |
| 1 | 191-A | 159 |  92% 5% . . |
| 1 | 192-A | 159 |  94% 6% . |
| 1 | 193-A | 159 |  89% 10% . |
| 1 | 194-A | 159 |  90% 7% . |
| 1 | 195-A | 159 |  91% 8% . . |
| 1 | 196-A | 159 |  91% 8% . |
| 1 | 197-A | 159 |  91% 8% . |










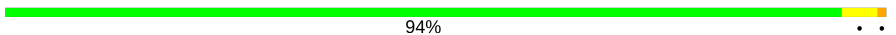







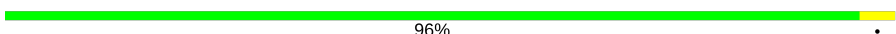







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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 198-A | 159 |  92% 6% . |
| 1 | 199-A | 159 |  88% 10% . |
| 1 | 2-A | 159 |  91% 8% . |
| 1 | 20-A | 159 |  89% 9% . |
| 1 | 200-A | 159 |  92% 6% . |
| 1 | 201-A | 159 |  88% 11% . |
| 1 | 202-A | 159 |  94% 5% . |
| 1 | 203-A | 159 |  91% 8% . |
| 1 | 204-A | 159 |  93% 6% . |
| 1 | 205-A | 159 |  89% 9% . |
| 1 | 206-A | 159 |  91% 6% . |
| 1 | 207-A | 159 |  92% 8% |
| 1 | 208-A | 159 |  89% 9% . |
| 1 | 209-A | 159 |  90% 9% . |
| 1 | 21-A | 159 |  92% 8% . |
| 1 | 210-A | 159 |  91% 7% .. |
| 1 | 211-A | 159 |  92% 8% . |
| 1 | 212-A | 159 |  89% 9% .. |
| 1 | 213-A | 159 |  88% 9% .. |
| 1 | 214-A | 159 |  90% 6% . |
| 1 | 215-A | 159 |  87% 10% . |
| 1 | 216-A | 159 |  87% 10% . |
| 1 | 217-A | 159 |  87% 11% . |
| 1 | 218-A | 159 |  86% 11% . |
| 1 | 219-A | 159 |  88% 9% . |















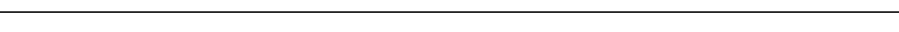

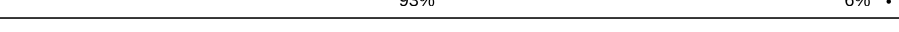
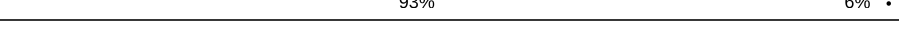
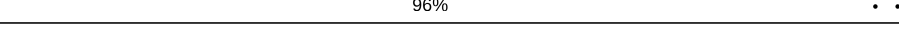
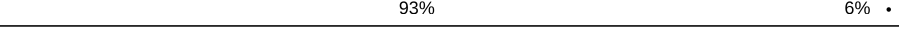





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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | 22-A | 159 |  93%5% • |
| 1 | 220-A | 159 |  89%9% • |
| 1 | 221-A | 159 |  88%8% • |
| 1 | 222-A | 159 |  90%8% • |
| 1 | 223-A | 159 |  91%6% •• |
| 1 | 224-A | 159 |  88%9% •• |
| 1 | 225-A | 159 |  90%6% • |
| 1 | 226-A | 159 |  89%8% • |
| 1 | 227-A | 159 |  91%8% • |
| 1 | 228-A | 159 |  94%•• |
| 1 | 229-A | 159 |  91%6% • |
| 1 | 23-A | 159 |  92%6% • |
| 1 | 230-A | 159 |  92%6% • |
| 1 | 231-A | 159 |  91%6% • |
| 1 | 232-A | 159 |  90%8% • |
| 1 | 233-A | 159 |  92%6% • |
| 1 | 234-A | 159 |  92%6% • |
| 1 | 235-A | 159 |  96%• |
| 1 | 236-A | 159 |  92%6% • |
| 1 | 237-A | 159 |  93%6% • |
| 1 | 238-A | 159 |  93%•• |
| 1 | 239-A | 159 |  94%5% • |
| 1 | 24-A | 159 |  89%10% • |
| 1 | 240-A | 159 |  92%7% • |
| 1 | 241-A | 159 |  95%5% |







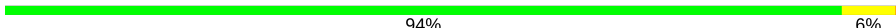


















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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | 242-A | 159 |  91% 8% . |
| 1 | 243-A | 159 |  92% 8% . |
| 1 | 244-A | 159 |  92% 6% . |
| 1 | 245-A | 159 |  91% 8% . |
| 1 | 246-A | 159 |  92% 7% . |
| 1 | 247-A | 159 |  92% 8% . |
| 1 | 248-A | 159 |  94% 5% . |
| 1 | 249-A | 159 |  91% 9% . |
| 1 | 25-A | 159 |  91% 8% . |
| 1 | 250-A | 159 |  92% 7% . |
| 1 | 26-A | 159 |  91% 8% . |
| 1 | 27-A | 159 |  94% 6% . |
| 1 | 28-A | 159 |  91% 8% . |
| 1 | 29-A | 159 |  94% 6% . |
| 1 | 3-A | 159 |  89% 7% . |
| 1 | 30-A | 159 |  93% 6% . |
| 1 | 31-A | 159 |  93% 6% . |
| 1 | 32-A | 159 |  96% . . |
| 1 | 33-A | 159 |  93% 6% . |
| 1 | 34-A | 159 |  91% 9% . |
| 1 | 35-A | 159 |  89% 9% . . |
| 1 | 36-A | 159 |  91% 7% . |
| 1 | 37-A | 159 |  93% 7% . |
| 1 | 38-A | 159 |  91% 8% . . |
| 1 | 39-A | 159 |  92% 8% . |


























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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 4-A | 159 |  92% 6% . |
| 1 | 40-A | 159 |  91% 6% . |
| 1 | 41-A | 159 |  89% 9% .. |
| 1 | 42-A | 159 |  91% 7% . |
| 1 | 43-A | 159 |  93% 6% . |
| 1 | 44-A | 159 |  92% 7% . |
| 1 | 45-A | 159 |  94% 6% . |
| 1 | 46-A | 159 |  92% 6% . |
| 1 | 47-A | 159 |  89% 8% . |
| 1 | 48-A | 159 |  90% 8% . |
| 1 | 49-A | 159 |  89% 9% . |
| 1 | 5-A | 159 |  93% . . |
| 1 | 50-A | 159 |  90% 8% . |
| 1 | 51-A | 159 |  89% 9% . |
| 1 | 52-A | 159 |  88% 10% . |
| 1 | 53-A | 159 |  88% 9% .. |
| 1 | 54-A | 159 |  88% 11% . |
| 1 | 55-A | 159 |  90% 8% . |
| 1 | 56-A | 159 |  91% 8% . |
| 1 | 57-A | 159 |  87% 8% . |
| 1 | 58-A | 159 |  89% 9% . |
| 1 | 59-A | 159 |  89% 8% . |
| 1 | 6-A | 159 |  94% 6% . |
| 1 | 60-A | 159 |  90% 8% . |
| 1 | 61-A | 159 |  91% 8% . |

















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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 1 | 62-A | 159 |  87% 10% .. |
| 1 | 63-A | 159 |  89% 8% .. |
| 1 | 64-A | 159 |  89% 9% .. |
| 1 | 65-A | 159 |  91% 7% .. |
| 1 | 66-A | 159 |  86% 10% .. |
| 1 | 67-A | 159 |  89% 8% . |
| 1 | 68-A | 159 |  91% 6% . |
| 1 | 69-A | 159 |  89% 9% .. |
| 1 | 7-A | 159 |  93% 5% . |
| 1 | 70-A | 159 |  87% 9% . |
| 1 | 71-A | 159 |  89% 7% . |
| 1 | 72-A | 159 |  92% 6% . |
| 1 | 73-A | 159 |  91% 7% . |
| 1 | 74-A | 159 |  89% 11% . |
| 1 | 75-A | 159 |  90% 7% . |
| 1 | 76-A | 159 |  88% 8% . |
| 1 | 77-A | 159 |  91% 6% . |
| 1 | 78-A | 159 |  89% 9% . |
| 1 | 79-A | 159 |  92% 8% . |
| 1 | 8-A | 159 |  91% 8% . |
| 1 | 80-A | 159 |  93% 6% . |
| 1 | 81-A | 159 |  92% 6% . |
| 1 | 82-A | 159 |  93% . . |
| 1 | 83-A | 159 |  88% 9% . |
| 1 | 84-A | 159 |  88% 10% .. |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | 85-A | 159 |  88% 11% . |
| 1 | 86-A | 159 |  91% 8% . |
| 1 | 87-A | 159 |  91% 8% . |
| 1 | 88-A | 159 |  89% 9% . |
| 1 | 89-A | 159 |  94% 6% . |
| 1 | 9-A | 159 |  91% 7% . |
| 1 | 90-A | 159 |  91% 7% .. |
| 1 | 91-A | 159 |  91% 8% . |
| 1 | 92-A | 159 |  92% 7% . |
| 1 | 93-A | 159 |  91% 9% . |
| 1 | 94-A | 159 |  90% 8% .. |
| 1 | 95-A | 159 |  92% 6% . |
| 1 | 96-A | 159 |  91% 8% . |
| 1 | 97-A | 159 |  88% 11% . |
| 1 | 98-A | 159 |  91% 9% |
| 1 | 99-A | 159 |  91% 8% . |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3 | NAP | 1-A | 202 | X | - | - | - |
| 3 | NAP | 103-A | 202 | X | - | - | - |
| 3 | NAP | 109-A | 202 | X | - | - | - |
| 3 | NAP | 118-A | 202 | X | - | - | - |
| 3 | NAP | 119-A | 202 | X | - | - | - |
| 3 | NAP | 120-A | 202 | X | - | - | - |
| 3 | NAP | 132-A | 202 | X | - | - | - |
| 3 | NAP | 141-A | 202 | X | - | - | - |
| 3 | NAP | 142-A | 202 | X | - | - | - |
| 3 | NAP | 143-A | 202 | X | - | - | - |

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| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 3 | NAP | 154-A | 202 | X | - | - | - |
| 3 | NAP | 163-A | 202 | X | - | - | - |
| 3 | NAP | 164-A | 202 | X | - | - | - |
| 3 | NAP | 178-A | 202 | X | - | - | - |
| 3 | NAP | 179-A | 202 | X | - | - | - |
| 3 | NAP | 18-A | 202 | X | - | - | - |
| 3 | NAP | 191-A | 202 | X | - | - | - |
| 3 | NAP | 192-A | 202 | X | - | - | - |
| 3 | NAP | 2-A | 202 | X | - | - | - |
| 3 | NAP | 205-A | 202 | X | - | - | - |
| 3 | NAP | 212-A | 202 | X | - | - | - |
| 3 | NAP | 213-A | 202 | X | - | - | - |
| 3 | NAP | 222-A | 202 | X | - | - | - |
| 3 | NAP | 223-A | 202 | X | - | - | - |
| 3 | NAP | 235-A | 202 | X | - | - | - |
| 3 | NAP | 236-A | 202 | X | - | - | - |
| 3 | NAP | 237-A | 202 | X | - | - | - |
| 3 | NAP | 238-A | 202 | X | - | - | - |
| 3 | NAP | 239-A | 202 | X | - | - | - |
| 3 | NAP | 29-A | 202 | X | - | - | - |
| 3 | NAP | 30-A | 202 | X | - | - | - |
| 3 | NAP | 41-A | 202 | X | - | - | - |
| 3 | NAP | 45-A | 202 | X | - | - | - |
| 3 | NAP | 55-A | 202 | X | - | - | - |
| 3 | NAP | 62-A | 202 | X | - | - | - |
| 3 | NAP | 63-A | 202 | X | - | - | - |
| 3 | NAP | 74-A | 202 | X | - | - | - |
| 3 | NAP | 85-A | 202 | X | - | - | - |
| 3 | NAP | 95-A | 202 | X | - | - | - |
| 3 | NAP | 96-A | 202 | X | - | - | - |

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 699653 atoms, of which 315500 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 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | | |
| 1 | 2-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | | |
| 1 | 3-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | | |
| 1 | 4-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | | |
| 1 | 5-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | | |
| 1 | 6-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | | |
| 1 | 7-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | | |
| 1 | 8-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | | |
| 1 | 9-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | | |
| 1 | 10-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | | |
| 1 | 11-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | | |
| 1 | 12-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | | |
| 1 | 13-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | | |
| 1 | 14-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | | |
| 1 | 15-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | | |
| 1 | 16-A | 159 | Total | C | H | N | O | S | | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 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 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 18-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 19-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 20-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 21-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 22-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 23-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 24-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 25-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 26-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 27-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 28-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 29-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 30-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 31-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 32-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 33-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 34-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 35-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 36-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 37-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 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 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 39-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 40-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 41-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 42-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 43-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 44-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 45-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 46-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 47-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 48-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 49-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 50-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 51-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 52-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 53-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 54-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 55-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 56-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 57-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 58-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 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 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 60-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 61-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 62-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 63-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 64-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 65-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 66-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 67-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 68-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 69-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 70-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 71-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 72-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 73-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 74-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 75-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 76-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 77-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 78-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 79-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 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 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 81-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 82-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 83-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 84-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 85-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 86-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 87-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 88-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 89-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 90-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 91-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 92-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 93-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 94-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 95-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 96-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 97-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 98-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 99-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 100-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 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 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 102-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 103-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 104-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 105-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 106-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 107-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 108-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 109-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 110-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 111-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 112-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 113-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 114-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 115-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 116-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 117-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 118-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 119-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 120-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 121-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 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 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 123-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 124-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 125-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 126-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 127-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 128-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 129-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 130-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 131-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 132-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 133-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 134-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 135-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 136-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 137-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 138-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 139-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 140-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 141-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 142-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 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 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 144-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 145-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 146-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 147-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 148-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 149-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 150-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 151-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 152-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 153-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 154-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 155-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 156-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 157-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 158-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 159-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 160-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 161-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 162-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 163-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 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 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 165-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 166-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 167-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 168-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 169-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 170-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 171-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 172-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 173-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 174-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 175-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 176-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 177-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 178-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 179-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 180-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 181-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 182-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 183-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 184-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 1 | 185-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 186-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 187-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 188-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 189-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 190-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 191-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 192-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 193-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 194-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 195-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 196-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 197-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 198-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 199-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 200-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 201-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 202-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 203-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 204-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 205-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 1 | 206-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 207-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 208-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 209-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 210-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 211-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 212-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 213-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 214-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 215-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 216-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 217-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 218-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 219-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 220-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 221-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 222-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 223-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 224-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 225-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 226-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |

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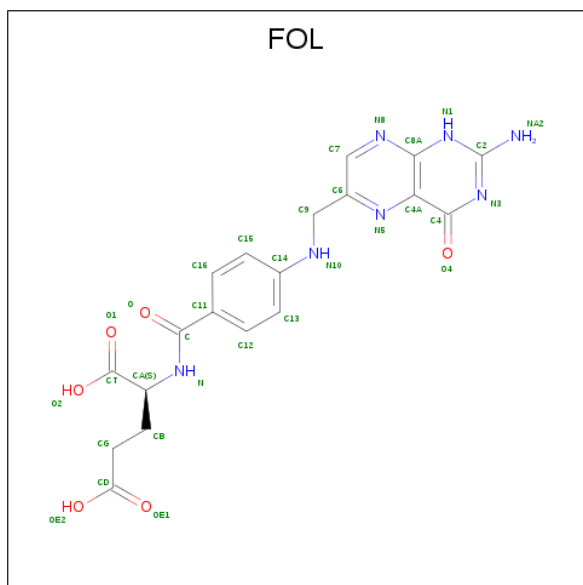
| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 1 | 227-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 228-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 229-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 230-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 231-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 232-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 233-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 234-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 235-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 236-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 237-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 238-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 239-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 240-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 241-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 242-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 243-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 244-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 245-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 246-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 247-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 1 | 248-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 249-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |
| 1 | 250-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2492 | 805 | 1224 | 217 | 239 | 7 | | | |

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



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | |
|-----|-------|----------|-------------|---------|---------|--------|---------|---------|---|
| 2 | 1-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 2-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 3-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 4-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 5-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 6-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 7-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 8-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 | 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 |
| 2 | 29-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 | 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 |
| 2 | 50-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 | 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 |
| 2 | 71-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 | 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 |
| 2 | 92-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 | 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 |
| 2 | 113-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 | 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 |
| 2 | 134-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 | 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 |
| 2 | 155-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 | 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 |
| 2 | 168-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 169-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 170-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 171-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 172-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 173-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 174-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 175-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 176-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 | 177-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 178-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 179-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 180-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 181-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 182-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 183-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 184-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 185-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 186-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 187-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 188-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 189-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 190-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 191-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 192-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 193-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 194-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 195-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 196-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 197-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 | 198-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 199-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 200-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 201-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 202-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 203-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 204-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 205-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 206-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 207-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 208-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 209-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 210-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 211-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 212-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 213-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 214-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 215-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 216-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 217-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 218-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |

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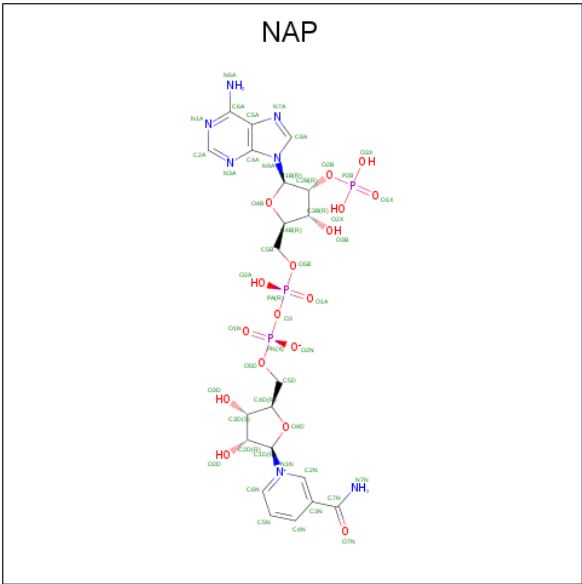
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 2 | 219-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 220-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 221-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 222-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 223-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 224-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 225-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 226-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 227-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 228-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 229-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 230-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 231-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 232-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 233-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 234-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 235-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 236-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 237-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 238-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 239-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 | 240-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 241-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 242-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 243-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 244-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 245-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 246-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 247-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 248-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 249-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |
| 2 | 250-A | 1 | Total | C | H | N | O | 0 | 0 |
| | | | 49 | 19 | 17 | 7 | 6 | | |

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



| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------|----|----|---|----|---|---------|---------|
| 3 | 1-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 2-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 3-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 4-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 5-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 6-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 7-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 8-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 9-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 10-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 11-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 12-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 13-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 14-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 15-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 16-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 17-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 18-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 19-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 20-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 21-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |
| 3 | 22-A | 1 | Total | C | H | N | O | P | 0 | 0 |
| | | | 69 | 21 | 21 | 7 | 17 | 3 | | |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 23-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 24-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 25-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 26-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 27-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 28-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 29-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 30-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 31-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 32-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 33-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 34-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 35-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 36-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 37-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 38-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 39-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 40-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 41-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 42-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 43-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 44-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 45-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 46-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 47-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 48-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 49-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 50-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 51-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 52-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 53-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 54-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 55-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 56-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 57-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 58-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 59-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 60-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 61-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 62-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 63-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 64-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 65-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 66-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 67-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 68-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 69-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 70-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 71-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 72-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 73-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 74-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 75-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 76-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 77-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 78-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 79-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 80-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 81-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 82-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 83-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 84-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 85-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 86-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 87-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 88-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 89-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 90-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 91-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 92-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 93-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 94-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 95-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 96-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 97-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 98-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 99-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 100-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 101-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 102-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 103-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 104-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 105-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 106-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 107-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 108-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 109-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 110-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 111-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 112-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 113-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 114-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 115-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 116-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 117-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 118-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 119-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 120-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 121-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 122-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 123-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 124-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 125-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 126-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 127-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 128-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 129-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 130-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 131-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 132-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 133-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 134-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 135-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 136-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 137-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 138-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 139-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 140-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 141-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 142-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 143-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 144-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 145-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 146-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 147-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 148-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 149-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 150-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 151-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 152-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 153-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 154-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 155-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 156-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 157-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 158-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 159-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 160-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 161-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 162-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 163-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 164-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 165-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 166-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 167-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 168-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 169-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 170-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 171-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 172-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 173-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 174-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 175-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 176-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 177-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 178-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 179-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 180-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 181-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 182-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 183-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 184-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 185-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 186-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 187-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 188-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 189-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 190-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 191-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 192-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 193-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 194-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 195-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 196-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 197-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 198-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 199-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 200-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 201-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 202-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 203-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 204-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 205-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 206-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 207-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 208-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 209-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 210-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 211-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 212-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 213-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 214-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 215-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 216-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 217-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 218-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 219-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 220-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 221-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 222-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 223-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 224-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 225-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 226-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 227-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 228-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 229-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 230-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 231-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 232-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|---------|--------|---------|---------|
| 3 | 233-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 234-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 235-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 236-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 237-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 238-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 239-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 240-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 241-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 242-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 243-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 244-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 245-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 246-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 247-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 248-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 249-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |
| 3 | 250-A | 1 | Total 69 | C 21 | H 21 | N 7 | O 17 | P 3 | 0 | 0 |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4 | 1-A | 200 | Total | O | 0 | 0 |
| | | | 200 | 200 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4 | 2-A | 206 | Total 206 | O 206 | 0 | 0 |
| 4 | 3-A | 185 | Total 185 | O 185 | 0 | 0 |
| 4 | 4-A | 175 | Total 175 | O 175 | 0 | 0 |
| 4 | 5-A | 186 | Total 186 | O 186 | 0 | 0 |
| 4 | 6-A | 185 | Total 185 | O 185 | 0 | 0 |
| 4 | 7-A | 202 | Total 202 | O 202 | 0 | 0 |
| 4 | 8-A | 200 | Total 200 | O 200 | 0 | 0 |
| 4 | 9-A | 201 | Total 201 | O 201 | 0 | 0 |
| 4 | 10-A | 204 | Total 204 | O 204 | 0 | 0 |
| 4 | 11-A | 205 | Total 205 | O 205 | 0 | 0 |
| 4 | 12-A | 197 | Total 197 | O 197 | 0 | 0 |
| 4 | 13-A | 192 | Total 192 | O 192 | 0 | 0 |
| 4 | 14-A | 189 | Total 189 | O 189 | 0 | 0 |
| 4 | 15-A | 173 | Total 173 | O 173 | 0 | 0 |
| 4 | 16-A | 176 | Total 176 | O 176 | 0 | 0 |
| 4 | 17-A | 188 | Total 188 | O 188 | 0 | 0 |
| 4 | 18-A | 195 | Total 195 | O 195 | 0 | 0 |
| 4 | 19-A | 196 | Total 196 | O 196 | 0 | 0 |
| 4 | 20-A | 211 | Total 211 | O 211 | 0 | 0 |
| 4 | 21-A | 189 | Total 189 | O 189 | 0 | 0 |
| 4 | 22-A | 191 | Total 191 | O 191 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4 | 23-A | 173 | Total 173 | O 173 | 0 | 0 |
| 4 | 24-A | 183 | Total 183 | O 183 | 0 | 0 |
| 4 | 25-A | 174 | Total 174 | O 174 | 0 | 0 |
| 4 | 26-A | 195 | Total 195 | O 195 | 0 | 0 |
| 4 | 27-A | 188 | Total 188 | O 188 | 0 | 0 |
| 4 | 28-A | 181 | Total 181 | O 181 | 0 | 0 |
| 4 | 29-A | 183 | Total 183 | O 183 | 0 | 0 |
| 4 | 30-A | 186 | Total 186 | O 186 | 0 | 0 |
| 4 | 31-A | 191 | Total 191 | O 191 | 0 | 0 |
| 4 | 32-A | 187 | Total 187 | O 187 | 0 | 0 |
| 4 | 33-A | 190 | Total 190 | O 190 | 0 | 0 |
| 4 | 34-A | 194 | Total 194 | O 194 | 0 | 0 |
| 4 | 35-A | 201 | Total 201 | O 201 | 0 | 0 |
| 4 | 36-A | 197 | Total 197 | O 197 | 0 | 0 |
| 4 | 37-A | 196 | Total 196 | O 196 | 0 | 0 |
| 4 | 38-A | 203 | Total 203 | O 203 | 0 | 0 |
| 4 | 39-A | 181 | Total 181 | O 181 | 0 | 0 |
| 4 | 40-A | 171 | Total 171 | O 171 | 0 | 0 |
| 4 | 41-A | 179 | Total 179 | O 179 | 0 | 0 |
| 4 | 42-A | 176 | Total 176 | O 176 | 0 | 0 |
| 4 | 43-A | 176 | Total 176 | O 176 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|-------|-----|---------|---------|
| 4 | 44-A | 183 | Total | O | 0 | 0 |
| | | | 183 | 183 | | |
| 4 | 45-A | 187 | Total | O | 0 | 0 |
| | | | 187 | 187 | | |
| 4 | 46-A | 197 | Total | O | 0 | 0 |
| | | | 197 | 197 | | |
| 4 | 47-A | 191 | Total | O | 0 | 0 |
| | | | 191 | 191 | | |
| 4 | 48-A | 184 | Total | O | 0 | 0 |
| | | | 184 | 184 | | |
| 4 | 49-A | 195 | Total | O | 0 | 0 |
| | | | 195 | 195 | | |
| 4 | 50-A | 189 | Total | O | 0 | 0 |
| | | | 189 | 189 | | |
| 4 | 51-A | 198 | Total | O | 0 | 0 |
| | | | 198 | 198 | | |
| 4 | 52-A | 190 | Total | O | 0 | 0 |
| | | | 190 | 190 | | |
| 4 | 53-A | 182 | Total | O | 0 | 0 |
| | | | 182 | 182 | | |
| 4 | 54-A | 180 | Total | O | 0 | 0 |
| | | | 180 | 180 | | |
| 4 | 55-A | 185 | Total | O | 0 | 0 |
| | | | 185 | 185 | | |
| 4 | 56-A | 184 | Total | O | 0 | 0 |
| | | | 184 | 184 | | |
| 4 | 57-A | 191 | Total | O | 0 | 0 |
| | | | 191 | 191 | | |
| 4 | 58-A | 187 | Total | O | 0 | 0 |
| | | | 187 | 187 | | |
| 4 | 59-A | 192 | Total | O | 0 | 0 |
| | | | 192 | 192 | | |
| 4 | 60-A | 173 | Total | O | 0 | 0 |
| | | | 173 | 173 | | |
| 4 | 61-A | 186 | Total | O | 0 | 0 |
| | | | 186 | 186 | | |
| 4 | 62-A | 201 | Total | O | 0 | 0 |
| | | | 201 | 201 | | |
| 4 | 63-A | 201 | Total | O | 0 | 0 |
| | | | 201 | 201 | | |
| 4 | 64-A | 188 | Total | O | 0 | 0 |
| | | | 188 | 188 | | |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4 | 65-A | 187 | Total 187 | O 187 | 0 | 0 |
| 4 | 66-A | 174 | Total 174 | O 174 | 0 | 0 |
| 4 | 67-A | 184 | Total 184 | O 184 | 0 | 0 |
| 4 | 68-A | 178 | Total 178 | O 178 | 0 | 0 |
| 4 | 69-A | 173 | Total 173 | O 173 | 0 | 0 |
| 4 | 70-A | 171 | Total 171 | O 171 | 0 | 0 |
| 4 | 71-A | 171 | Total 171 | O 171 | 0 | 0 |
| 4 | 72-A | 196 | Total 196 | O 196 | 0 | 0 |
| 4 | 73-A | 207 | Total 207 | O 207 | 0 | 0 |
| 4 | 74-A | 191 | Total 191 | O 191 | 0 | 0 |
| 4 | 75-A | 193 | Total 193 | O 193 | 0 | 0 |
| 4 | 76-A | 182 | Total 182 | O 182 | 0 | 0 |
| 4 | 77-A | 176 | Total 176 | O 176 | 0 | 0 |
| 4 | 78-A | 184 | Total 184 | O 184 | 0 | 0 |
| 4 | 79-A | 193 | Total 193 | O 193 | 0 | 0 |
| 4 | 80-A | 201 | Total 201 | O 201 | 0 | 0 |
| 4 | 81-A | 187 | Total 187 | O 187 | 0 | 0 |
| 4 | 82-A | 175 | Total 175 | O 175 | 0 | 0 |
| 4 | 83-A | 175 | Total 175 | O 175 | 0 | 0 |
| 4 | 84-A | 172 | Total 172 | O 172 | 0 | 0 |
| 4 | 85-A | 186 | Total 186 | O 186 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4 | 86-A | 199 | Total 199 | O 199 | 0 | 0 |
| 4 | 87-A | 200 | Total 200 | O 200 | 0 | 0 |
| 4 | 88-A | 191 | Total 191 | O 191 | 0 | 0 |
| 4 | 89-A | 189 | Total 189 | O 189 | 0 | 0 |
| 4 | 90-A | 180 | Total 180 | O 180 | 0 | 0 |
| 4 | 91-A | 190 | Total 190 | O 190 | 0 | 0 |
| 4 | 92-A | 181 | Total 181 | O 181 | 0 | 0 |
| 4 | 93-A | 177 | Total 177 | O 177 | 0 | 0 |
| 4 | 94-A | 189 | Total 189 | O 189 | 0 | 0 |
| 4 | 95-A | 173 | Total 173 | O 173 | 0 | 0 |
| 4 | 96-A | 182 | Total 182 | O 182 | 0 | 0 |
| 4 | 97-A | 188 | Total 188 | O 188 | 0 | 0 |
| 4 | 98-A | 191 | Total 191 | O 191 | 0 | 0 |
| 4 | 99-A | 198 | Total 198 | O 198 | 0 | 0 |
| 4 | 100-A | 200 | Total 200 | O 200 | 0 | 0 |
| 4 | 101-A | 204 | Total 204 | O 204 | 0 | 0 |
| 4 | 102-A | 189 | Total 189 | O 189 | 0 | 0 |
| 4 | 103-A | 211 | Total 211 | O 211 | 0 | 0 |
| 4 | 104-A | 202 | Total 202 | O 202 | 0 | 0 |
| 4 | 105-A | 196 | Total 196 | O 196 | 0 | 0 |
| 4 | 106-A | 189 | Total 189 | O 189 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4 | 107-A | 179 | Total 179 | O 179 | 0 | 0 |
| 4 | 108-A | 185 | Total 185 | O 185 | 0 | 0 |
| 4 | 109-A | 186 | Total 186 | O 186 | 0 | 0 |
| 4 | 110-A | 186 | Total 186 | O 186 | 0 | 0 |
| 4 | 111-A | 181 | Total 181 | O 181 | 0 | 0 |
| 4 | 112-A | 175 | Total 175 | O 175 | 0 | 0 |
| 4 | 113-A | 183 | Total 183 | O 183 | 0 | 0 |
| 4 | 114-A | 189 | Total 189 | O 189 | 0 | 0 |
| 4 | 115-A | 183 | Total 183 | O 183 | 0 | 0 |
| 4 | 116-A | 194 | Total 194 | O 194 | 0 | 0 |
| 4 | 117-A | 190 | Total 190 | O 190 | 0 | 0 |
| 4 | 118-A | 194 | Total 194 | O 194 | 0 | 0 |
| 4 | 119-A | 194 | Total 194 | O 194 | 0 | 0 |
| 4 | 120-A | 204 | Total 204 | O 204 | 0 | 0 |
| 4 | 121-A | 191 | Total 191 | O 191 | 0 | 0 |
| 4 | 122-A | 192 | Total 192 | O 192 | 0 | 0 |
| 4 | 123-A | 195 | Total 195 | O 195 | 0 | 0 |
| 4 | 124-A | 186 | Total 186 | O 186 | 0 | 0 |
| 4 | 125-A | 185 | Total 185 | O 185 | 0 | 0 |
| 4 | 126-A | 178 | Total 178 | O 178 | 0 | 0 |
| 4 | 127-A | 185 | Total 185 | O 185 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4 | 128-A | 175 | Total 175 | O 175 | 0 | 0 |
| 4 | 129-A | 180 | Total 180 | O 180 | 0 | 0 |
| 4 | 130-A | 186 | Total 186 | O 186 | 0 | 0 |
| 4 | 131-A | 201 | Total 201 | O 201 | 0 | 0 |
| 4 | 132-A | 205 | Total 205 | O 205 | 0 | 0 |
| 4 | 133-A | 205 | Total 205 | O 205 | 0 | 0 |
| 4 | 134-A | 209 | Total 209 | O 209 | 0 | 0 |
| 4 | 135-A | 195 | Total 195 | O 195 | 0 | 0 |
| 4 | 136-A | 205 | Total 205 | O 205 | 0 | 0 |
| 4 | 137-A | 190 | Total 190 | O 190 | 0 | 0 |
| 4 | 138-A | 174 | Total 174 | O 174 | 0 | 0 |
| 4 | 139-A | 186 | Total 186 | O 186 | 0 | 0 |
| 4 | 140-A | 186 | Total 186 | O 186 | 0 | 0 |
| 4 | 141-A | 196 | Total 196 | O 196 | 0 | 0 |
| 4 | 142-A | 203 | Total 203 | O 203 | 0 | 0 |
| 4 | 143-A | 192 | Total 192 | O 192 | 0 | 0 |
| 4 | 144-A | 187 | Total 187 | O 187 | 0 | 0 |
| 4 | 145-A | 176 | Total 176 | O 176 | 0 | 0 |
| 4 | 146-A | 176 | Total 176 | O 176 | 0 | 0 |
| 4 | 147-A | 162 | Total 162 | O 162 | 0 | 0 |
| 4 | 148-A | 163 | Total 163 | O 163 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4 | 149-A | 178 | Total 178 | O 178 | 0 | 0 |
| 4 | 150-A | 190 | Total 190 | O 190 | 0 | 0 |
| 4 | 151-A | 204 | Total 204 | O 204 | 0 | 0 |
| 4 | 152-A | 187 | Total 187 | O 187 | 0 | 0 |
| 4 | 153-A | 191 | Total 191 | O 191 | 0 | 0 |
| 4 | 154-A | 190 | Total 190 | O 190 | 0 | 0 |
| 4 | 155-A | 187 | Total 187 | O 187 | 0 | 0 |
| 4 | 156-A | 190 | Total 190 | O 190 | 0 | 0 |
| 4 | 157-A | 193 | Total 193 | O 193 | 0 | 0 |
| 4 | 158-A | 181 | Total 181 | O 181 | 0 | 0 |
| 4 | 159-A | 176 | Total 176 | O 176 | 0 | 0 |
| 4 | 160-A | 185 | Total 185 | O 185 | 0 | 0 |
| 4 | 161-A | 187 | Total 187 | O 187 | 0 | 0 |
| 4 | 162-A | 196 | Total 196 | O 196 | 0 | 0 |
| 4 | 163-A | 204 | Total 204 | O 204 | 0 | 0 |
| 4 | 164-A | 198 | Total 198 | O 198 | 0 | 0 |
| 4 | 165-A | 215 | Total 215 | O 215 | 0 | 0 |
| 4 | 166-A | 194 | Total 194 | O 194 | 0 | 0 |
| 4 | 167-A | 175 | Total 175 | O 175 | 0 | 0 |
| 4 | 168-A | 176 | Total 176 | O 176 | 0 | 0 |
| 4 | 169-A | 184 | Total 184 | O 184 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4 | 170-A | 190 | Total 190 | O 190 | 0 | 0 |
| 4 | 171-A | 187 | Total 187 | O 187 | 0 | 0 |
| 4 | 172-A | 187 | Total 187 | O 187 | 0 | 0 |
| 4 | 173-A | 191 | Total 191 | O 191 | 0 | 0 |
| 4 | 174-A | 199 | Total 199 | O 199 | 0 | 0 |
| 4 | 175-A | 196 | Total 196 | O 196 | 0 | 0 |
| 4 | 176-A | 194 | Total 194 | O 194 | 0 | 0 |
| 4 | 177-A | 203 | Total 203 | O 203 | 0 | 0 |
| 4 | 178-A | 188 | Total 188 | O 188 | 0 | 0 |
| 4 | 179-A | 175 | Total 175 | O 175 | 0 | 0 |
| 4 | 180-A | 169 | Total 169 | O 169 | 0 | 0 |
| 4 | 181-A | 192 | Total 192 | O 192 | 0 | 0 |
| 4 | 182-A | 187 | Total 187 | O 187 | 0 | 0 |
| 4 | 183-A | 185 | Total 185 | O 185 | 0 | 0 |
| 4 | 184-A | 179 | Total 179 | O 179 | 0 | 0 |
| 4 | 185-A | 197 | Total 197 | O 197 | 0 | 0 |
| 4 | 186-A | 187 | Total 187 | O 187 | 0 | 0 |
| 4 | 187-A | 191 | Total 191 | O 191 | 0 | 0 |
| 4 | 188-A | 203 | Total 203 | O 203 | 0 | 0 |
| 4 | 189-A | 209 | Total 209 | O 209 | 0 | 0 |
| 4 | 190-A | 197 | Total 197 | O 197 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4 | 191-A | 179 | Total 179 | O 179 | 0 | 0 |
| 4 | 192-A | 185 | Total 185 | O 185 | 0 | 0 |
| 4 | 193-A | 183 | Total 183 | O 183 | 0 | 0 |
| 4 | 194-A | 182 | Total 182 | O 182 | 0 | 0 |
| 4 | 195-A | 173 | Total 173 | O 173 | 0 | 0 |
| 4 | 196-A | 184 | Total 184 | O 184 | 0 | 0 |
| 4 | 197-A | 181 | Total 181 | O 181 | 0 | 0 |
| 4 | 198-A | 181 | Total 181 | O 181 | 0 | 0 |
| 4 | 199-A | 184 | Total 184 | O 184 | 0 | 0 |
| 4 | 200-A | 192 | Total 192 | O 192 | 0 | 0 |
| 4 | 201-A | 207 | Total 207 | O 207 | 0 | 0 |
| 4 | 202-A | 194 | Total 194 | O 194 | 0 | 0 |
| 4 | 203-A | 184 | Total 184 | O 184 | 0 | 0 |
| 4 | 204-A | 182 | Total 182 | O 182 | 0 | 0 |
| 4 | 205-A | 193 | Total 193 | O 193 | 0 | 0 |
| 4 | 206-A | 190 | Total 190 | O 190 | 0 | 0 |
| 4 | 207-A | 180 | Total 180 | O 180 | 0 | 0 |
| 4 | 208-A | 178 | Total 178 | O 178 | 0 | 0 |
| 4 | 209-A | 185 | Total 185 | O 185 | 0 | 0 |
| 4 | 210-A | 184 | Total 184 | O 184 | 0 | 0 |
| 4 | 211-A | 184 | Total 184 | O 184 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4 | 212-A | 191 | Total O 191 191 | 0 | 0 |
| 4 | 213-A | 202 | Total O 202 202 | 0 | 0 |
| 4 | 214-A | 190 | Total O 190 190 | 0 | 0 |
| 4 | 215-A | 193 | Total O 193 193 | 0 | 0 |
| 4 | 216-A | 195 | Total O 195 195 | 0 | 0 |
| 4 | 217-A | 197 | Total O 197 197 | 0 | 0 |
| 4 | 218-A | 197 | Total O 197 197 | 0 | 0 |
| 4 | 219-A | 192 | Total O 192 192 | 0 | 0 |
| 4 | 220-A | 177 | Total O 177 177 | 0 | 0 |
| 4 | 221-A | 183 | Total O 183 183 | 0 | 0 |
| 4 | 222-A | 182 | Total O 182 182 | 0 | 0 |
| 4 | 223-A | 181 | Total O 181 181 | 0 | 0 |
| 4 | 224-A | 203 | Total O 203 203 | 0 | 0 |
| 4 | 225-A | 205 | Total O 205 205 | 0 | 0 |
| 4 | 226-A | 202 | Total O 202 202 | 0 | 0 |
| 4 | 227-A | 189 | Total O 189 189 | 0 | 0 |
| 4 | 228-A | 162 | Total O 162 162 | 0 | 0 |
| 4 | 229-A | 180 | Total O 180 180 | 0 | 0 |
| 4 | 230-A | 174 | Total O 174 174 | 0 | 0 |
| 4 | 231-A | 206 | Total O 206 206 | 0 | 0 |
| 4 | 232-A | 211 | Total O 211 211 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 4 | 233-A | 195 | Total 195 | O 195 | 0 | 0 |
| 4 | 234-A | 184 | Total 184 | O 184 | 0 | 0 |
| 4 | 235-A | 167 | Total 167 | O 167 | 0 | 0 |
| 4 | 236-A | 172 | Total 172 | O 172 | 0 | 0 |
| 4 | 237-A | 184 | Total 184 | O 184 | 0 | 0 |
| 4 | 238-A | 198 | Total 198 | O 198 | 0 | 0 |
| 4 | 239-A | 194 | Total 194 | O 194 | 0 | 0 |
| 4 | 240-A | 206 | Total 206 | O 206 | 0 | 0 |
| 4 | 241-A | 208 | Total 208 | O 208 | 0 | 0 |
| 4 | 242-A | 179 | Total 179 | O 179 | 0 | 0 |
| 4 | 243-A | 184 | Total 184 | O 184 | 0 | 0 |
| 4 | 244-A | 181 | Total 181 | O 181 | 0 | 0 |
| 4 | 245-A | 178 | Total 178 | O 178 | 0 | 0 |
| 4 | 246-A | 197 | Total 197 | O 197 | 0 | 0 |
| 4 | 247-A | 186 | Total 186 | O 186 | 0 | 0 |
| 4 | 248-A | 182 | Total 182 | O 182 | 0 | 0 |
| 4 | 249-A | 195 | Total 195 | O 195 | 0 | 0 |
| 4 | 250-A | 202 | Total 202 | O 202 | 0 | 0 |

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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:  92% 5% . .




- Molecule 1: Dihydrofolate reductase

Chain 2-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 3-A:  89% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 4-A:  92% 6% .



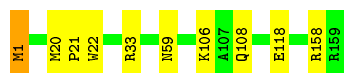
- Molecule 1: Dihydrofolate reductase

Chain 5-A:  93% . .



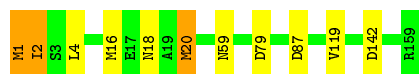
- Molecule 1: Dihydrofolate reductase

Chain 6-A:  94% 6% •



- Molecule 1: Dihydrofolate reductase

Chain 7-A:  93% 5% •



- Molecule 1: Dihydrofolate reductase

Chain 8-A:  91% 8% •



- Molecule 1: Dihydrofolate reductase

Chain 9-A:  91% 7% •



- Molecule 1: Dihydrofolate reductase

Chain 10-A:  92% 6% •



- Molecule 1: Dihydrofolate reductase

Chain 11-A:  93% 6% •




- Molecule 1: Dihydrofolate reductase

Chain 12-A:  91% 9% •



- Molecule 1: Dihydrofolate reductase

Chain 13-A:  89% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 14-A:  92% 6% .



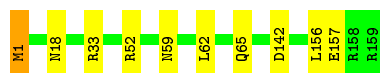
- Molecule 1: Dihydrofolate reductase

Chain 15-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 16-A:  94% 6% .



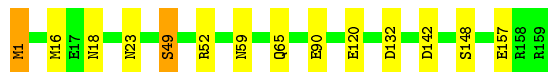
- Molecule 1: Dihydrofolate reductase

Chain 17-A:  92% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 18-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 19-A:  89% 9% .



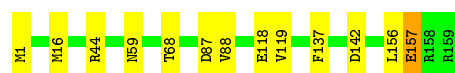
- Molecule 1: Dihydrofolate reductase

Chain 20-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 21-A:  92% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 22-A:  93% 5% .



- Molecule 1: Dihydrofolate reductase

Chain 23-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 24-A:  89% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 25-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 26-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 27-A:  94% 6%



- Molecule 1: Dihydrofolate reductase

Chain 28-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 29-A:  94% 6% .



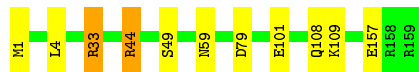
- Molecule 1: Dihydrofolate reductase

Chain 30-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 31-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 32-A:  96% . .



- Molecule 1: Dihydrofolate reductase

Chain 33-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 34-A:  91% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 35-A:  89% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 36-A:  91% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 37-A:  93% 7%



- Molecule 1: Dihydrofolate reductase

Chain 38-A:  91% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 39-A:  92% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 40-A:  91% 6% .



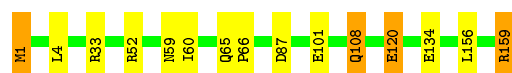
- Molecule 1: Dihydrofolate reductase

Chain 41-A:  89% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 42-A:  91% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 43-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 44-A:  92% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 45-A:  94% 6% .



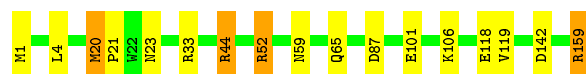
- Molecule 1: Dihydrofolate reductase

Chain 46-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 47-A:  89% 8% .



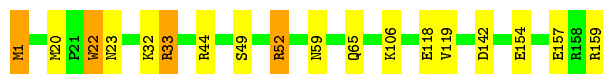
- Molecule 1: Dihydrofolate reductase

Chain 48-A:  90% 8% .



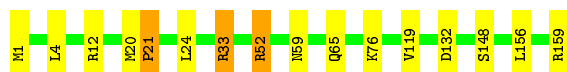
- Molecule 1: Dihydrofolate reductase

Chain 49-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 50-A:  90% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 51-A:  89% 9% .



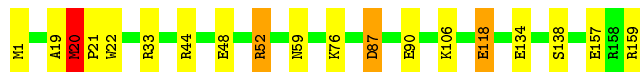
- Molecule 1: Dihydrofolate reductase

Chain 52-A:  88% 10% .



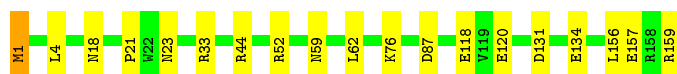
- Molecule 1: Dihydrofolate reductase

Chain 53-A:  88% 9% ..



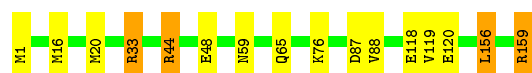
- Molecule 1: Dihydrofolate reductase

Chain 54-A:  88% 11% .



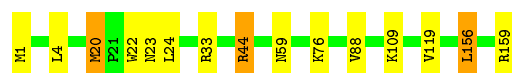
- Molecule 1: Dihydrofolate reductase

Chain 55-A:  90% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 56-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 57-A:  87% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 58-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 59-A:  89% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 60-A:  90% 8% .




- Molecule 1: Dihydrofolate reductase

Chain 61-A:  91% 8% .



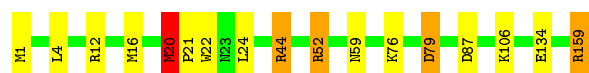
- Molecule 1: Dihydrofolate reductase

Chain 62-A:  87% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 63-A:  89% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 64-A:  89% 9% ..




- Molecule 1: Dihydrofolate reductase

Chain 65-A:  91% 7% ..



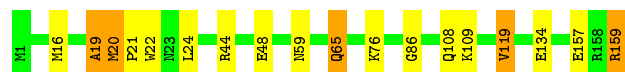
- Molecule 1: Dihydrofolate reductase

Chain 66-A:  86% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 67-A:  89% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 68-A:  91% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 69-A:  89% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 70-A:  87% 9% .



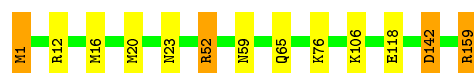
- Molecule 1: Dihydrofolate reductase

Chain 71-A:  89% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 72-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 73-A:  91% 7% .



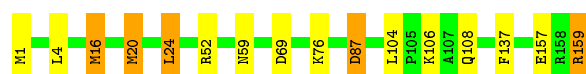
- Molecule 1: Dihydrofolate reductase

Chain 74-A:  89% 11% .




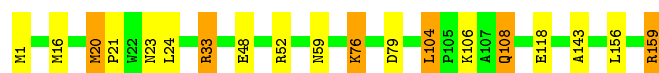
- Molecule 1: Dihydrofolate reductase

Chain 75-A:  90% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 76-A:  88% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 77-A:  91% 6% .



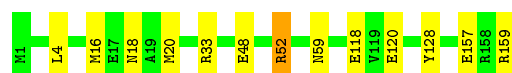
- Molecule 1: Dihydrofolate reductase

Chain 78-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 79-A:  92% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 80-A:  93% 6% .



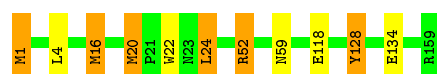
- Molecule 1: Dihydrofolate reductase

Chain 81-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 82-A:  93% . .



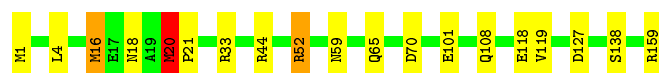
- Molecule 1: Dihydrofolate reductase

Chain 83-A:  88% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 84-A:  88% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 85-A:  88% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 86-A:  91% 8% .



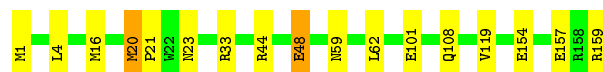
- Molecule 1: Dihydrofolate reductase

Chain 87-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 88-A:  89% 9% .




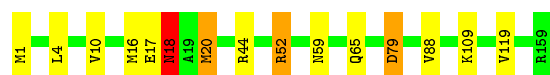
- Molecule 1: Dihydrofolate reductase

Chain 89-A:  94% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 90-A:  91% 7% ..



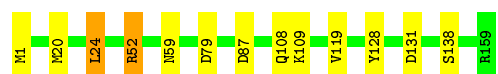
- Molecule 1: Dihydrofolate reductase

Chain 91-A:  91% 8% .



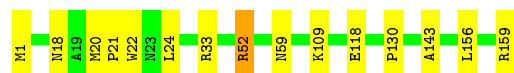
- Molecule 1: Dihydrofolate reductase

Chain 92-A:  92% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 93-A:  91% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 94-A:  90% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 95-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 96-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 97-A:  88% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 98-A:  91% 9%



- Molecule 1: Dihydrofolate reductase

Chain 99-A:  91% 8% .



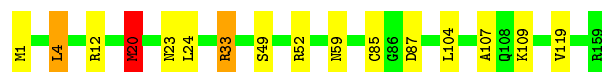
- Molecule 1: Dihydrofolate reductase

Chain 100-A:  92% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 101-A:  90% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 102-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 103-A:  87% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 104-A:  89% 9% •



- Molecule 1: Dihydrofolate reductase

Chain 105-A:  91% 9%



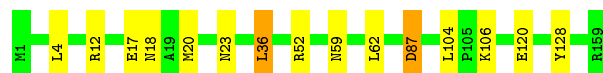
- Molecule 1: Dihydrofolate reductase

Chain 106-A:  92% 6% •



- Molecule 1: Dihydrofolate reductase

Chain 107-A:  91% 8% •



- Molecule 1: Dihydrofolate reductase

Chain 108-A:  91% 8% •



- Molecule 1: Dihydrofolate reductase

Chain 109-A:  89% 9% ••



- Molecule 1: Dihydrofolate reductase

Chain 110-A:  88% 10% •



- Molecule 1: Dihydrofolate reductase

Chain 111-A:  88% 11% .



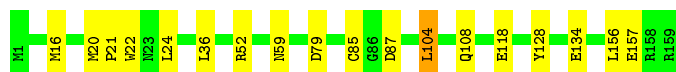
- Molecule 1: Dihydrofolate reductase

Chain 112-A:  90% 9% .



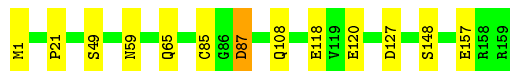
- Molecule 1: Dihydrofolate reductase

Chain 113-A:  89% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 114-A:  92% 8% .



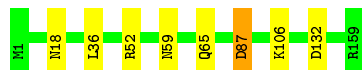
- Molecule 1: Dihydrofolate reductase

Chain 115-A:  92% 5% ..



- Molecule 1: Dihydrofolate reductase

Chain 116-A:  95% ..



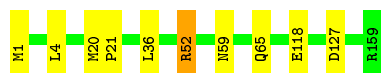
- Molecule 1: Dihydrofolate reductase

Chain 117-A:  93% 7% .



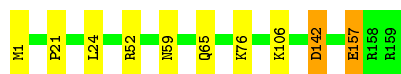
- Molecule 1: Dihydrofolate reductase

Chain 118-A:  94% 6% •



- Molecule 1: Dihydrofolate reductase

Chain 119-A:  94% 5% •



- Molecule 1: Dihydrofolate reductase

Chain 120-A:  91% 7% •



- Molecule 1: Dihydrofolate reductase

Chain 121-A:  88% 9% ••



- Molecule 1: Dihydrofolate reductase

Chain 122-A:  92% 6% ••



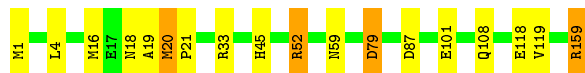
- Molecule 1: Dihydrofolate reductase

Chain 123-A:  91% 7% •



- Molecule 1: Dihydrofolate reductase

Chain 124-A:  89% 9% •



- Molecule 1: Dihydrofolate reductase

Chain 125-A:  92% 7% ..



- Molecule 1: Dihydrofolate reductase

Chain 126-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 127-A:  91% 6% ..



- Molecule 1: Dihydrofolate reductase

Chain 128-A:  92% 5% ..



- Molecule 1: Dihydrofolate reductase

Chain 129-A:  88% 12%



- Molecule 1: Dihydrofolate reductase

Chain 130-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 131-A:  89% 8% ..



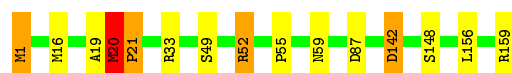
- Molecule 1: Dihydrofolate reductase

Chain 132-A:  87% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 133-A:  91% 6% ..



- Molecule 1: Dihydrofolate reductase

Chain 134-A:  93% 5% ..



- Molecule 1: Dihydrofolate reductase

Chain 135-A:  92% 6% .



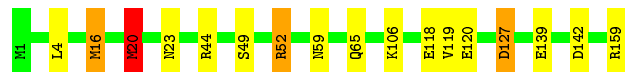
- Molecule 1: Dihydrofolate reductase

Chain 136-A:  89% 10% ..



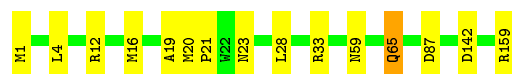
- Molecule 1: Dihydrofolate reductase

Chain 137-A:  89% 8% ..



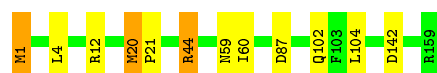
- Molecule 1: Dihydrofolate reductase

Chain 138-A:  91% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 139-A:  92% 6% .



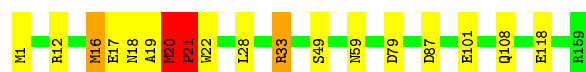
- Molecule 1: Dihydrofolate reductase

Chain 140-A:  87% 10% ..



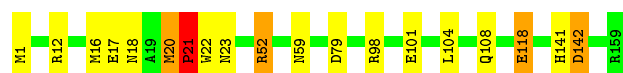
- Molecule 1: Dihydrofolate reductase

Chain 141-A:  89% 9% ..



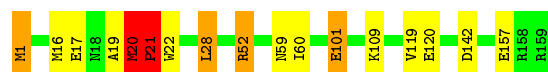
- Molecule 1: Dihydrofolate reductase

Chain 142-A:  88% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 143-A:  89% 7% ..



- Molecule 1: Dihydrofolate reductase

Chain 144-A:  89% 8% ..



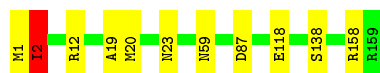
- Molecule 1: Dihydrofolate reductase

Chain 145-A:  91% 9% .



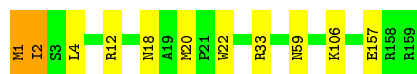
- Molecule 1: Dihydrofolate reductase

Chain 146-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 147-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 148-A:  93% 5% ..



- Molecule 1: Dihydrofolate reductase

Chain 149-A:  89% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 150-A:  90% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 151-A:  91% 6% ..



- Molecule 1: Dihydrofolate reductase

Chain 152-A:  91% 9% .



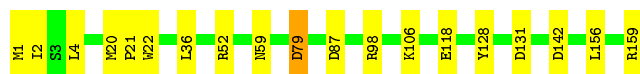
- Molecule 1: Dihydrofolate reductase

Chain 153-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 154-A:  88% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 155-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 156-A:  91% 7% .



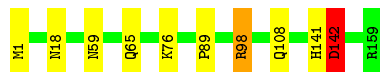
- Molecule 1: Dihydrofolate reductase

Chain 157-A:  90% 9% .



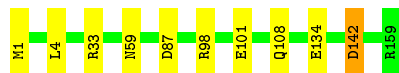
- Molecule 1: Dihydrofolate reductase

Chain 158-A:  94% 5% ..



- Molecule 1: Dihydrofolate reductase

Chain 159-A:  94% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 160-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 161-A:  94% 5% .



- Molecule 1: Dihydrofolate reductase

Chain 162-A:  91% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 163-A:  89% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 164-A:  91% 8% .



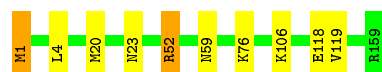
- Molecule 1: Dihydrofolate reductase

Chain 165-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 166-A:  94% 5% .



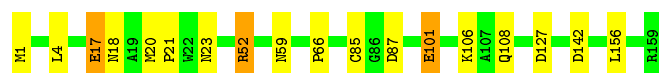
- Molecule 1: Dihydrofolate reductase

Chain 167-A:  94% 5% .



- Molecule 1: Dihydrofolate reductase

Chain 168-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 169-A:  96% . .



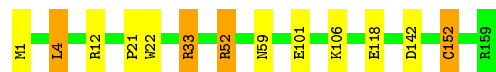
- Molecule 1: Dihydrofolate reductase

Chain 170-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 171-A:  92% 6% .



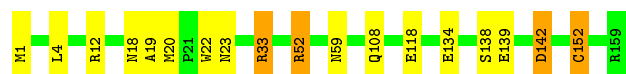
- Molecule 1: Dihydrofolate reductase

Chain 172-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 173-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 174-A:  90% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 175-A:  90% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 176-A:  92% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 177-A:  94% . .



- Molecule 1: Dihydrofolate reductase

Chain 178-A:  91% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 179-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 180-A:  91% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 181-A:  90% 8% .



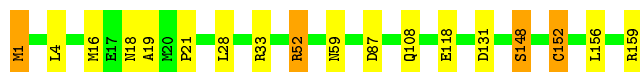
- Molecule 1: Dihydrofolate reductase

Chain 182-A:  91% 8% .



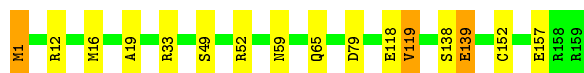
- Molecule 1: Dihydrofolate reductase

Chain 183-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 184-A:  90% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 185-A:  89% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 186-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 187-A:  89% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 188-A:  89% 10% .



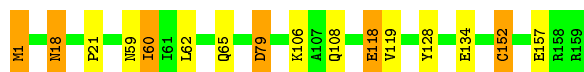
- Molecule 1: Dihydrofolate reductase

Chain 189-A:  92% 7% .



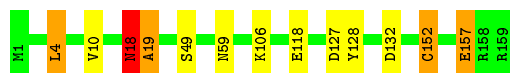
- Molecule 1: Dihydrofolate reductase

Chain 190-A:  90% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 191-A:  92% 5% . .



- Molecule 1: Dihydrofolate reductase

Chain 192-A:  94% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 193-A:  89% 10% .




- Molecule 1: Dihydrofolate reductase

Chain 194-A:  90% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 195-A:  91% 8% ..



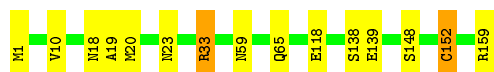
- Molecule 1: Dihydrofolate reductase

Chain 196-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 197-A:  91% 8% .



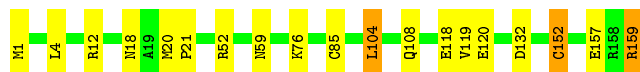
- Molecule 1: Dihydrofolate reductase

Chain 198-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 199-A:  88% 10% .



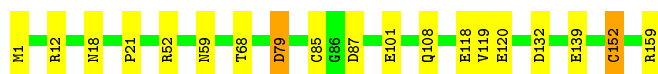
- Molecule 1: Dihydrofolate reductase

Chain 200-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 201-A:  88% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 202-A:  94% 5%



- Molecule 1: Dihydrofolate reductase

Chain 203-A:  91% 8%



- Molecule 1: Dihydrofolate reductase

Chain 204-A:  93% 6%



- Molecule 1: Dihydrofolate reductase

Chain 205-A:  89% 9%



- Molecule 1: Dihydrofolate reductase

Chain 206-A:  91% 6%



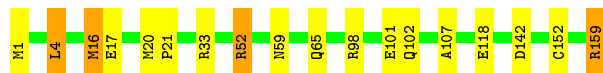
- Molecule 1: Dihydrofolate reductase

Chain 207-A:  92% 8%



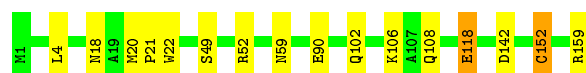
- Molecule 1: Dihydrofolate reductase

Chain 208-A:  89% 9%



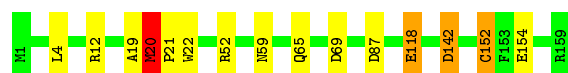
- Molecule 1: Dihydrofolate reductase

Chain 209-A:  90% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 210-A:  91% 7% ..



- Molecule 1: Dihydrofolate reductase

Chain 211-A:  92% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 212-A:  89% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 213-A:  88% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 214-A:  90% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 215-A:  87% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 216-A:  87% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 217-A:  87% 11% .



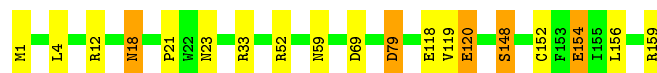
- Molecule 1: Dihydrofolate reductase

Chain 218-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 219-A:  88% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 220-A:  89% 9% .



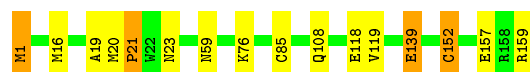
- Molecule 1: Dihydrofolate reductase

Chain 221-A:  88% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 222-A:  90% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 223-A:  91% 6% ..



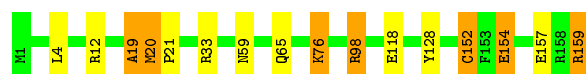
- Molecule 1: Dihydrofolate reductase

Chain 224-A:  88% 9% ..



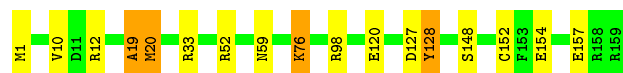
- Molecule 1: Dihydrofolate reductase

Chain 225-A:  90% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 226-A:  89% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 227-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 228-A:  94% ..



- Molecule 1: Dihydrofolate reductase

Chain 229-A:  91% 6% .



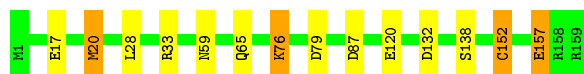
- Molecule 1: Dihydrofolate reductase

Chain 230-A:  92% 6% •



- Molecule 1: Dihydrofolate reductase

Chain 231-A:  91% 6% •



- Molecule 1: Dihydrofolate reductase

Chain 232-A:  90% 8% •



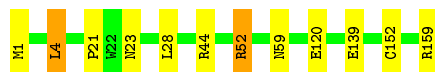
- Molecule 1: Dihydrofolate reductase

Chain 233-A:  92% 6% •



- Molecule 1: Dihydrofolate reductase

Chain 234-A:  92% 6% •



- Molecule 1: Dihydrofolate reductase

Chain 235-A:  96% •



- Molecule 1: Dihydrofolate reductase

Chain 236-A:  92% 6% •



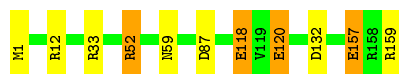
- Molecule 1: Dihydrofolate reductase

Chain 237-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 238-A:  93% . .



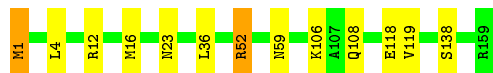
- Molecule 1: Dihydrofolate reductase

Chain 239-A:  94% 5% .



- Molecule 1: Dihydrofolate reductase

Chain 240-A:  92% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 241-A:  95% 5%



- Molecule 1: Dihydrofolate reductase

Chain 242-A:  91% 8% .



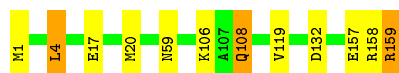
- Molecule 1: Dihydrofolate reductase

Chain 243-A:  92% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 244-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 245-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 246-A:  92% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 247-A:  92% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 248-A:  94% 5% .



- Molecule 1: Dihydrofolate reductase

Chain 249-A:  91% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 250-A:  92% 7% .



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 34.04Å 44.82Å 98.20Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 40.77 – 1.15 | Depositor |
| % Data completeness (in resolution range) | 94.4 (40.77-1.15) | Depositor |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 4.99 (at 1.15Å) | Xtriage |
| Refinement program | PHENIX (phenix.ensemble_refinement: 1.8.4_1496) | Depositor |
| R, R_{free} | 0.109 , 0.136 | Depositor |
| Wilson B-factor (Å ²) | 6.9 | Xtriage |
| Anisotropy | 0.279 | Xtriage |
| L-test for twinning ² | $\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 699653 | wwPDB-VP |
| Average B, all atoms (Å ²) | 5.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.90% 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, 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 | 0.82 | 3/1302 (0.2%) | 1.13 | 7/1770 (0.4%) |
| 1 | 2-A | 0.78 | 1/1302 (0.1%) | 1.00 | 6/1770 (0.3%) |
| 1 | 3-A | 0.80 | 2/1302 (0.2%) | 0.95 | 6/1770 (0.3%) |
| 1 | 4-A | 0.71 | 1/1302 (0.1%) | 0.96 | 3/1770 (0.2%) |
| 1 | 5-A | 0.77 | 1/1302 (0.1%) | 0.97 | 6/1770 (0.3%) |
| 1 | 6-A | 0.76 | 0/1302 | 0.95 | 5/1770 (0.3%) |
| 1 | 7-A | 0.77 | 2/1302 (0.2%) | 0.92 | 3/1770 (0.2%) |
| 1 | 8-A | 0.83 | 3/1302 (0.2%) | 0.97 | 8/1770 (0.5%) |
| 1 | 9-A | 0.79 | 2/1302 (0.2%) | 1.02 | 5/1770 (0.3%) |
| 1 | 10-A | 0.88 | 6/1302 (0.5%) | 0.93 | 3/1770 (0.2%) |
| 1 | 11-A | 0.75 | 2/1302 (0.2%) | 0.95 | 5/1770 (0.3%) |
| 1 | 12-A | 0.78 | 2/1302 (0.2%) | 0.98 | 4/1770 (0.2%) |
| 1 | 13-A | 0.91 | 4/1302 (0.3%) | 1.01 | 8/1770 (0.5%) |
| 1 | 14-A | 0.76 | 1/1302 (0.1%) | 0.99 | 5/1770 (0.3%) |
| 1 | 15-A | 0.77 | 2/1302 (0.2%) | 0.91 | 1/1770 (0.1%) |
| 1 | 16-A | 0.66 | 0/1302 | 0.91 | 1/1770 (0.1%) |
| 1 | 17-A | 0.70 | 0/1302 | 0.88 | 0/1770 |
| 1 | 18-A | 0.72 | 2/1302 (0.2%) | 0.95 | 3/1770 (0.2%) |
| 1 | 19-A | 0.71 | 2/1302 (0.2%) | 0.94 | 3/1770 (0.2%) |
| 1 | 20-A | 0.75 | 2/1302 (0.2%) | 0.97 | 4/1770 (0.2%) |
| 1 | 21-A | 0.77 | 1/1302 (0.1%) | 0.89 | 2/1770 (0.1%) |
| 1 | 22-A | 0.76 | 1/1302 (0.1%) | 1.03 | 6/1770 (0.3%) |
| 1 | 23-A | 0.74 | 1/1302 (0.1%) | 1.00 | 6/1770 (0.3%) |
| 1 | 24-A | 0.88 | 5/1302 (0.4%) | 1.27 | 10/1770 (0.6%) |
| 1 | 25-A | 0.78 | 2/1302 (0.2%) | 0.96 | 4/1770 (0.2%) |
| 1 | 26-A | 0.81 | 3/1302 (0.2%) | 1.04 | 7/1770 (0.4%) |
| 1 | 27-A | 0.73 | 0/1302 | 0.88 | 2/1770 (0.1%) |
| 1 | 28-A | 0.73 | 1/1302 (0.1%) | 0.97 | 7/1770 (0.4%) |
| 1 | 29-A | 0.78 | 3/1302 (0.2%) | 0.91 | 2/1770 (0.1%) |
| 1 | 30-A | 0.71 | 1/1302 (0.1%) | 0.92 | 4/1770 (0.2%) |
| 1 | 31-A | 0.89 | 5/1302 (0.4%) | 0.97 | 4/1770 (0.2%) |
| 1 | 32-A | 0.70 | 1/1302 (0.1%) | 0.89 | 1/1770 (0.1%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 33-A | 0.70 | 0/1302 | 0.94 | 4/1770 (0.2%) |
| 1 | 34-A | 0.84 | 3/1302 (0.2%) | 0.99 | 3/1770 (0.2%) |
| 1 | 35-A | 0.77 | 2/1302 (0.2%) | 1.00 | 5/1770 (0.3%) |
| 1 | 36-A | 0.79 | 2/1302 (0.2%) | 1.02 | 9/1770 (0.5%) |
| 1 | 37-A | 0.77 | 2/1302 (0.2%) | 0.87 | 0/1770 |
| 1 | 38-A | 0.83 | 3/1302 (0.2%) | 0.96 | 5/1770 (0.3%) |
| 1 | 39-A | 0.81 | 5/1302 (0.4%) | 0.95 | 3/1770 (0.2%) |
| 1 | 40-A | 0.93 | 9/1302 (0.7%) | 0.99 | 5/1770 (0.3%) |
| 1 | 41-A | 0.95 | 4/1302 (0.3%) | 0.98 | 4/1770 (0.2%) |
| 1 | 42-A | 0.88 | 5/1302 (0.4%) | 0.95 | 5/1770 (0.3%) |
| 1 | 43-A | 0.78 | 3/1302 (0.2%) | 0.91 | 3/1770 (0.2%) |
| 1 | 44-A | 0.84 | 5/1302 (0.4%) | 0.91 | 2/1770 (0.1%) |
| 1 | 45-A | 0.70 | 1/1302 (0.1%) | 1.03 | 4/1770 (0.2%) |
| 1 | 46-A | 0.78 | 2/1302 (0.2%) | 1.18 | 10/1770 (0.6%) |
| 1 | 47-A | 0.75 | 1/1302 (0.1%) | 1.00 | 7/1770 (0.4%) |
| 1 | 48-A | 0.73 | 0/1302 | 0.95 | 3/1770 (0.2%) |
| 1 | 49-A | 0.83 | 3/1302 (0.2%) | 1.04 | 5/1770 (0.3%) |
| 1 | 50-A | 0.76 | 0/1302 | 0.93 | 5/1770 (0.3%) |
| 1 | 51-A | 0.88 | 5/1302 (0.4%) | 1.01 | 4/1770 (0.2%) |
| 1 | 52-A | 0.76 | 1/1302 (0.1%) | 1.00 | 6/1770 (0.3%) |
| 1 | 53-A | 0.81 | 1/1302 (0.1%) | 0.98 | 5/1770 (0.3%) |
| 1 | 54-A | 0.75 | 0/1302 | 0.90 | 2/1770 (0.1%) |
| 1 | 55-A | 0.75 | 0/1302 | 0.96 | 4/1770 (0.2%) |
| 1 | 56-A | 0.76 | 2/1302 (0.2%) | 1.06 | 7/1770 (0.4%) |
| 1 | 57-A | 0.90 | 6/1302 (0.5%) | 1.08 | 5/1770 (0.3%) |
| 1 | 58-A | 0.78 | 1/1302 (0.1%) | 1.00 | 6/1770 (0.3%) |
| 1 | 59-A | 0.84 | 5/1302 (0.4%) | 1.00 | 9/1770 (0.5%) |
| 1 | 60-A | 0.84 | 6/1302 (0.5%) | 0.98 | 5/1770 (0.3%) |
| 1 | 61-A | 0.75 | 3/1302 (0.2%) | 0.99 | 7/1770 (0.4%) |
| 1 | 62-A | 0.74 | 1/1302 (0.1%) | 0.99 | 9/1770 (0.5%) |
| 1 | 63-A | 0.85 | 1/1302 (0.1%) | 1.03 | 10/1770 (0.6%) |
| 1 | 64-A | 0.89 | 5/1302 (0.4%) | 1.01 | 6/1770 (0.3%) |
| 1 | 65-A | 0.75 | 1/1302 (0.1%) | 1.00 | 6/1770 (0.3%) |
| 1 | 66-A | 0.92 | 5/1302 (0.4%) | 1.12 | 10/1770 (0.6%) |
| 1 | 67-A | 0.83 | 3/1302 (0.2%) | 1.06 | 8/1770 (0.5%) |
| 1 | 68-A | 0.78 | 0/1302 | 1.06 | 8/1770 (0.5%) |
| 1 | 69-A | 0.87 | 2/1302 (0.2%) | 1.21 | 9/1770 (0.5%) |
| 1 | 70-A | 0.89 | 4/1302 (0.3%) | 1.05 | 6/1770 (0.3%) |
| 1 | 71-A | 0.80 | 1/1302 (0.1%) | 1.06 | 7/1770 (0.4%) |
| 1 | 72-A | 0.74 | 1/1302 (0.1%) | 0.99 | 7/1770 (0.4%) |
| 1 | 73-A | 0.77 | 2/1302 (0.2%) | 0.95 | 8/1770 (0.5%) |
| 1 | 74-A | 0.74 | 2/1302 (0.2%) | 0.95 | 5/1770 (0.3%) |
| 1 | 75-A | 0.75 | 2/1302 (0.2%) | 1.04 | 8/1770 (0.5%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 76-A | 0.82 | 2/1302 (0.2%) | 1.08 | 12/1770 (0.7%) |
| 1 | 77-A | 0.77 | 2/1302 (0.2%) | 0.98 | 5/1770 (0.3%) |
| 1 | 78-A | 0.82 | 3/1302 (0.2%) | 1.08 | 12/1770 (0.7%) |
| 1 | 79-A | 0.84 | 5/1302 (0.4%) | 1.00 | 7/1770 (0.4%) |
| 1 | 80-A | 0.75 | 1/1302 (0.1%) | 0.87 | 2/1770 (0.1%) |
| 1 | 81-A | 0.76 | 1/1302 (0.1%) | 0.95 | 4/1770 (0.2%) |
| 1 | 82-A | 0.79 | 1/1302 (0.1%) | 1.02 | 6/1770 (0.3%) |
| 1 | 83-A | 0.77 | 1/1302 (0.1%) | 1.03 | 5/1770 (0.3%) |
| 1 | 84-A | 0.80 | 2/1302 (0.2%) | 1.10 | 13/1770 (0.7%) |
| 1 | 85-A | 0.82 | 3/1302 (0.2%) | 0.97 | 7/1770 (0.4%) |
| 1 | 86-A | 0.79 | 3/1302 (0.2%) | 0.97 | 5/1770 (0.3%) |
| 1 | 87-A | 0.80 | 2/1302 (0.2%) | 0.97 | 1/1770 (0.1%) |
| 1 | 88-A | 0.92 | 6/1302 (0.5%) | 1.05 | 8/1770 (0.5%) |
| 1 | 89-A | 0.76 | 1/1302 (0.1%) | 0.98 | 5/1770 (0.3%) |
| 1 | 90-A | 0.84 | 3/1302 (0.2%) | 0.96 | 8/1770 (0.5%) |
| 1 | 91-A | 0.95 | 5/1302 (0.4%) | 1.04 | 7/1770 (0.4%) |
| 1 | 92-A | 0.69 | 0/1302 | 0.91 | 4/1770 (0.2%) |
| 1 | 93-A | 0.74 | 0/1302 | 0.94 | 3/1770 (0.2%) |
| 1 | 94-A | 0.82 | 3/1302 (0.2%) | 1.02 | 8/1770 (0.5%) |
| 1 | 95-A | 0.70 | 1/1302 (0.1%) | 0.94 | 7/1770 (0.4%) |
| 1 | 96-A | 0.80 | 3/1302 (0.2%) | 0.93 | 3/1770 (0.2%) |
| 1 | 97-A | 0.81 | 6/1302 (0.5%) | 0.98 | 5/1770 (0.3%) |
| 1 | 98-A | 0.71 | 0/1302 | 0.93 | 2/1770 (0.1%) |
| 1 | 99-A | 0.77 | 3/1302 (0.2%) | 1.00 | 6/1770 (0.3%) |
| 1 | 100-A | 0.75 | 0/1302 | 0.94 | 4/1770 (0.2%) |
| 1 | 101-A | 0.83 | 2/1302 (0.2%) | 1.06 | 9/1770 (0.5%) |
| 1 | 102-A | 0.81 | 3/1302 (0.2%) | 0.97 | 6/1770 (0.3%) |
| 1 | 103-A | 0.78 | 2/1302 (0.2%) | 1.05 | 8/1770 (0.5%) |
| 1 | 104-A | 0.71 | 0/1302 | 0.94 | 3/1770 (0.2%) |
| 1 | 105-A | 0.74 | 1/1302 (0.1%) | 0.94 | 3/1770 (0.2%) |
| 1 | 106-A | 0.79 | 2/1302 (0.2%) | 1.01 | 5/1770 (0.3%) |
| 1 | 107-A | 0.76 | 2/1302 (0.2%) | 0.96 | 4/1770 (0.2%) |
| 1 | 108-A | 0.72 | 1/1302 (0.1%) | 1.05 | 4/1770 (0.2%) |
| 1 | 109-A | 0.76 | 0/1302 | 1.01 | 4/1770 (0.2%) |
| 1 | 110-A | 0.78 | 1/1302 (0.1%) | 1.08 | 9/1770 (0.5%) |
| 1 | 111-A | 0.81 | 2/1302 (0.2%) | 1.01 | 7/1770 (0.4%) |
| 1 | 112-A | 0.74 | 2/1302 (0.2%) | 0.99 | 3/1770 (0.2%) |
| 1 | 113-A | 0.73 | 1/1302 (0.1%) | 1.00 | 4/1770 (0.2%) |
| 1 | 114-A | 0.75 | 1/1302 (0.1%) | 0.93 | 2/1770 (0.1%) |
| 1 | 115-A | 0.81 | 3/1302 (0.2%) | 0.91 | 2/1770 (0.1%) |
| 1 | 116-A | 0.70 | 0/1302 | 0.90 | 2/1770 (0.1%) |
| 1 | 117-A | 0.75 | 3/1302 (0.2%) | 0.87 | 0/1770 |
| 1 | 118-A | 0.78 | 1/1302 (0.1%) | 0.97 | 3/1770 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 119-A | 0.81 | 1/1302 (0.1%) | 0.96 | 1/1770 (0.1%) |
| 1 | 120-A | 0.75 | 1/1302 (0.1%) | 0.99 | 6/1770 (0.3%) |
| 1 | 121-A | 0.75 | 2/1302 (0.2%) | 1.06 | 10/1770 (0.6%) |
| 1 | 122-A | 0.77 | 3/1302 (0.2%) | 0.99 | 6/1770 (0.3%) |
| 1 | 123-A | 0.75 | 1/1302 (0.1%) | 0.98 | 7/1770 (0.4%) |
| 1 | 124-A | 0.82 | 2/1302 (0.2%) | 1.04 | 13/1770 (0.7%) |
| 1 | 125-A | 0.84 | 6/1302 (0.5%) | 1.06 | 7/1770 (0.4%) |
| 1 | 126-A | 0.83 | 7/1302 (0.5%) | 0.93 | 2/1770 (0.1%) |
| 1 | 127-A | 0.79 | 3/1302 (0.2%) | 1.00 | 4/1770 (0.2%) |
| 1 | 128-A | 0.75 | 2/1302 (0.2%) | 0.97 | 3/1770 (0.2%) |
| 1 | 129-A | 0.81 | 2/1302 (0.2%) | 0.95 | 6/1770 (0.3%) |
| 1 | 130-A | 0.77 | 0/1302 | 1.03 | 10/1770 (0.6%) |
| 1 | 131-A | 0.79 | 1/1302 (0.1%) | 1.08 | 10/1770 (0.6%) |
| 1 | 132-A | 0.77 | 0/1302 | 1.04 | 10/1770 (0.6%) |
| 1 | 133-A | 0.74 | 1/1302 (0.1%) | 1.00 | 7/1770 (0.4%) |
| 1 | 134-A | 0.74 | 0/1302 | 1.00 | 6/1770 (0.3%) |
| 1 | 135-A | 0.74 | 0/1302 | 0.99 | 3/1770 (0.2%) |
| 1 | 136-A | 0.77 | 1/1302 (0.1%) | 1.02 | 8/1770 (0.5%) |
| 1 | 137-A | 0.74 | 0/1302 | 1.04 | 9/1770 (0.5%) |
| 1 | 138-A | 0.76 | 1/1302 (0.1%) | 1.04 | 8/1770 (0.5%) |
| 1 | 139-A | 0.71 | 1/1302 (0.1%) | 0.95 | 5/1770 (0.3%) |
| 1 | 140-A | 0.78 | 4/1302 (0.3%) | 1.02 | 10/1770 (0.6%) |
| 1 | 141-A | 0.78 | 1/1302 (0.1%) | 1.04 | 9/1770 (0.5%) |
| 1 | 142-A | 0.88 | 2/1302 (0.2%) | 1.07 | 10/1770 (0.6%) |
| 1 | 143-A | 0.93 | 9/1302 (0.7%) | 1.15 | 12/1770 (0.7%) |
| 1 | 144-A | 0.84 | 4/1302 (0.3%) | 1.03 | 8/1770 (0.5%) |
| 1 | 145-A | 0.83 | 4/1302 (0.3%) | 1.11 | 10/1770 (0.6%) |
| 1 | 146-A | 0.73 | 1/1302 (0.1%) | 0.97 | 3/1770 (0.2%) |
| 1 | 147-A | 0.75 | 0/1302 | 0.90 | 3/1770 (0.2%) |
| 1 | 148-A | 0.74 | 1/1302 (0.1%) | 0.92 | 3/1770 (0.2%) |
| 1 | 149-A | 0.85 | 1/1302 (0.1%) | 1.04 | 6/1770 (0.3%) |
| 1 | 150-A | 0.82 | 3/1302 (0.2%) | 1.08 | 7/1770 (0.4%) |
| 1 | 151-A | 0.77 | 2/1302 (0.2%) | 0.96 | 7/1770 (0.4%) |
| 1 | 152-A | 0.77 | 0/1302 | 0.95 | 4/1770 (0.2%) |
| 1 | 153-A | 0.72 | 0/1302 | 0.94 | 5/1770 (0.3%) |
| 1 | 154-A | 0.74 | 0/1302 | 1.01 | 5/1770 (0.3%) |
| 1 | 155-A | 0.82 | 4/1302 (0.3%) | 0.97 | 4/1770 (0.2%) |
| 1 | 156-A | 0.88 | 6/1302 (0.5%) | 0.98 | 7/1770 (0.4%) |
| 1 | 157-A | 0.75 | 1/1302 (0.1%) | 0.96 | 5/1770 (0.3%) |
| 1 | 158-A | 0.73 | 0/1302 | 0.92 | 3/1770 (0.2%) |
| 1 | 159-A | 0.75 | 1/1302 (0.1%) | 0.93 | 3/1770 (0.2%) |
| 1 | 160-A | 0.74 | 1/1302 (0.1%) | 1.03 | 8/1770 (0.5%) |
| 1 | 161-A | 0.69 | 0/1302 | 0.97 | 4/1770 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 162-A | 0.76 | 2/1302 (0.2%) | 0.93 | 5/1770 (0.3%) |
| 1 | 163-A | 0.93 | 6/1302 (0.5%) | 0.93 | 5/1770 (0.3%) |
| 1 | 164-A | 0.72 | 1/1302 (0.1%) | 1.01 | 6/1770 (0.3%) |
| 1 | 165-A | 0.81 | 0/1302 | 1.01 | 4/1770 (0.2%) |
| 1 | 166-A | 0.74 | 0/1302 | 0.96 | 4/1770 (0.2%) |
| 1 | 167-A | 0.78 | 1/1302 (0.1%) | 1.03 | 7/1770 (0.4%) |
| 1 | 168-A | 0.79 | 4/1302 (0.3%) | 0.93 | 3/1770 (0.2%) |
| 1 | 169-A | 0.67 | 0/1302 | 0.92 | 3/1770 (0.2%) |
| 1 | 170-A | 0.73 | 1/1302 (0.1%) | 0.95 | 2/1770 (0.1%) |
| 1 | 171-A | 0.77 | 2/1302 (0.2%) | 0.98 | 7/1770 (0.4%) |
| 1 | 172-A | 0.71 | 1/1302 (0.1%) | 0.88 | 3/1770 (0.2%) |
| 1 | 173-A | 0.82 | 3/1302 (0.2%) | 0.98 | 6/1770 (0.3%) |
| 1 | 174-A | 0.80 | 3/1302 (0.2%) | 1.03 | 7/1770 (0.4%) |
| 1 | 175-A | 0.89 | 1/1302 (0.1%) | 1.02 | 8/1770 (0.5%) |
| 1 | 176-A | 0.79 | 2/1302 (0.2%) | 0.94 | 2/1770 (0.1%) |
| 1 | 177-A | 0.67 | 0/1302 | 0.95 | 5/1770 (0.3%) |
| 1 | 178-A | 0.80 | 1/1302 (0.1%) | 1.05 | 10/1770 (0.6%) |
| 1 | 179-A | 0.78 | 4/1302 (0.3%) | 0.99 | 7/1770 (0.4%) |
| 1 | 180-A | 0.70 | 0/1302 | 0.98 | 7/1770 (0.4%) |
| 1 | 181-A | 0.93 | 3/1302 (0.2%) | 1.09 | 7/1770 (0.4%) |
| 1 | 182-A | 0.81 | 2/1302 (0.2%) | 1.04 | 8/1770 (0.5%) |
| 1 | 183-A | 0.94 | 1/1302 (0.1%) | 1.03 | 11/1770 (0.6%) |
| 1 | 184-A | 0.71 | 0/1302 | 0.96 | 7/1770 (0.4%) |
| 1 | 185-A | 0.83 | 3/1302 (0.2%) | 1.09 | 8/1770 (0.5%) |
| 1 | 186-A | 0.93 | 4/1302 (0.3%) | 1.01 | 6/1770 (0.3%) |
| 1 | 187-A | 0.72 | 0/1302 | 1.01 | 5/1770 (0.3%) |
| 1 | 188-A | 0.80 | 2/1302 (0.2%) | 0.97 | 5/1770 (0.3%) |
| 1 | 189-A | 0.71 | 1/1302 (0.1%) | 0.92 | 5/1770 (0.3%) |
| 1 | 190-A | 0.82 | 2/1302 (0.2%) | 1.03 | 7/1770 (0.4%) |
| 1 | 191-A | 0.89 | 3/1302 (0.2%) | 0.96 | 4/1770 (0.2%) |
| 1 | 192-A | 0.81 | 2/1302 (0.2%) | 0.97 | 5/1770 (0.3%) |
| 1 | 193-A | 0.93 | 2/1302 (0.2%) | 1.03 | 6/1770 (0.3%) |
| 1 | 194-A | 0.75 | 2/1302 (0.2%) | 1.02 | 5/1770 (0.3%) |
| 1 | 195-A | 0.84 | 2/1302 (0.2%) | 1.15 | 12/1770 (0.7%) |
| 1 | 196-A | 0.86 | 1/1302 (0.1%) | 0.97 | 6/1770 (0.3%) |
| 1 | 197-A | 0.70 | 1/1302 (0.1%) | 0.98 | 6/1770 (0.3%) |
| 1 | 198-A | 0.93 | 2/1302 (0.2%) | 0.98 | 4/1770 (0.2%) |
| 1 | 199-A | 0.89 | 3/1302 (0.2%) | 0.96 | 7/1770 (0.4%) |
| 1 | 200-A | 0.78 | 2/1302 (0.2%) | 0.98 | 4/1770 (0.2%) |
| 1 | 201-A | 0.88 | 5/1302 (0.4%) | 1.00 | 7/1770 (0.4%) |
| 1 | 202-A | 0.73 | 0/1302 | 0.95 | 2/1770 (0.1%) |
| 1 | 203-A | 1.04 | 5/1302 (0.4%) | 1.00 | 6/1770 (0.3%) |
| 1 | 204-A | 0.82 | 1/1302 (0.1%) | 1.06 | 7/1770 (0.4%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------------|-------------|----------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 205-A | 0.97 | 2/1302 (0.2%) | 1.11 | 6/1770 (0.3%) |
| 1 | 206-A | 1.05 | 2/1302 (0.2%) | 1.05 | 7/1770 (0.4%) |
| 1 | 207-A | 0.73 | 1/1302 (0.1%) | 0.98 | 2/1770 (0.1%) |
| 1 | 208-A | 0.94 | 5/1302 (0.4%) | 0.96 | 6/1770 (0.3%) |
| 1 | 209-A | 0.78 | 1/1302 (0.1%) | 0.96 | 3/1770 (0.2%) |
| 1 | 210-A | 0.79 | 3/1302 (0.2%) | 1.09 | 7/1770 (0.4%) |
| 1 | 211-A | 1.14 | 4/1302 (0.3%) | 1.08 | 5/1770 (0.3%) |
| 1 | 212-A | 0.95 | 3/1302 (0.2%) | 1.09 | 10/1770 (0.6%) |
| 1 | 213-A | 0.80 | 3/1302 (0.2%) | 1.04 | 9/1770 (0.5%) |
| 1 | 214-A | 0.81 | 4/1302 (0.3%) | 1.01 | 9/1770 (0.5%) |
| 1 | 215-A | 0.78 | 2/1302 (0.2%) | 1.05 | 10/1770 (0.6%) |
| 1 | 216-A | 0.95 | 7/1302 (0.5%) | 1.07 | 13/1770 (0.7%) |
| 1 | 217-A | 0.77 | 1/1302 (0.1%) | 1.16 | 15/1770 (0.8%) |
| 1 | 218-A | 0.84 | 4/1302 (0.3%) | 1.06 | 9/1770 (0.5%) |
| 1 | 219-A | 0.86 | 4/1302 (0.3%) | 0.99 | 7/1770 (0.4%) |
| 1 | 220-A | 0.92 | 5/1302 (0.4%) | 1.05 | 5/1770 (0.3%) |
| 1 | 221-A | 1.28 | 7/1302 (0.5%) | 1.14 | 5/1770 (0.3%) |
| 1 | 222-A | 0.86 | 4/1302 (0.3%) | 1.03 | 6/1770 (0.3%) |
| 1 | 223-A | 0.92 | 6/1302 (0.5%) | 0.97 | 5/1770 (0.3%) |
| 1 | 224-A | 1.23 | 4/1302 (0.3%) | 1.08 | 7/1770 (0.4%) |
| 1 | 225-A | 0.91 | 3/1302 (0.2%) | 1.04 | 8/1770 (0.5%) |
| 1 | 226-A | 0.88 | 3/1302 (0.2%) | 1.06 | 8/1770 (0.5%) |
| 1 | 227-A | 0.94 | 3/1302 (0.2%) | 0.98 | 3/1770 (0.2%) |
| 1 | 228-A | 0.75 | 1/1302 (0.1%) | 0.94 | 2/1770 (0.1%) |
| 1 | 229-A | 0.89 | 3/1302 (0.2%) | 0.98 | 5/1770 (0.3%) |
| 1 | 230-A | 0.95 | 4/1302 (0.3%) | 1.05 | 7/1770 (0.4%) |
| 1 | 231-A | 0.90 | 4/1302 (0.3%) | 1.00 | 6/1770 (0.3%) |
| 1 | 232-A | 0.81 | 3/1302 (0.2%) | 0.99 | 5/1770 (0.3%) |
| 1 | 233-A | 0.83 | 4/1302 (0.3%) | 0.99 | 4/1770 (0.2%) |
| 1 | 234-A | 0.95 | 2/1302 (0.2%) | 1.05 | 7/1770 (0.4%) |
| 1 | 235-A | 0.73 | 1/1302 (0.1%) | 0.91 | 1/1770 (0.1%) |
| 1 | 236-A | 0.77 | 2/1302 (0.2%) | 0.94 | 3/1770 (0.2%) |
| 1 | 237-A | 0.70 | 0/1302 | 0.95 | 4/1770 (0.2%) |
| 1 | 238-A | 0.77 | 3/1302 (0.2%) | 1.00 | 8/1770 (0.5%) |
| 1 | 239-A | 0.74 | 1/1302 (0.1%) | 0.90 | 4/1770 (0.2%) |
| 1 | 240-A | 0.73 | 2/1302 (0.2%) | 0.90 | 3/1770 (0.2%) |
| 1 | 241-A | 0.69 | 0/1302 | 0.84 | 1/1770 (0.1%) |
| 1 | 242-A | 0.66 | 0/1302 | 0.91 | 4/1770 (0.2%) |
| 1 | 243-A | 0.72 | 1/1302 (0.1%) | 0.89 | 1/1770 (0.1%) |
| 1 | 244-A | 0.76 | 4/1302 (0.3%) | 0.98 | 6/1770 (0.3%) |
| 1 | 245-A | 0.70 | 1/1302 (0.1%) | 0.96 | 6/1770 (0.3%) |
| 1 | 246-A | 0.79 | 1/1302 (0.1%) | 0.93 | 3/1770 (0.2%) |
| 1 | 247-A | 0.77 | 2/1302 (0.2%) | 1.00 | 3/1770 (0.2%) |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-------------------|-------------|--------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | 248-A | 0.68 | 0/1302 | 0.92 | 3/1770 (0.2%) |
| 1 | 249-A | 0.76 | 2/1302 (0.2%) | 1.00 | 5/1770 (0.3%) |
| 1 | 250-A | 0.75 | 0/1302 | 0.95 | 2/1770 (0.1%) |
| All | All | 0.80 | 539/325500 (0.2%) | 0.99 | 1403/442500 (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 | 3-A | 0 | 1 |
| 1 | 4-A | 0 | 1 |
| 1 | 5-A | 0 | 1 |
| 1 | 8-A | 0 | 1 |
| 1 | 13-A | 0 | 1 |
| 1 | 22-A | 0 | 1 |
| 1 | 25-A | 0 | 1 |
| 1 | 34-A | 0 | 1 |
| 1 | 35-A | 0 | 1 |
| 1 | 41-A | 0 | 1 |
| 1 | 46-A | 0 | 1 |
| 1 | 47-A | 0 | 1 |
| 1 | 48-A | 0 | 1 |
| 1 | 53-A | 0 | 1 |
| 1 | 57-A | 0 | 2 |
| 1 | 58-A | 0 | 1 |
| 1 | 59-A | 0 | 1 |
| 1 | 62-A | 0 | 1 |
| 1 | 65-A | 0 | 2 |
| 1 | 66-A | 0 | 3 |
| 1 | 67-A | 0 | 3 |
| 1 | 68-A | 0 | 2 |
| 1 | 69-A | 0 | 1 |
| 1 | 70-A | 0 | 1 |
| 1 | 71-A | 0 | 1 |
| 1 | 78-A | 0 | 1 |
| 1 | 82-A | 0 | 1 |
| 1 | 83-A | 0 | 1 |
| 1 | 84-A | 0 | 1 |
| 1 | 85-A | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 94-A | 0 | 1 |
| 1 | 96-A | 0 | 2 |
| 1 | 100-A | 0 | 1 |
| 1 | 101-A | 0 | 1 |
| 1 | 109-A | 0 | 2 |
| 1 | 113-A | 0 | 1 |
| 1 | 114-A | 0 | 1 |
| 1 | 115-A | 0 | 2 |
| 1 | 120-A | 0 | 2 |
| 1 | 121-A | 0 | 2 |
| 1 | 122-A | 0 | 3 |
| 1 | 123-A | 0 | 1 |
| 1 | 124-A | 0 | 3 |
| 1 | 125-A | 0 | 1 |
| 1 | 126-A | 0 | 2 |
| 1 | 127-A | 0 | 1 |
| 1 | 128-A | 0 | 2 |
| 1 | 129-A | 0 | 2 |
| 1 | 130-A | 0 | 1 |
| 1 | 131-A | 0 | 2 |
| 1 | 133-A | 0 | 2 |
| 1 | 134-A | 0 | 2 |
| 1 | 138-A | 0 | 2 |
| 1 | 140-A | 0 | 2 |
| 1 | 141-A | 0 | 1 |
| 1 | 142-A | 0 | 2 |
| 1 | 143-A | 0 | 1 |
| 1 | 144-A | 0 | 2 |
| 1 | 146-A | 0 | 1 |
| 1 | 147-A | 0 | 1 |
| 1 | 148-A | 0 | 1 |
| 1 | 149-A | 0 | 1 |
| 1 | 151-A | 0 | 1 |
| 1 | 152-A | 0 | 1 |
| 1 | 154-A | 0 | 1 |
| 1 | 155-A | 0 | 1 |
| 1 | 157-A | 0 | 1 |
| 1 | 158-A | 0 | 1 |
| 1 | 160-A | 0 | 1 |
| 1 | 164-A | 0 | 1 |
| 1 | 173-A | 0 | 1 |
| 1 | 174-A | 0 | 1 |

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| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | 175-A | 0 | 2 |
| 1 | 176-A | 0 | 1 |
| 1 | 177-A | 0 | 1 |
| 1 | 178-A | 0 | 2 |
| 1 | 180-A | 0 | 1 |
| 1 | 181-A | 0 | 1 |
| 1 | 182-A | 0 | 2 |
| 1 | 183-A | 0 | 1 |
| 1 | 184-A | 0 | 1 |
| 1 | 185-A | 0 | 2 |
| 1 | 186-A | 0 | 1 |
| 1 | 187-A | 0 | 3 |
| 1 | 188-A | 0 | 2 |
| 1 | 190-A | 0 | 1 |
| 1 | 191-A | 0 | 1 |
| 1 | 192-A | 0 | 1 |
| 1 | 193-A | 0 | 1 |
| 1 | 194-A | 0 | 2 |
| 1 | 195-A | 0 | 1 |
| 1 | 197-A | 0 | 1 |
| 1 | 205-A | 0 | 1 |
| 1 | 209-A | 0 | 1 |
| 1 | 210-A | 0 | 2 |
| 1 | 212-A | 0 | 1 |
| 1 | 213-A | 0 | 2 |
| 1 | 214-A | 0 | 2 |
| 1 | 215-A | 0 | 1 |
| 1 | 216-A | 0 | 1 |
| 1 | 217-A | 0 | 2 |
| 1 | 218-A | 0 | 1 |
| 1 | 219-A | 0 | 1 |
| 1 | 220-A | 0 | 1 |
| 1 | 221-A | 0 | 1 |
| 1 | 222-A | 0 | 1 |
| 1 | 223-A | 0 | 2 |
| 1 | 224-A | 0 | 3 |
| 1 | 225-A | 0 | 1 |
| 1 | 226-A | 0 | 2 |
| 1 | 229-A | 0 | 1 |
| 1 | 247-A | 0 | 1 |
| All | All | 0 | 155 |

All (539) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|--------|-------------|----------|
| 1 | 221-A | 152 | CYS | CB-SG | 33.07 | 2.38 | 1.82 |
| 1 | 224-A | 152 | CYS | CB-SG | 32.84 | 2.38 | 1.82 |
| 1 | 211-A | 152 | CYS | CB-SG | 29.74 | 2.32 | 1.82 |
| 1 | 206-A | 152 | CYS | CB-SG | -26.18 | 1.37 | 1.82 |
| 1 | 203-A | 152 | CYS | CB-SG | 24.07 | 2.23 | 1.82 |
| 1 | 205-A | 152 | CYS | CB-SG | -22.82 | 1.43 | 1.82 |
| 1 | 234-A | 152 | CYS | CB-SG | -21.73 | 1.45 | 1.82 |
| 1 | 198-A | 152 | CYS | CB-SG | 19.88 | 2.16 | 1.82 |
| 1 | 183-A | 152 | CYS | CB-SG | 19.23 | 2.15 | 1.82 |
| 1 | 186-A | 152 | CYS | CB-SG | 18.77 | 2.14 | 1.82 |
| 1 | 196-A | 152 | CYS | CB-SG | -18.16 | 1.51 | 1.82 |
| 1 | 175-A | 152 | CYS | CB-SG | -17.08 | 1.53 | 1.82 |
| 1 | 193-A | 152 | CYS | CB-SG | -16.84 | 1.53 | 1.82 |
| 1 | 212-A | 152 | CYS | CB-SG | 16.64 | 2.10 | 1.82 |
| 1 | 229-A | 152 | CYS | CB-SG | -16.39 | 1.54 | 1.82 |
| 1 | 227-A | 152 | CYS | CB-SG | -16.36 | 1.54 | 1.82 |
| 1 | 181-A | 148 | SER | CB-OG | 15.67 | 1.62 | 1.42 |
| 1 | 199-A | 152 | CYS | CB-SG | -15.49 | 1.55 | 1.82 |
| 1 | 225-A | 152 | CYS | CB-SG | -14.78 | 1.57 | 1.82 |
| 1 | 230-A | 152 | CYS | CB-SG | 14.13 | 2.06 | 1.82 |
| 1 | 191-A | 152 | CYS | CB-SG | -13.89 | 1.58 | 1.82 |
| 1 | 208-A | 152 | CYS | CB-SG | -13.39 | 1.59 | 1.82 |
| 1 | 204-A | 152 | CYS | CB-SG | 12.81 | 2.04 | 1.82 |
| 1 | 218-A | 152 | CYS | CB-SG | -12.52 | 1.60 | 1.82 |
| 1 | 41-A | 120 | GLU | CB-CG | 12.46 | 1.75 | 1.52 |
| 1 | 13-A | 120 | GLU | CB-CG | -12.39 | 1.28 | 1.52 |
| 1 | 231-A | 152 | CYS | CB-SG | 12.12 | 2.02 | 1.82 |
| 1 | 220-A | 154 | GLU | CB-CG | 12.09 | 1.75 | 1.52 |
| 1 | 101-A | 85 | CYS | CB-SG | -11.88 | 1.62 | 1.82 |
| 1 | 178-A | 152 | CYS | CB-SG | -11.76 | 1.62 | 1.82 |
| 1 | 40-A | 101 | GLU | CB-CG | 11.72 | 1.74 | 1.52 |
| 1 | 41-A | 120 | GLU | CD-OE1 | 11.55 | 1.38 | 1.25 |
| 1 | 222-A | 152 | CYS | CB-SG | 11.22 | 2.01 | 1.82 |
| 1 | 192-A | 152 | CYS | CB-SG | 11.18 | 2.01 | 1.82 |
| 1 | 163-A | 106 | LYS | CD-CE | 11.16 | 1.79 | 1.51 |
| 1 | 223-A | 152 | CYS | CB-SG | 10.75 | 2.00 | 1.82 |
| 1 | 88-A | 16 | MET | CG-SD | 10.65 | 2.08 | 1.81 |
| 1 | 13-A | 120 | GLU | CG-CD | 10.61 | 1.67 | 1.51 |
| 1 | 195-A | 152 | CYS | CB-SG | 10.22 | 1.99 | 1.82 |
| 1 | 181-A | 152 | CYS | CB-SG | -10.12 | 1.65 | 1.82 |
| 1 | 31-A | 44 | ARG | CG-CD | 10.00 | 1.76 | 1.51 |
| 1 | 185-A | 101 | GLU | CG-CD | -9.96 | 1.37 | 1.51 |
| 1 | 171-A | 152 | CYS | CB-SG | 9.93 | 1.99 | 1.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 90-A | 16 | MET | CB-CG | 9.81 | 1.82 | 1.51 |
| 1 | 176-A | 152 | CYS | CB-SG | -9.79 | 1.65 | 1.82 |
| 1 | 171-A | 101 | GLU | CB-CG | 9.77 | 1.70 | 1.52 |
| 1 | 182-A | 152 | CYS | CB-SG | -9.77 | 1.65 | 1.82 |
| 1 | 42-A | 120 | GLU | CB-CG | 9.69 | 1.70 | 1.52 |
| 1 | 25-A | 157 | GLU | CB-CG | 9.64 | 1.70 | 1.52 |
| 1 | 230-A | 157 | GLU | CB-CG | 9.62 | 1.70 | 1.52 |
| 1 | 230-A | 101 | GLU | CB-CG | 9.61 | 1.70 | 1.52 |
| 1 | 8-A | 157 | GLU | CG-CD | 9.60 | 1.66 | 1.51 |
| 1 | 155-A | 120 | GLU | CB-CG | 9.58 | 1.70 | 1.52 |
| 1 | 39-A | 120 | GLU | CB-CG | 9.54 | 1.70 | 1.52 |
| 1 | 208-A | 118 | GLU | CB-CG | 9.51 | 1.70 | 1.52 |
| 1 | 220-A | 152 | CYS | CB-SG | 9.48 | 1.98 | 1.82 |
| 1 | 201-A | 118 | GLU | CG-CD | 9.34 | 1.66 | 1.51 |
| 1 | 216-A | 142 | ASP | CB-CG | -9.33 | 1.32 | 1.51 |
| 1 | 129-A | 101 | GLU | CB-CG | 9.32 | 1.69 | 1.52 |
| 1 | 44-A | 119 | VAL | CB-CG1 | -9.30 | 1.33 | 1.52 |
| 1 | 21-A | 157 | GLU | CB-CG | 9.28 | 1.69 | 1.52 |
| 1 | 233-A | 152 | CYS | CB-SG | 9.27 | 1.98 | 1.82 |
| 1 | 150-A | 157 | GLU | CG-CD | 9.27 | 1.65 | 1.51 |
| 1 | 41-A | 44 | ARG | CG-CD | 9.24 | 1.75 | 1.51 |
| 1 | 49-A | 142 | ASP | CB-CG | -9.11 | 1.32 | 1.51 |
| 1 | 247-A | 85 | CYS | CB-SG | 9.09 | 1.97 | 1.82 |
| 1 | 78-A | 48 | GLU | CB-CG | 9.07 | 1.69 | 1.52 |
| 1 | 78-A | 85 | CYS | CB-SG | 9.07 | 1.97 | 1.82 |
| 1 | 40-A | 44 | ARG | CG-CD | 9.04 | 1.74 | 1.51 |
| 1 | 70-A | 159 | ARG | CG-CD | -9.04 | 1.29 | 1.51 |
| 1 | 230-A | 157 | GLU | CG-CD | 8.96 | 1.65 | 1.51 |
| 1 | 209-A | 152 | CYS | CB-SG | 8.95 | 1.97 | 1.82 |
| 1 | 91-A | 16 | MET | CB-CG | 8.82 | 1.79 | 1.51 |
| 1 | 226-A | 152 | CYS | CB-SG | 8.81 | 1.97 | 1.82 |
| 1 | 219-A | 152 | CYS | CB-SG | -8.80 | 1.67 | 1.82 |
| 1 | 179-A | 152 | CYS | CB-SG | -8.77 | 1.67 | 1.82 |
| 1 | 143-A | 101 | GLU | CB-CG | 8.75 | 1.68 | 1.52 |
| 1 | 216-A | 1 | MET | CB-CG | 8.69 | 1.79 | 1.51 |
| 1 | 235-A | 101 | GLU | CB-CG | -8.67 | 1.35 | 1.52 |
| 1 | 44-A | 120 | GLU | CB-CG | 8.63 | 1.68 | 1.52 |
| 1 | 238-A | 157 | GLU | CB-CG | 8.58 | 1.68 | 1.52 |
| 1 | 84-A | 16 | MET | CG-SD | 8.58 | 2.03 | 1.81 |
| 1 | 69-A | 101 | GLU | CB-CG | 8.57 | 1.68 | 1.52 |
| 1 | 46-A | 118 | GLU | CG-CD | 8.57 | 1.64 | 1.51 |
| 1 | 226-A | 154 | GLU | CG-CD | 8.54 | 1.64 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 42-A | 120 | GLU | CD-OE1 | 8.49 | 1.34 | 1.25 |
| 1 | 201-A | 85 | CYS | CB-SG | 8.47 | 1.96 | 1.82 |
| 1 | 88-A | 16 | MET | CB-CG | 8.41 | 1.78 | 1.51 |
| 1 | 208-A | 17 | GLU | CB-CG | 8.39 | 1.68 | 1.52 |
| 1 | 2-A | 152 | CYS | CB-SG | 8.33 | 1.96 | 1.82 |
| 1 | 121-A | 85 | CYS | CB-SG | 8.23 | 1.96 | 1.82 |
| 1 | 223-A | 154 | GLU | CG-CD | 8.22 | 1.64 | 1.51 |
| 1 | 36-A | 101 | GLU | CB-CG | 8.21 | 1.67 | 1.52 |
| 1 | 163-A | 118 | GLU | CB-CG | 8.20 | 1.67 | 1.52 |
| 1 | 144-A | 20 | MET | CG-SD | 8.17 | 2.02 | 1.81 |
| 1 | 115-A | 85 | CYS | CB-SG | -8.16 | 1.68 | 1.82 |
| 1 | 64-A | 44 | ARG | CB-CG | 8.13 | 1.74 | 1.52 |
| 1 | 64-A | 101 | GLU | CB-CG | 8.05 | 1.67 | 1.52 |
| 1 | 163-A | 118 | GLU | CG-CD | 8.05 | 1.64 | 1.51 |
| 1 | 76-A | 48 | GLU | CG-CD | 8.04 | 1.64 | 1.51 |
| 1 | 143-A | 20 | MET | CG-SD | 8.04 | 2.02 | 1.81 |
| 1 | 167-A | 52 | ARG | CG-CD | 8.03 | 1.72 | 1.51 |
| 1 | 24-A | 157 | GLU | CB-CG | 7.99 | 1.67 | 1.52 |
| 1 | 43-A | 120 | GLU | CB-CG | 7.99 | 1.67 | 1.52 |
| 1 | 201-A | 101 | GLU | CB-CG | -7.99 | 1.36 | 1.52 |
| 1 | 39-A | 120 | GLU | CD-OE1 | 7.91 | 1.34 | 1.25 |
| 1 | 145-A | 20 | MET | CA-CB | 7.86 | 1.71 | 1.53 |
| 1 | 107-A | 120 | GLU | CG-CD | 7.85 | 1.63 | 1.51 |
| 1 | 249-A | 85 | CYS | CB-SG | -7.84 | 1.69 | 1.82 |
| 1 | 143-A | 20 | MET | CB-CG | 7.83 | 1.76 | 1.51 |
| 1 | 191-A | 157 | GLU | CB-CG | 7.80 | 1.67 | 1.52 |
| 1 | 40-A | 120 | GLU | CB-CG | 7.80 | 1.67 | 1.52 |
| 1 | 126-A | 120 | GLU | CG-CD | 7.78 | 1.63 | 1.51 |
| 1 | 229-A | 101 | GLU | CB-CG | 7.78 | 1.67 | 1.52 |
| 1 | 200-A | 152 | CYS | CB-SG | 7.75 | 1.95 | 1.82 |
| 1 | 29-A | 154 | GLU | CB-CG | 7.69 | 1.66 | 1.52 |
| 1 | 199-A | 85 | CYS | CB-SG | 7.68 | 1.95 | 1.82 |
| 1 | 173-A | 152 | CYS | CB-SG | 7.67 | 1.95 | 1.82 |
| 1 | 62-A | 44 | ARG | CB-CG | 7.64 | 1.73 | 1.52 |
| 1 | 218-A | 154 | GLU | CB-CG | 7.64 | 1.66 | 1.52 |
| 1 | 96-A | 118 | GLU | CB-CG | 7.60 | 1.66 | 1.52 |
| 1 | 57-A | 159 | ARG | CB-CG | 7.59 | 1.73 | 1.52 |
| 1 | 8-A | 157 | GLU | CB-CG | 7.58 | 1.66 | 1.52 |
| 1 | 144-A | 20 | MET | CB-CG | 7.57 | 1.75 | 1.51 |
| 1 | 89-A | 16 | MET | CB-CG | 7.57 | 1.75 | 1.51 |
| 1 | 44-A | 120 | GLU | CG-CD | 7.55 | 1.63 | 1.51 |
| 1 | 191-A | 19 | ALA | CA-CB | 7.55 | 1.68 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 141-A | 22 | TRP | CB-CG | -7.48 | 1.36 | 1.50 |
| 1 | 26-A | 44 | ARG | CG-CD | -7.46 | 1.33 | 1.51 |
| 1 | 34-A | 44 | ARG | CG-CD | 7.45 | 1.70 | 1.51 |
| 1 | 110-A | 101 | GLU | CG-CD | 7.42 | 1.63 | 1.51 |
| 1 | 88-A | 119 | VAL | CB-CG1 | -7.42 | 1.37 | 1.52 |
| 1 | 144-A | 16 | MET | CB-CG | -7.40 | 1.27 | 1.51 |
| 1 | 99-A | 142 | ASP | CB-CG | -7.39 | 1.36 | 1.51 |
| 1 | 214-A | 152 | CYS | CB-SG | -7.38 | 1.69 | 1.82 |
| 1 | 120-A | 79 | ASP | CB-CG | 7.36 | 1.67 | 1.51 |
| 1 | 156-A | 157 | GLU | CG-CD | -7.33 | 1.41 | 1.51 |
| 1 | 227-A | 101 | GLU | CG-CD | 7.33 | 1.62 | 1.51 |
| 1 | 145-A | 20 | MET | CB-CG | 7.31 | 1.74 | 1.51 |
| 1 | 10-A | 101 | GLU | CB-CG | 7.27 | 1.66 | 1.52 |
| 1 | 91-A | 20 | MET | CB-CG | 7.26 | 1.74 | 1.51 |
| 1 | 223-A | 119 | VAL | CB-CG2 | -7.24 | 1.37 | 1.52 |
| 1 | 77-A | 118 | GLU | CG-CD | -7.23 | 1.41 | 1.51 |
| 1 | 57-A | 101 | GLU | CB-CG | 7.22 | 1.65 | 1.52 |
| 1 | 97-A | 157 | GLU | CG-CD | 7.21 | 1.62 | 1.51 |
| 1 | 211-A | 101 | GLU | CB-CG | 7.21 | 1.65 | 1.52 |
| 1 | 41-A | 120 | GLU | CG-CD | 7.21 | 1.62 | 1.51 |
| 1 | 44-A | 101 | GLU | CB-CG | -7.20 | 1.38 | 1.52 |
| 1 | 4-A | 101 | GLU | CB-CG | -7.18 | 1.38 | 1.52 |
| 1 | 10-A | 108 | GLN | CG-CD | -7.17 | 1.34 | 1.51 |
| 1 | 11-A | 120 | GLU | CB-CG | 7.16 | 1.65 | 1.52 |
| 1 | 213-A | 101 | GLU | CB-CG | 7.12 | 1.65 | 1.52 |
| 1 | 59-A | 44 | ARG | CZ-NH2 | 7.10 | 1.42 | 1.33 |
| 1 | 10-A | 120 | GLU | CD-OE1 | 7.10 | 1.33 | 1.25 |
| 1 | 232-A | 49 | SER | CA-CB | 7.08 | 1.63 | 1.52 |
| 1 | 105-A | 148 | SER | CA-CB | 7.08 | 1.63 | 1.52 |
| 1 | 156-A | 118 | GLU | CG-CD | 7.00 | 1.62 | 1.51 |
| 1 | 42-A | 101 | GLU | CB-CG | -6.99 | 1.38 | 1.52 |
| 1 | 66-A | 20 | MET | CB-CG | 6.99 | 1.73 | 1.51 |
| 1 | 215-A | 120 | GLU | CB-CG | 6.99 | 1.65 | 1.52 |
| 1 | 10-A | 157 | GLU | CB-CG | -6.97 | 1.39 | 1.52 |
| 1 | 201-A | 118 | GLU | CB-CG | 6.94 | 1.65 | 1.52 |
| 1 | 29-A | 44 | ARG | CB-CG | 6.94 | 1.71 | 1.52 |
| 1 | 94-A | 101 | GLU | CB-CG | 6.92 | 1.65 | 1.52 |
| 1 | 115-A | 157 | GLU | CB-CG | 6.92 | 1.65 | 1.52 |
| 1 | 243-A | 108 | GLN | CB-CG | 6.90 | 1.71 | 1.52 |
| 1 | 79-A | 118 | GLU | CG-CD | 6.88 | 1.62 | 1.51 |
| 1 | 43-A | 120 | GLU | CD-OE1 | 6.88 | 1.33 | 1.25 |
| 1 | 233-A | 85 | CYS | CB-SG | -6.87 | 1.70 | 1.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 51-A | 101 | GLU | CG-CD | -6.83 | 1.41 | 1.51 |
| 1 | 231-A | 157 | GLU | CB-CG | 6.80 | 1.65 | 1.52 |
| 1 | 126-A | 118 | GLU | CB-CG | 6.78 | 1.65 | 1.52 |
| 1 | 225-A | 154 | GLU | CG-CD | 6.76 | 1.62 | 1.51 |
| 1 | 39-A | 120 | GLU | CG-CD | 6.75 | 1.62 | 1.51 |
| 1 | 203-A | 119 | VAL | CB-CG1 | -6.75 | 1.38 | 1.52 |
| 1 | 53-A | 118 | GLU | CB-CG | 6.75 | 1.65 | 1.52 |
| 1 | 127-A | 118 | GLU | CB-CG | 6.73 | 1.65 | 1.52 |
| 1 | 225-A | 76 | LYS | CB-CG | -6.73 | 1.34 | 1.52 |
| 1 | 195-A | 157 | GLU | CB-CG | 6.71 | 1.65 | 1.52 |
| 1 | 28-A | 49 | SER | CA-CB | 6.71 | 1.63 | 1.52 |
| 1 | 11-A | 120 | GLU | CG-CD | 6.69 | 1.61 | 1.51 |
| 1 | 224-A | 154 | GLU | CG-CD | 6.67 | 1.61 | 1.51 |
| 1 | 73-A | 157 | GLU | CB-CG | 6.67 | 1.64 | 1.52 |
| 1 | 1-A | 98 | ARG | CZ-NH1 | 6.65 | 1.41 | 1.33 |
| 1 | 14-A | 118 | GLU | CB-CG | 6.63 | 1.64 | 1.52 |
| 1 | 244-A | 108 | GLN | CB-CG | 6.63 | 1.70 | 1.52 |
| 1 | 37-A | 120 | GLU | CB-CG | 6.63 | 1.64 | 1.52 |
| 1 | 143-A | 101 | GLU | CG-CD | 6.62 | 1.61 | 1.51 |
| 1 | 163-A | 139 | GLU | CG-CD | 6.62 | 1.61 | 1.51 |
| 1 | 19-A | 79 | ASP | CB-CG | 6.62 | 1.65 | 1.51 |
| 1 | 78-A | 16 | MET | CB-CG | 6.61 | 1.72 | 1.51 |
| 1 | 205-A | 119 | VAL | CB-CG1 | -6.61 | 1.39 | 1.52 |
| 1 | 30-A | 109 | LYS | CD-CE | 6.61 | 1.67 | 1.51 |
| 1 | 115-A | 119 | VAL | CB-CG2 | -6.60 | 1.39 | 1.52 |
| 1 | 127-A | 118 | GLU | CG-CD | 6.59 | 1.61 | 1.51 |
| 1 | 63-A | 22 | TRP | CB-CG | 6.58 | 1.62 | 1.50 |
| 1 | 97-A | 49 | SER | CA-CB | 6.58 | 1.62 | 1.52 |
| 1 | 121-A | 22 | TRP | CB-CG | -6.58 | 1.38 | 1.50 |
| 1 | 140-A | 16 | MET | CB-CG | 6.57 | 1.72 | 1.51 |
| 1 | 70-A | 20 | MET | CB-CG | 6.57 | 1.72 | 1.51 |
| 1 | 179-A | 119 | VAL | CB-CG2 | -6.57 | 1.39 | 1.52 |
| 1 | 193-A | 52 | ARG | CG-CD | -6.56 | 1.35 | 1.51 |
| 1 | 217-A | 79 | ASP | CB-CG | 6.55 | 1.65 | 1.51 |
| 1 | 66-A | 19 | ALA | C-O | 6.52 | 1.35 | 1.23 |
| 1 | 150-A | 139 | GLU | CB-CG | -6.51 | 1.39 | 1.52 |
| 1 | 216-A | 120 | GLU | CB-CG | 6.51 | 1.64 | 1.52 |
| 1 | 142-A | 118 | GLU | CG-CD | 6.50 | 1.61 | 1.51 |
| 1 | 213-A | 157 | GLU | CG-CD | 6.49 | 1.61 | 1.51 |
| 1 | 59-A | 139 | GLU | CB-CG | 6.48 | 1.64 | 1.52 |
| 1 | 102-A | 157 | GLU | CB-CG | 6.48 | 1.64 | 1.52 |
| 1 | 160-A | 139 | GLU | CG-CD | 6.46 | 1.61 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | 60-A | 20 | MET | CB-CG | 6.46 | 1.72 | 1.51 |
| 1 | 106-A | 17 | GLU | CG-CD | 6.42 | 1.61 | 1.51 |
| 1 | 156-A | 120 | GLU | CB-CG | 6.42 | 1.64 | 1.52 |
| 1 | 25-A | 157 | GLU | CG-CD | 6.42 | 1.61 | 1.51 |
| 1 | 236-A | 118 | GLU | CG-CD | 6.41 | 1.61 | 1.51 |
| 1 | 24-A | 127 | ASP | CB-CG | 6.41 | 1.65 | 1.51 |
| 1 | 49-A | 1 | MET | N-CA | 6.40 | 1.59 | 1.46 |
| 1 | 24-A | 20 | MET | CB-CG | 6.38 | 1.71 | 1.51 |
| 1 | 91-A | 128 | TYR | CB-CG | 6.38 | 1.61 | 1.51 |
| 1 | 39-A | 85 | CYS | CB-SG | 6.37 | 1.93 | 1.82 |
| 1 | 210-A | 118 | GLU | CG-CD | 6.37 | 1.61 | 1.51 |
| 1 | 186-A | 101 | GLU | CB-CG | -6.35 | 1.40 | 1.52 |
| 1 | 128-A | 48 | GLU | CB-CG | 6.33 | 1.64 | 1.52 |
| 1 | 13-A | 118 | GLU | CB-CG | -6.33 | 1.40 | 1.52 |
| 1 | 23-A | 101 | GLU | CG-CD | 6.31 | 1.61 | 1.51 |
| 1 | 106-A | 17 | GLU | CB-CG | 6.30 | 1.64 | 1.52 |
| 1 | 111-A | 101 | GLU | CB-CG | 6.30 | 1.64 | 1.52 |
| 1 | 66-A | 16 | MET | CG-SD | 6.30 | 1.97 | 1.81 |
| 1 | 208-A | 107 | ALA | CA-CB | -6.29 | 1.39 | 1.52 |
| 1 | 34-A | 101 | GLU | CB-CG | 6.28 | 1.64 | 1.52 |
| 1 | 150-A | 157 | GLU | CB-CG | 6.27 | 1.64 | 1.52 |
| 1 | 126-A | 134 | GLU | CG-CD | 6.27 | 1.61 | 1.51 |
| 1 | 240-A | 52 | ARG | CG-CD | 6.27 | 1.67 | 1.51 |
| 1 | 186-A | 79 | ASP | CB-CG | 6.26 | 1.65 | 1.51 |
| 1 | 190-A | 128 | TYR | CD2-CE2 | -6.25 | 1.29 | 1.39 |
| 1 | 226-A | 157 | GLU | CB-CG | 6.24 | 1.64 | 1.52 |
| 1 | 155-A | 118 | GLU | CB-CG | 6.23 | 1.64 | 1.52 |
| 1 | 31-A | 33 | ARG | CZ-NH2 | -6.23 | 1.25 | 1.33 |
| 1 | 249-A | 33 | ARG | CZ-NH1 | 6.23 | 1.41 | 1.33 |
| 1 | 99-A | 109 | LYS | CD-CE | -6.22 | 1.35 | 1.51 |
| 1 | 162-A | 85 | CYS | CB-SG | -6.21 | 1.71 | 1.82 |
| 1 | 58-A | 20 | MET | CG-SD | 6.20 | 1.97 | 1.81 |
| 1 | 10-A | 101 | GLU | CG-CD | 6.19 | 1.61 | 1.51 |
| 1 | 189-A | 152 | CYS | CB-SG | 6.18 | 1.92 | 1.82 |
| 1 | 190-A | 152 | CYS | CB-SG | 6.17 | 1.92 | 1.82 |
| 1 | 231-A | 17 | GLU | CG-CD | 6.17 | 1.61 | 1.51 |
| 1 | 12-A | 118 | GLU | CG-CD | -6.17 | 1.42 | 1.51 |
| 1 | 31-A | 33 | ARG | CD-NE | 6.16 | 1.56 | 1.46 |
| 1 | 57-A | 48 | GLU | CG-CD | 6.15 | 1.61 | 1.51 |
| 1 | 197-A | 152 | CYS | CB-SG | 6.14 | 1.92 | 1.82 |
| 1 | 70-A | 76 | LYS | CE-NZ | 6.14 | 1.64 | 1.49 |
| 1 | 185-A | 49 | SER | CA-CB | 6.13 | 1.62 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 145-A | 20 | MET | CG-SD | 6.11 | 1.97 | 1.81 |
| 1 | 13-A | 134 | GLU | CB-CG | -6.11 | 1.40 | 1.52 |
| 1 | 38-A | 120 | GLU | CG-CD | 6.11 | 1.61 | 1.51 |
| 1 | 51-A | 52 | ARG | CG-CD | -6.11 | 1.36 | 1.51 |
| 1 | 138-A | 65 | GLN | CB-CG | -6.10 | 1.36 | 1.52 |
| 1 | 224-A | 76 | LYS | CB-CG | -6.07 | 1.36 | 1.52 |
| 1 | 173-A | 142 | ASP | CB-CG | 6.06 | 1.64 | 1.51 |
| 1 | 47-A | 44 | ARG | CB-CG | 6.04 | 1.68 | 1.52 |
| 1 | 5-A | 108 | GLN | CB-CG | 6.04 | 1.68 | 1.52 |
| 1 | 192-A | 134 | GLU | CG-CD | 6.04 | 1.61 | 1.51 |
| 1 | 67-A | 48 | GLU | CG-CD | 6.03 | 1.60 | 1.51 |
| 1 | 119-A | 157 | GLU | CG-CD | 6.03 | 1.60 | 1.51 |
| 1 | 216-A | 1 | MET | CG-SD | 6.03 | 1.96 | 1.81 |
| 1 | 124-A | 118 | GLU | CB-CG | -6.02 | 1.40 | 1.52 |
| 1 | 7-A | 20 | MET | CB-CG | 6.02 | 1.70 | 1.51 |
| 1 | 94-A | 101 | GLU | CG-CD | 6.01 | 1.60 | 1.51 |
| 1 | 45-A | 120 | GLU | CB-CG | 6.01 | 1.63 | 1.52 |
| 1 | 57-A | 48 | GLU | CB-CG | 6.01 | 1.63 | 1.52 |
| 1 | 61-A | 49 | SER | CB-OG | -6.01 | 1.34 | 1.42 |
| 1 | 67-A | 134 | GLU | CG-CD | -6.00 | 1.43 | 1.51 |
| 1 | 87-A | 49 | SER | CA-CB | 6.00 | 1.61 | 1.52 |
| 1 | 151-A | 1 | MET | C-O | 5.99 | 1.34 | 1.23 |
| 1 | 221-A | 19 | ALA | CA-CB | 5.99 | 1.65 | 1.52 |
| 1 | 117-A | 157 | GLU | CD-OE2 | -5.98 | 1.19 | 1.25 |
| 1 | 40-A | 154 | GLU | CG-CD | 5.97 | 1.60 | 1.51 |
| 1 | 168-A | 101 | GLU | CB-CG | 5.97 | 1.63 | 1.52 |
| 1 | 87-A | 119 | VAL | CB-CG1 | -5.96 | 1.40 | 1.52 |
| 1 | 203-A | 101 | GLU | CB-CG | 5.95 | 1.63 | 1.52 |
| 1 | 181-A | 159 | ARG | CG-CD | 5.95 | 1.66 | 1.51 |
| 1 | 221-A | 19 | ALA | N-CA | 5.95 | 1.58 | 1.46 |
| 1 | 15-A | 142 | ASP | CB-CG | 5.94 | 1.64 | 1.51 |
| 1 | 156-A | 120 | GLU | CG-CD | 5.94 | 1.60 | 1.51 |
| 1 | 179-A | 49 | SER | CA-CB | 5.93 | 1.61 | 1.52 |
| 1 | 214-A | 159 | ARG | CG-CD | 5.93 | 1.66 | 1.51 |
| 1 | 194-A | 119 | VAL | CB-CG1 | -5.92 | 1.40 | 1.52 |
| 1 | 122-A | 76 | LYS | CB-CG | 5.90 | 1.68 | 1.52 |
| 1 | 246-A | 157 | GLU | CG-CD | -5.90 | 1.43 | 1.51 |
| 1 | 64-A | 44 | ARG | CG-CD | 5.89 | 1.66 | 1.51 |
| 1 | 85-A | 16 | MET | CB-CG | -5.88 | 1.32 | 1.51 |
| 1 | 90-A | 18 | ASN | CB-CG | 5.88 | 1.64 | 1.51 |
| 1 | 44-A | 120 | GLU | CD-OE1 | 5.88 | 1.32 | 1.25 |
| 1 | 66-A | 16 | MET | CB-CG | 5.88 | 1.70 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | 142-A | 101 | GLU | CD-OE2 | 5.87 | 1.32 | 1.25 |
| 1 | 86-A | 48 | GLU | CB-CG | 5.86 | 1.63 | 1.52 |
| 1 | 51-A | 128 | TYR | CD1-CE1 | 5.86 | 1.48 | 1.39 |
| 1 | 1-A | 157 | GLU | CB-CG | 5.85 | 1.63 | 1.52 |
| 1 | 144-A | 20 | MET | CA-CB | 5.85 | 1.66 | 1.53 |
| 1 | 59-A | 137 | PHE | CB-CG | -5.85 | 1.41 | 1.51 |
| 1 | 222-A | 19 | ALA | N-CA | 5.84 | 1.58 | 1.46 |
| 1 | 37-A | 17 | GLU | CG-CD | 5.83 | 1.60 | 1.51 |
| 1 | 99-A | 20 | MET | CB-CG | 5.83 | 1.70 | 1.51 |
| 1 | 200-A | 4 | LEU | CG-CD1 | -5.82 | 1.30 | 1.51 |
| 1 | 91-A | 1 | MET | CG-SD | -5.82 | 1.66 | 1.81 |
| 1 | 223-A | 16 | MET | CB-CG | 5.82 | 1.70 | 1.51 |
| 1 | 42-A | 108 | GLN | CB-CG | 5.82 | 1.68 | 1.52 |
| 1 | 218-A | 101 | GLU | CB-CG | -5.81 | 1.41 | 1.52 |
| 1 | 40-A | 118 | GLU | CB-CG | 5.80 | 1.63 | 1.52 |
| 1 | 219-A | 120 | GLU | CG-CD | 5.80 | 1.60 | 1.51 |
| 1 | 40-A | 120 | GLU | CG-CD | 5.78 | 1.60 | 1.51 |
| 1 | 232-A | 79 | ASP | CB-CG | 5.77 | 1.63 | 1.51 |
| 1 | 64-A | 17 | GLU | CB-CG | 5.77 | 1.63 | 1.52 |
| 1 | 74-A | 106 | LYS | CD-CE | 5.76 | 1.65 | 1.51 |
| 1 | 143-A | 101 | GLU | CA-CB | 5.75 | 1.66 | 1.53 |
| 1 | 117-A | 157 | GLU | CB-CG | -5.74 | 1.41 | 1.52 |
| 1 | 214-A | 101 | GLU | CB-CG | 5.74 | 1.63 | 1.52 |
| 1 | 220-A | 157 | GLU | CG-CD | 5.74 | 1.60 | 1.51 |
| 1 | 96-A | 118 | GLU | CG-CD | 5.73 | 1.60 | 1.51 |
| 1 | 64-A | 139 | GLU | CB-CG | 5.72 | 1.63 | 1.52 |
| 1 | 174-A | 154 | GLU | CG-CD | 5.72 | 1.60 | 1.51 |
| 1 | 198-A | 118 | GLU | CB-CG | 5.71 | 1.62 | 1.52 |
| 1 | 22-A | 85 | CYS | CB-SG | -5.71 | 1.72 | 1.81 |
| 1 | 149-A | 134 | GLU | CG-CD | -5.70 | 1.43 | 1.51 |
| 1 | 31-A | 157 | GLU | CB-CG | 5.70 | 1.62 | 1.52 |
| 1 | 86-A | 24 | LEU | CG-CD1 | -5.69 | 1.30 | 1.51 |
| 1 | 224-A | 21 | PRO | CB-CG | 5.69 | 1.78 | 1.50 |
| 1 | 238-A | 118 | GLU | CG-CD | 5.69 | 1.60 | 1.51 |
| 1 | 73-A | 157 | GLU | CG-CD | 5.69 | 1.60 | 1.51 |
| 1 | 103-A | 101 | GLU | CD-OE2 | -5.69 | 1.19 | 1.25 |
| 1 | 168-A | 52 | ARG | CB-CG | 5.69 | 1.68 | 1.52 |
| 1 | 210-A | 118 | GLU | CB-CG | 5.68 | 1.62 | 1.52 |
| 1 | 35-A | 157 | GLU | CB-CG | 5.67 | 1.62 | 1.52 |
| 1 | 133-A | 142 | ASP | CB-CG | 5.67 | 1.63 | 1.51 |
| 1 | 208-A | 118 | GLU | CG-CD | 5.66 | 1.60 | 1.51 |
| 1 | 7-A | 20 | MET | CG-SD | 5.66 | 1.95 | 1.81 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 9-A | 139 | GLU | CB-CG | -5.65 | 1.41 | 1.52 |
| 1 | 125-A | 20 | MET | CB-CG | 5.65 | 1.69 | 1.51 |
| 1 | 57-A | 118 | GLU | CB-CG | 5.64 | 1.62 | 1.52 |
| 1 | 124-A | 87 | ASP | CB-CG | 5.64 | 1.63 | 1.51 |
| 1 | 88-A | 108 | GLN | CB-CG | 5.64 | 1.67 | 1.52 |
| 1 | 140-A | 119 | VAL | CB-CG2 | -5.63 | 1.41 | 1.52 |
| 1 | 112-A | 120 | GLU | CB-CG | 5.62 | 1.62 | 1.52 |
| 1 | 157-A | 138 | SER | CA-CB | 5.62 | 1.61 | 1.52 |
| 1 | 81-A | 24 | LEU | CG-CD1 | -5.61 | 1.31 | 1.51 |
| 1 | 126-A | 118 | GLU | CG-CD | 5.61 | 1.60 | 1.51 |
| 1 | 145-A | 18 | ASN | CB-CG | -5.61 | 1.38 | 1.51 |
| 1 | 210-A | 154 | GLU | CG-CD | 5.61 | 1.60 | 1.51 |
| 1 | 170-A | 20 | MET | CG-SD | 5.61 | 1.95 | 1.81 |
| 1 | 61-A | 44 | ARG | CB-CG | 5.60 | 1.67 | 1.52 |
| 1 | 66-A | 20 | MET | CA-CB | 5.60 | 1.66 | 1.53 |
| 1 | 143-A | 20 | MET | CA-CB | 5.60 | 1.66 | 1.53 |
| 1 | 82-A | 118 | GLU | CG-CD | 5.60 | 1.60 | 1.51 |
| 1 | 207-A | 4 | LEU | CG-CD1 | -5.60 | 1.31 | 1.51 |
| 1 | 236-A | 118 | GLU | CB-CG | 5.60 | 1.62 | 1.52 |
| 1 | 125-A | 48 | GLU | CB-CG | 5.59 | 1.62 | 1.52 |
| 1 | 65-A | 19 | ALA | C-O | 5.59 | 1.33 | 1.23 |
| 1 | 51-A | 101 | GLU | CB-CG | -5.58 | 1.41 | 1.52 |
| 1 | 212-A | 33 | ARG | CB-CG | 5.58 | 1.67 | 1.52 |
| 1 | 43-A | 119 | VAL | CB-CG1 | -5.58 | 1.41 | 1.52 |
| 1 | 108-A | 106 | LYS | CB-CG | 5.58 | 1.67 | 1.52 |
| 1 | 59-A | 44 | ARG | CG-CD | 5.57 | 1.65 | 1.51 |
| 1 | 194-A | 108 | GLN | CB-CG | 5.57 | 1.67 | 1.52 |
| 1 | 56-A | 20 | MET | CB-CG | 5.57 | 1.69 | 1.51 |
| 1 | 143-A | 119 | VAL | CB-CG2 | -5.56 | 1.41 | 1.52 |
| 1 | 213-A | 157 | GLU | CB-CG | 5.56 | 1.62 | 1.52 |
| 1 | 156-A | 118 | GLU | CB-CG | 5.55 | 1.62 | 1.52 |
| 1 | 168-A | 85 | CYS | CB-SG | -5.55 | 1.72 | 1.81 |
| 1 | 60-A | 108 | GLN | CG-CD | 5.55 | 1.63 | 1.51 |
| 1 | 185-A | 152 | CYS | CB-SG | 5.55 | 1.91 | 1.82 |
| 1 | 39-A | 139 | GLU | CD-OE2 | 5.54 | 1.31 | 1.25 |
| 1 | 79-A | 33 | ARG | CB-CG | 5.54 | 1.67 | 1.52 |
| 1 | 143-A | 101 | GLU | CD-OE2 | 5.53 | 1.31 | 1.25 |
| 1 | 159-A | 101 | GLU | CG-CD | 5.53 | 1.60 | 1.51 |
| 1 | 233-A | 79 | ASP | CB-CG | 5.53 | 1.63 | 1.51 |
| 1 | 126-A | 9 | ALA | CA-CB | -5.52 | 1.40 | 1.52 |
| 1 | 238-A | 120 | GLU | CB-CG | 5.52 | 1.62 | 1.52 |
| 1 | 186-A | 17 | GLU | CG-CD | 5.51 | 1.60 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 31-A | 33 | ARG | CB-CG | -5.51 | 1.37 | 1.52 |
| 1 | 162-A | 139 | GLU | CG-CD | 5.50 | 1.60 | 1.51 |
| 1 | 91-A | 16 | MET | CG-SD | 5.50 | 1.95 | 1.81 |
| 1 | 40-A | 154 | GLU | CB-CG | 5.49 | 1.62 | 1.52 |
| 1 | 203-A | 101 | GLU | CG-CD | 5.49 | 1.60 | 1.51 |
| 1 | 232-A | 152 | CYS | CB-SG | 5.49 | 1.91 | 1.82 |
| 1 | 94-A | 119 | VAL | CB-CG1 | -5.49 | 1.41 | 1.52 |
| 1 | 20-A | 101 | GLU | CG-CD | 5.49 | 1.60 | 1.51 |
| 1 | 102-A | 157 | GLU | CG-CD | 5.48 | 1.60 | 1.51 |
| 1 | 174-A | 152 | CYS | CB-SG | 5.48 | 1.91 | 1.82 |
| 1 | 221-A | 152 | CYS | CA-CB | 5.48 | 1.66 | 1.53 |
| 1 | 176-A | 154 | GLU | CB-CG | -5.47 | 1.41 | 1.52 |
| 1 | 80-A | 48 | GLU | CB-CG | 5.47 | 1.62 | 1.52 |
| 1 | 85-A | 20 | MET | CB-CG | 5.47 | 1.68 | 1.51 |
| 1 | 46-A | 1 | MET | CB-CG | 5.46 | 1.68 | 1.51 |
| 1 | 155-A | 120 | GLU | CG-CD | 5.45 | 1.60 | 1.51 |
| 1 | 26-A | 44 | ARG | CB-CG | -5.45 | 1.37 | 1.52 |
| 1 | 211-A | 101 | GLU | CG-CD | 5.45 | 1.60 | 1.51 |
| 1 | 77-A | 48 | GLU | CG-CD | 5.45 | 1.60 | 1.51 |
| 1 | 86-A | 108 | GLN | CG-CD | 5.45 | 1.63 | 1.51 |
| 1 | 96-A | 138 | SER | CA-CB | 5.45 | 1.61 | 1.52 |
| 1 | 126-A | 118 | GLU | CD-OE2 | 5.45 | 1.31 | 1.25 |
| 1 | 203-A | 152 | CYS | CA-CB | 5.45 | 1.66 | 1.53 |
| 1 | 71-A | 20 | MET | CB-CG | 5.45 | 1.68 | 1.51 |
| 1 | 35-A | 157 | GLU | CD-OE2 | -5.44 | 1.19 | 1.25 |
| 1 | 60-A | 48 | GLU | CG-CD | 5.44 | 1.60 | 1.51 |
| 1 | 219-A | 154 | GLU | CB-CG | 5.44 | 1.62 | 1.52 |
| 1 | 40-A | 4 | LEU | CG-CD2 | -5.44 | 1.31 | 1.51 |
| 1 | 18-A | 49 | SER | CA-CB | 5.44 | 1.61 | 1.52 |
| 1 | 32-A | 85 | CYS | CB-SG | -5.44 | 1.73 | 1.81 |
| 1 | 247-A | 157 | GLU | CB-CG | 5.43 | 1.62 | 1.52 |
| 1 | 59-A | 120 | GLU | CB-CG | 5.43 | 1.62 | 1.52 |
| 1 | 221-A | 157 | GLU | CB-CG | 5.42 | 1.62 | 1.52 |
| 1 | 83-A | 33 | ARG | CB-CG | 5.42 | 1.67 | 1.52 |
| 1 | 163-A | 106 | LYS | CG-CD | -5.42 | 1.34 | 1.52 |
| 1 | 3-A | 52 | ARG | CG-CD | -5.41 | 1.38 | 1.51 |
| 1 | 101-A | 107 | ALA | CA-CB | -5.41 | 1.41 | 1.52 |
| 1 | 218-A | 154 | GLU | CG-CD | 5.41 | 1.60 | 1.51 |
| 1 | 1-A | 119 | VAL | CB-CG2 | -5.41 | 1.41 | 1.52 |
| 1 | 9-A | 120 | GLU | CB-CG | 5.41 | 1.62 | 1.52 |
| 1 | 88-A | 157 | GLU | CG-CD | 5.40 | 1.60 | 1.51 |
| 1 | 239-A | 108 | GLN | CB-CG | 5.40 | 1.67 | 1.52 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1 | 79-A | 128 | TYR | CD1-CE1 | 5.40 | 1.47 | 1.39 |
| 1 | 146-A | 118 | GLU | CB-CG | 5.40 | 1.62 | 1.52 |
| 1 | 42-A | 120 | GLU | CG-CD | 5.40 | 1.60 | 1.51 |
| 1 | 139-A | 102 | GLN | CG-CD | -5.40 | 1.38 | 1.51 |
| 1 | 206-A | 79 | ASP | CB-CG | 5.40 | 1.63 | 1.51 |
| 1 | 245-A | 107 | ALA | CA-CB | -5.39 | 1.41 | 1.52 |
| 1 | 60-A | 118 | GLU | CB-CG | 5.39 | 1.62 | 1.52 |
| 1 | 26-A | 154 | GLU | CB-CG | 5.38 | 1.62 | 1.52 |
| 1 | 114-A | 157 | GLU | CB-CG | 5.38 | 1.62 | 1.52 |
| 1 | 67-A | 119 | VAL | CB-CG1 | 5.37 | 1.64 | 1.52 |
| 1 | 60-A | 108 | GLN | CB-CG | 5.37 | 1.67 | 1.52 |
| 1 | 136-A | 20 | MET | CB-CG | 5.37 | 1.68 | 1.51 |
| 1 | 61-A | 48 | GLU | CG-CD | 5.37 | 1.59 | 1.51 |
| 1 | 222-A | 119 | VAL | CB-CG2 | -5.37 | 1.41 | 1.52 |
| 1 | 155-A | 120 | GLU | CD-OE2 | 5.36 | 1.31 | 1.25 |
| 1 | 88-A | 48 | GLU | CB-CG | 5.36 | 1.62 | 1.52 |
| 1 | 221-A | 20 | MET | CG-SD | 5.35 | 1.95 | 1.81 |
| 1 | 90-A | 52 | ARG | CG-CD | 5.34 | 1.65 | 1.51 |
| 1 | 125-A | 157 | GLU | CD-OE2 | 5.34 | 1.31 | 1.25 |
| 1 | 216-A | 120 | GLU | CG-CD | 5.34 | 1.59 | 1.51 |
| 1 | 229-A | 76 | LYS | CD-CE | 5.34 | 1.64 | 1.51 |
| 1 | 240-A | 1 | MET | N-CA | 5.34 | 1.57 | 1.46 |
| 1 | 234-A | 1 | MET | N-CA | 5.33 | 1.57 | 1.46 |
| 1 | 173-A | 139 | GLU | CB-CG | -5.32 | 1.42 | 1.52 |
| 1 | 223-A | 87 | ASP | CB-CG | 5.32 | 1.62 | 1.51 |
| 1 | 8-A | 159 | ARG | CG-CD | -5.32 | 1.38 | 1.51 |
| 1 | 34-A | 159 | ARG | CG-CD | 5.32 | 1.65 | 1.51 |
| 1 | 111-A | 108 | GLN | CB-CG | -5.32 | 1.38 | 1.52 |
| 1 | 15-A | 120 | GLU | CG-CD | 5.31 | 1.59 | 1.51 |
| 1 | 29-A | 44 | ARG | CG-CD | 5.31 | 1.65 | 1.51 |
| 1 | 74-A | 76 | LYS | CD-CE | 5.31 | 1.64 | 1.51 |
| 1 | 12-A | 157 | GLU | CB-CG | 5.30 | 1.62 | 1.52 |
| 1 | 102-A | 1 | MET | CG-SD | 5.30 | 1.95 | 1.81 |
| 1 | 125-A | 33 | ARG | CG-CD | 5.30 | 1.65 | 1.51 |
| 1 | 51-A | 17 | GLU | CG-CD | 5.30 | 1.59 | 1.51 |
| 1 | 216-A | 49 | SER | CA-CB | 5.30 | 1.60 | 1.52 |
| 1 | 10-A | 20 | MET | CG-SD | -5.30 | 1.67 | 1.81 |
| 1 | 103-A | 154 | GLU | CD-OE2 | -5.29 | 1.19 | 1.25 |
| 1 | 113-A | 157 | GLU | CB-CG | 5.29 | 1.62 | 1.52 |
| 1 | 156-A | 98 | ARG | CB-CG | -5.29 | 1.38 | 1.52 |
| 1 | 174-A | 154 | GLU | CB-CG | 5.29 | 1.62 | 1.52 |
| 1 | 140-A | 20 | MET | CB-CG | -5.28 | 1.34 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 122-A | 76 | LYS | CD-CE | 5.27 | 1.64 | 1.51 |
| 1 | 85-A | 108 | GLN | CG-CD | 5.27 | 1.63 | 1.51 |
| 1 | 57-A | 159 | ARG | CG-CD | 5.27 | 1.65 | 1.51 |
| 1 | 125-A | 20 | MET | CG-SD | 5.26 | 1.94 | 1.81 |
| 1 | 95-A | 120 | GLU | CG-CD | 5.26 | 1.59 | 1.51 |
| 1 | 19-A | 157 | GLU | CG-CD | 5.26 | 1.59 | 1.51 |
| 1 | 148-A | 2 | ILE | CA-CB | 5.25 | 1.67 | 1.54 |
| 1 | 75-A | 76 | LYS | CE-NZ | 5.25 | 1.62 | 1.49 |
| 1 | 24-A | 157 | GLU | CG-CD | 5.24 | 1.59 | 1.51 |
| 1 | 76-A | 48 | GLU | CB-CG | 5.24 | 1.62 | 1.52 |
| 1 | 140-A | 16 | MET | CG-SD | 5.24 | 1.94 | 1.81 |
| 1 | 128-A | 118 | GLU | CG-CD | 5.24 | 1.59 | 1.51 |
| 1 | 228-A | 101 | GLU | CG-CD | -5.24 | 1.44 | 1.51 |
| 1 | 179-A | 17 | GLU | CB-CG | 5.23 | 1.62 | 1.52 |
| 1 | 227-A | 1 | MET | CB-CG | 5.23 | 1.68 | 1.51 |
| 1 | 52-A | 52 | ARG | CG-CD | 5.22 | 1.65 | 1.51 |
| 1 | 117-A | 101 | GLU | CG-CD | 5.22 | 1.59 | 1.51 |
| 1 | 97-A | 154 | GLU | CG-CD | 5.22 | 1.59 | 1.51 |
| 1 | 20-A | 134 | GLU | CB-CG | 5.22 | 1.62 | 1.52 |
| 1 | 122-A | 48 | GLU | CB-CG | 5.22 | 1.62 | 1.52 |
| 1 | 151-A | 159 | ARG | CG-CD | 5.22 | 1.65 | 1.51 |
| 1 | 126-A | 22 | TRP | CB-CG | 5.22 | 1.59 | 1.50 |
| 1 | 182-A | 101 | GLU | CG-CD | 5.20 | 1.59 | 1.51 |
| 1 | 79-A | 33 | ARG | CG-CD | 5.20 | 1.65 | 1.51 |
| 1 | 172-A | 132 | ASP | CB-CG | 5.18 | 1.62 | 1.51 |
| 1 | 215-A | 108 | GLN | CB-CG | 5.18 | 1.66 | 1.52 |
| 1 | 212-A | 20 | MET | CB-CG | 5.18 | 1.68 | 1.51 |
| 1 | 125-A | 33 | ARG | CB-CG | 5.17 | 1.66 | 1.52 |
| 1 | 40-A | 17 | GLU | CG-CD | 5.17 | 1.59 | 1.51 |
| 1 | 118-A | 127 | ASP | CB-CG | 5.17 | 1.62 | 1.51 |
| 1 | 211-A | 152 | CYS | CA-CB | 5.16 | 1.65 | 1.53 |
| 1 | 222-A | 85 | CYS | CB-SG | -5.16 | 1.73 | 1.81 |
| 1 | 69-A | 1 | MET | CG-SD | 5.16 | 1.94 | 1.81 |
| 1 | 38-A | 118 | GLU | CB-CG | 5.16 | 1.61 | 1.52 |
| 1 | 199-A | 159 | ARG | CG-CD | 5.16 | 1.64 | 1.51 |
| 1 | 70-A | 134 | GLU | CG-CD | 5.15 | 1.59 | 1.51 |
| 1 | 112-A | 101 | GLU | CD-OE1 | 5.15 | 1.31 | 1.25 |
| 1 | 201-A | 139 | GLU | CB-CG | -5.14 | 1.42 | 1.52 |
| 1 | 129-A | 22 | TRP | CB-CG | 5.14 | 1.59 | 1.50 |
| 1 | 220-A | 85 | CYS | CB-SG | -5.13 | 1.73 | 1.81 |
| 1 | 163-A | 101 | GLU | CG-CD | -5.13 | 1.44 | 1.51 |
| 1 | 233-A | 23 | ASN | CB-CG | 5.12 | 1.62 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1 | 164-A | 65 | GLN | CG-CD | 5.12 | 1.62 | 1.51 |
| 1 | 49-A | 154 | GLU | CB-CG | 5.12 | 1.61 | 1.52 |
| 1 | 143-A | 16 | MET | CB-CG | -5.12 | 1.34 | 1.51 |
| 1 | 244-A | 4 | LEU | CG-CD2 | -5.12 | 1.32 | 1.51 |
| 1 | 18-A | 1 | MET | CB-CG | 5.11 | 1.67 | 1.51 |
| 1 | 223-A | 16 | MET | CG-SD | 5.11 | 1.94 | 1.81 |
| 1 | 24-A | 120 | GLU | CD-OE2 | 5.11 | 1.31 | 1.25 |
| 1 | 97-A | 119 | VAL | CB-CG1 | 5.11 | 1.63 | 1.52 |
| 1 | 220-A | 154 | GLU | CG-CD | 5.11 | 1.59 | 1.51 |
| 1 | 221-A | 19 | ALA | C-O | 5.11 | 1.33 | 1.23 |
| 1 | 97-A | 154 | GLU | CB-CG | 5.10 | 1.61 | 1.52 |
| 1 | 84-A | 33 | ARG | CG-CD | 5.10 | 1.64 | 1.51 |
| 1 | 107-A | 120 | GLU | CB-CG | 5.10 | 1.61 | 1.52 |
| 1 | 123-A | 128 | TYR | CB-CG | 5.10 | 1.59 | 1.51 |
| 1 | 36-A | 157 | GLU | CG-CD | 5.09 | 1.59 | 1.51 |
| 1 | 244-A | 132 | ASP | CB-CG | 5.08 | 1.62 | 1.51 |
| 1 | 56-A | 119 | VAL | CB-CG2 | 5.08 | 1.63 | 1.52 |
| 1 | 131-A | 16 | MET | CB-CG | 5.08 | 1.67 | 1.51 |
| 1 | 72-A | 118 | GLU | CG-CD | 5.08 | 1.59 | 1.51 |
| 1 | 79-A | 157 | GLU | CD-OE1 | 5.07 | 1.31 | 1.25 |
| 1 | 214-A | 20 | MET | N-CA | 5.07 | 1.56 | 1.46 |
| 1 | 188-A | 101 | GLU | CG-CD | 5.07 | 1.59 | 1.51 |
| 1 | 97-A | 101 | GLU | CG-CD | 5.07 | 1.59 | 1.51 |
| 1 | 219-A | 154 | GLU | CG-CD | 5.06 | 1.59 | 1.51 |
| 1 | 216-A | 1 | MET | CA-C | 5.05 | 1.66 | 1.52 |
| 1 | 60-A | 159 | ARG | CB-CG | 5.05 | 1.66 | 1.52 |
| 1 | 75-A | 157 | GLU | CB-CG | -5.04 | 1.42 | 1.52 |
| 1 | 231-A | 76 | LYS | CB-CG | -5.04 | 1.39 | 1.52 |
| 1 | 244-A | 159 | ARG | CA-CB | -5.04 | 1.42 | 1.53 |
| 1 | 168-A | 52 | ARG | CG-CD | 5.03 | 1.64 | 1.51 |
| 1 | 127-A | 118 | GLU | CD-OE2 | 5.02 | 1.31 | 1.25 |
| 1 | 3-A | 118 | GLU | CB-CG | 5.02 | 1.61 | 1.52 |
| 1 | 188-A | 79 | ASP | CB-CG | 5.02 | 1.62 | 1.51 |
| 1 | 38-A | 120 | GLU | CD-OE1 | 5.01 | 1.31 | 1.25 |

All (1403) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | 69-A | 44 | ARG | NE-CZ-NH2 | -22.77 | 108.92 | 120.30 |
| 1 | 24-A | 44 | ARG | NE-CZ-NH2 | -21.25 | 109.67 | 120.30 |
| 1 | 46-A | 44 | ARG | NE-CZ-NH2 | -21.14 | 109.73 | 120.30 |
| 1 | 24-A | 44 | ARG | NE-CZ-NH1 | 19.11 | 129.85 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | 56-A | 44 | ARG | NE-CZ-NH2 | -17.13 | 111.74 | 120.30 |
| 1 | 131-A | 16 | MET | CG-SD-CE | 16.87 | 127.19 | 100.20 |
| 1 | 221-A | 152 | CYS | CA-CB-SG | 16.81 | 144.26 | 114.00 |
| 1 | 145-A | 20 | MET | C-N-CD | -16.73 | 83.79 | 120.60 |
| 1 | 211-A | 152 | CYS | CA-CB-SG | 16.25 | 143.26 | 114.00 |
| 1 | 1-A | 98 | ARG | NE-CZ-NH2 | -16.25 | 112.17 | 120.30 |
| 1 | 210-A | 52 | ARG | NE-CZ-NH1 | 16.16 | 128.38 | 120.30 |
| 1 | 195-A | 52 | ARG | NE-CZ-NH1 | 15.71 | 128.16 | 120.30 |
| 1 | 57-A | 44 | ARG | NE-CZ-NH2 | -15.51 | 112.54 | 120.30 |
| 1 | 103-A | 20 | MET | CG-SD-CE | -15.28 | 75.75 | 100.20 |
| 1 | 222-A | 152 | CYS | CA-CB-SG | 15.16 | 141.29 | 114.00 |
| 1 | 210-A | 52 | ARG | NE-CZ-NH2 | -14.85 | 112.88 | 120.30 |
| 1 | 217-A | 159 | ARG | NE-CZ-NH2 | -14.26 | 113.17 | 120.30 |
| 1 | 68-A | 159 | ARG | NE-CZ-NH2 | -14.25 | 113.17 | 120.30 |
| 1 | 26-A | 44 | ARG | NE-CZ-NH2 | -14.17 | 113.21 | 120.30 |
| 1 | 204-A | 152 | CYS | CA-CB-SG | 14.06 | 139.31 | 114.00 |
| 1 | 227-A | 152 | CYS | CA-CB-SG | -13.70 | 89.34 | 114.00 |
| 1 | 143-A | 20 | MET | C-N-CD | -13.70 | 90.47 | 120.60 |
| 1 | 231-A | 152 | CYS | CA-CB-SG | 13.65 | 138.57 | 114.00 |
| 1 | 45-A | 44 | ARG | NE-CZ-NH2 | -13.27 | 113.66 | 120.30 |
| 1 | 68-A | 159 | ARG | NE-CZ-NH1 | 13.25 | 126.92 | 120.30 |
| 1 | 1-A | 98 | ARG | NE-CZ-NH1 | 13.18 | 126.89 | 120.30 |
| 1 | 192-A | 152 | CYS | CA-CB-SG | 13.14 | 137.66 | 114.00 |
| 1 | 185-A | 52 | ARG | NE-CZ-NH1 | 13.13 | 126.86 | 120.30 |
| 1 | 205-A | 152 | CYS | CA-CB-SG | -13.02 | 90.57 | 114.00 |
| 1 | 78-A | 159 | ARG | NE-CZ-NH2 | -13.01 | 113.80 | 120.30 |
| 1 | 45-A | 44 | ARG | NE-CZ-NH1 | 12.78 | 126.69 | 120.30 |
| 1 | 249-A | 33 | ARG | NE-CZ-NH1 | 12.73 | 126.67 | 120.30 |
| 1 | 150-A | 159 | ARG | NE-CZ-NH1 | 12.72 | 126.66 | 120.30 |
| 1 | 35-A | 52 | ARG | NE-CZ-NH2 | -12.58 | 114.01 | 120.30 |
| 1 | 206-A | 152 | CYS | CA-CB-SG | -12.54 | 91.43 | 114.00 |
| 1 | 57-A | 44 | ARG | NE-CZ-NH1 | 12.37 | 126.48 | 120.30 |
| 1 | 178-A | 52 | ARG | NE-CZ-NH2 | -11.90 | 114.35 | 120.30 |
| 1 | 205-A | 16 | MET | CG-SD-CE | 11.88 | 119.21 | 100.20 |
| 1 | 164-A | 52 | ARG | NE-CZ-NH2 | -11.83 | 114.39 | 120.30 |
| 1 | 101-A | 33 | ARG | NE-CZ-NH1 | 11.70 | 126.15 | 120.30 |
| 1 | 69-A | 1 | MET | CG-SD-CE | 11.63 | 118.81 | 100.20 |
| 1 | 193-A | 152 | CYS | CA-CB-SG | -11.51 | 93.28 | 114.00 |
| 1 | 78-A | 159 | ARG | NE-CZ-NH1 | 11.46 | 126.03 | 120.30 |
| 1 | 84-A | 159 | ARG | NE-CZ-NH2 | 11.39 | 125.99 | 120.30 |
| 1 | 166-A | 52 | ARG | NE-CZ-NH1 | 11.36 | 125.98 | 120.30 |
| 1 | 165-A | 52 | ARG | NE-CZ-NH1 | 11.35 | 125.97 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|--------|-------------|----------|
| 1 | 234-A | 152 | CYS | CA-CB-SG | -11.30 | 93.66 | 114.00 |
| 1 | 14-A | 1 | MET | CG-SD-CE | 11.27 | 118.23 | 100.20 |
| 1 | 121-A | 159 | ARG | NE-CZ-NH2 | -11.26 | 114.67 | 120.30 |
| 1 | 22-A | 44 | ARG | NE-CZ-NH2 | -11.24 | 114.68 | 120.30 |
| 1 | 229-A | 1 | MET | CG-SD-CE | 11.23 | 118.17 | 100.20 |
| 1 | 195-A | 18 | ASN | CB-CA-C | -11.20 | 88.00 | 110.40 |
| 1 | 218-A | 159 | ARG | NE-CZ-NH1 | -11.19 | 114.71 | 120.30 |
| 1 | 181-A | 52 | ARG | NE-CZ-NH1 | 11.17 | 125.88 | 120.30 |
| 1 | 31-A | 33 | ARG | NE-CZ-NH1 | 11.14 | 125.87 | 120.30 |
| 1 | 9-A | 79 | ASP | CB-CG-OD2 | 11.11 | 128.30 | 118.30 |
| 1 | 175-A | 152 | CYS | CA-CB-SG | -11.07 | 94.07 | 114.00 |
| 1 | 230-A | 159 | ARG | NE-CZ-NH1 | -11.06 | 114.77 | 120.30 |
| 1 | 112-A | 36 | LEU | CA-CB-CG | 10.99 | 140.58 | 115.30 |
| 1 | 190-A | 79 | ASP | CB-CG-OD2 | 10.99 | 128.19 | 118.30 |
| 1 | 72-A | 159 | ARG | NE-CZ-NH1 | 10.96 | 125.78 | 120.30 |
| 1 | 23-A | 52 | ARG | NE-CZ-NH1 | 10.96 | 125.78 | 120.30 |
| 1 | 46-A | 44 | ARG | NE-CZ-NH1 | 10.94 | 125.77 | 120.30 |
| 1 | 230-A | 159 | ARG | NE-CZ-NH2 | 10.93 | 125.77 | 120.30 |
| 1 | 75-A | 159 | ARG | NE-CZ-NH1 | 10.91 | 125.75 | 120.30 |
| 1 | 230-A | 152 | CYS | CA-CB-SG | 10.86 | 133.55 | 114.00 |
| 1 | 187-A | 159 | ARG | NE-CZ-NH1 | 10.82 | 125.71 | 120.30 |
| 1 | 195-A | 52 | ARG | NE-CZ-NH2 | -10.80 | 114.90 | 120.30 |
| 1 | 61-A | 20 | MET | CG-SD-CE | -10.78 | 82.95 | 100.20 |
| 1 | 75-A | 159 | ARG | NE-CZ-NH2 | -10.78 | 114.91 | 120.30 |
| 1 | 82-A | 16 | MET | CG-SD-CE | 10.72 | 117.35 | 100.20 |
| 1 | 222-A | 159 | ARG | NE-CZ-NH2 | -10.68 | 114.96 | 120.30 |
| 1 | 146-A | 2 | ILE | CB-CA-C | -10.51 | 90.57 | 111.60 |
| 1 | 212-A | 152 | CYS | CA-CB-SG | 10.51 | 132.92 | 114.00 |
| 1 | 193-A | 52 | ARG | NE-CZ-NH1 | 10.49 | 125.55 | 120.30 |
| 1 | 1-A | 119 | VAL | CB-CA-C | -10.46 | 91.52 | 111.40 |
| 1 | 76-A | 52 | ARG | NE-CZ-NH2 | -10.46 | 115.07 | 120.30 |
| 1 | 211-A | 20 | MET | C-N-CD | -10.43 | 97.65 | 120.60 |
| 1 | 160-A | 33 | ARG | NE-CZ-NH1 | 10.40 | 125.50 | 120.30 |
| 1 | 160-A | 33 | ARG | NE-CZ-NH2 | -10.40 | 115.10 | 120.30 |
| 1 | 224-A | 152 | CYS | CA-CB-SG | 10.39 | 132.70 | 114.00 |
| 1 | 224-A | 19 | ALA | N-CA-C | 10.37 | 138.99 | 111.00 |
| 1 | 84-A | 159 | ARG | NE-CZ-NH1 | -10.31 | 115.15 | 120.30 |
| 1 | 247-A | 159 | ARG | NE-CZ-NH2 | -10.29 | 115.15 | 120.30 |
| 1 | 125-A | 20 | MET | C-N-CD | -10.29 | 97.96 | 120.60 |
| 1 | 238-A | 159 | ARG | NE-CZ-NH1 | 10.28 | 125.44 | 120.30 |
| 1 | 9-A | 79 | ASP | CB-CG-OD1 | -10.27 | 109.06 | 118.30 |
| 1 | 132-A | 19 | ALA | N-CA-C | -10.17 | 83.54 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 67-A | 20 | MET | CG-SD-CE | 10.12 | 116.38 | 100.20 |
| 1 | 71-A | 159 | ARG | NE-CZ-NH1 | 10.09 | 125.35 | 120.30 |
| 1 | 144-A | 20 | MET | CA-CB-CG | 10.05 | 130.39 | 113.30 |
| 1 | 181-A | 159 | ARG | NE-CZ-NH1 | 10.04 | 125.32 | 120.30 |
| 1 | 171-A | 152 | CYS | CA-CB-SG | 10.03 | 132.05 | 114.00 |
| 1 | 83-A | 4 | LEU | CB-CG-CD2 | 10.01 | 128.01 | 111.00 |
| 1 | 178-A | 19 | ALA | N-CA-C | 9.89 | 137.72 | 111.00 |
| 1 | 234-A | 159 | ARG | NE-CZ-NH2 | -9.89 | 115.36 | 120.30 |
| 1 | 230-A | 1 | MET | CG-SD-CE | 9.85 | 115.95 | 100.20 |
| 1 | 185-A | 52 | ARG | NE-CZ-NH2 | -9.81 | 115.39 | 120.30 |
| 1 | 98-A | 159 | ARG | NE-CZ-NH2 | 9.79 | 125.20 | 120.30 |
| 1 | 164-A | 52 | ARG | NE-CZ-NH1 | 9.78 | 125.19 | 120.30 |
| 1 | 18-A | 132 | ASP | CB-CG-OD2 | 9.74 | 127.06 | 118.30 |
| 1 | 63-A | 52 | ARG | NE-CZ-NH2 | -9.73 | 115.43 | 120.30 |
| 1 | 57-A | 44 | ARG | CG-CD-NE | -9.68 | 91.47 | 111.80 |
| 1 | 69-A | 44 | ARG | NE-CZ-NH1 | 9.63 | 125.12 | 120.30 |
| 1 | 36-A | 52 | ARG | NE-CZ-NH1 | 9.59 | 125.10 | 120.30 |
| 1 | 156-A | 101 | GLU | OE1-CD-OE2 | 9.59 | 134.80 | 123.30 |
| 1 | 190-A | 79 | ASP | CB-CG-OD1 | -9.57 | 109.69 | 118.30 |
| 1 | 156-A | 1 | MET | CB-CG-SD | -9.56 | 83.72 | 112.40 |
| 1 | 51-A | 159 | ARG | NE-CZ-NH1 | 9.55 | 125.08 | 120.30 |
| 1 | 82-A | 52 | ARG | NE-CZ-NH2 | -9.54 | 115.53 | 120.30 |
| 1 | 178-A | 152 | CYS | CA-CB-SG | -9.53 | 96.85 | 114.00 |
| 1 | 11-A | 52 | ARG | NE-CZ-NH1 | 9.52 | 125.06 | 120.30 |
| 1 | 91-A | 16 | MET | CA-CB-CG | 9.51 | 129.47 | 113.30 |
| 1 | 203-A | 152 | CYS | CA-CB-SG | 9.51 | 131.12 | 114.00 |
| 1 | 33-A | 159 | ARG | NE-CZ-NH1 | 9.49 | 125.05 | 120.30 |
| 1 | 11-A | 52 | ARG | NE-CZ-NH2 | -9.49 | 115.56 | 120.30 |
| 1 | 217-A | 159 | ARG | NE-CZ-NH1 | 9.48 | 125.04 | 120.30 |
| 1 | 212-A | 159 | ARG | NE-CZ-NH2 | -9.48 | 115.56 | 120.30 |
| 1 | 183-A | 52 | ARG | NE-CZ-NH1 | 9.47 | 125.04 | 120.30 |
| 1 | 247-A | 159 | ARG | NE-CZ-NH1 | 9.44 | 125.02 | 120.30 |
| 1 | 91-A | 24 | LEU | CB-CG-CD2 | 9.39 | 126.96 | 111.00 |
| 1 | 124-A | 16 | MET | CA-CB-CG | 9.36 | 129.20 | 113.30 |
| 1 | 145-A | 20 | MET | CA-CB-CG | 9.34 | 129.18 | 113.30 |
| 1 | 84-A | 16 | MET | CB-CG-SD | -9.33 | 84.41 | 112.40 |
| 1 | 194-A | 152 | CYS | CA-CB-SG | 9.33 | 130.79 | 114.00 |
| 1 | 124-A | 52 | ARG | NE-CZ-NH2 | -9.32 | 115.64 | 120.30 |
| 1 | 25-A | 44 | ARG | NE-CZ-NH2 | -9.30 | 115.65 | 120.30 |
| 1 | 161-A | 52 | ARG | NE-CZ-NH2 | -9.30 | 115.65 | 120.30 |
| 1 | 186-A | 52 | ARG | NE-CZ-NH1 | 9.29 | 124.94 | 120.30 |
| 1 | 167-A | 142 | ASP | CB-CG-OD1 | -9.29 | 109.94 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 248-A | 159 | ARG | NE-CZ-NH2 | -9.29 | 115.66 | 120.30 |
| 1 | 232-A | 152 | CYS | CA-CB-SG | 9.28 | 130.70 | 114.00 |
| 1 | 100-A | 20 | MET | CG-SD-CE | 9.27 | 115.03 | 100.20 |
| 1 | 233-A | 152 | CYS | CA-CB-SG | 9.26 | 130.66 | 114.00 |
| 1 | 52-A | 20 | MET | CG-SD-CE | 9.25 | 115.00 | 100.20 |
| 1 | 125-A | 20 | MET | CB-CG-SD | 9.23 | 140.08 | 112.40 |
| 1 | 36-A | 52 | ARG | NE-CZ-NH2 | -9.22 | 115.69 | 120.30 |
| 1 | 75-A | 16 | MET | CG-SD-CE | 9.20 | 114.92 | 100.20 |
| 1 | 143-A | 20 | MET | CA-CB-CG | 9.20 | 128.94 | 113.30 |
| 1 | 8-A | 79 | ASP | CB-CG-OD2 | 9.19 | 126.57 | 118.30 |
| 1 | 89-A | 20 | MET | CG-SD-CE | -9.18 | 85.52 | 100.20 |
| 1 | 138-A | 159 | ARG | NE-CZ-NH2 | -9.16 | 115.72 | 120.30 |
| 1 | 131-A | 20 | MET | CG-SD-CE | -9.13 | 85.59 | 100.20 |
| 1 | 142-A | 20 | MET | CA-CB-CG | 9.12 | 128.81 | 113.30 |
| 1 | 110-A | 149 | HIS | CB-CA-C | 9.11 | 128.62 | 110.40 |
| 1 | 119-A | 142 | ASP | CB-CG-OD1 | -9.11 | 110.10 | 118.30 |
| 1 | 181-A | 152 | CYS | CA-CB-SG | -9.06 | 97.68 | 114.00 |
| 1 | 238-A | 159 | ARG | NE-CZ-NH2 | -9.00 | 115.80 | 120.30 |
| 1 | 212-A | 159 | ARG | NE-CZ-NH1 | 8.96 | 124.78 | 120.30 |
| 1 | 247-A | 20 | MET | CG-SD-CE | -8.96 | 85.87 | 100.20 |
| 1 | 109-A | 16 | MET | CB-CG-SD | -8.94 | 85.59 | 112.40 |
| 1 | 52-A | 52 | ARG | NE-CZ-NH2 | -8.93 | 115.83 | 120.30 |
| 1 | 138-A | 159 | ARG | NE-CZ-NH1 | 8.93 | 124.76 | 120.30 |
| 1 | 64-A | 24 | LEU | CB-CG-CD2 | 8.91 | 126.14 | 111.00 |
| 1 | 9-A | 142 | ASP | CB-CG-OD2 | 8.90 | 126.31 | 118.30 |
| 1 | 101-A | 4 | LEU | CB-CG-CD1 | 8.89 | 126.11 | 111.00 |
| 1 | 108-A | 24 | LEU | CB-CG-CD1 | 8.88 | 126.10 | 111.00 |
| 1 | 108-A | 104 | LEU | CB-CG-CD2 | 8.87 | 126.09 | 111.00 |
| 1 | 233-A | 52 | ARG | NE-CZ-NH1 | 8.88 | 124.74 | 120.30 |
| 1 | 88-A | 16 | MET | CB-CG-SD | 8.87 | 139.02 | 112.40 |
| 1 | 220-A | 152 | CYS | CA-CB-SG | 8.84 | 129.91 | 114.00 |
| 1 | 197-A | 152 | CYS | CA-CB-SG | 8.84 | 129.91 | 114.00 |
| 1 | 69-A | 44 | ARG | CD-NE-CZ | 8.83 | 135.97 | 123.60 |
| 1 | 5-A | 20 | MET | CG-SD-CE | -8.82 | 86.09 | 100.20 |
| 1 | 238-A | 1 | MET | CG-SD-CE | 8.82 | 114.31 | 100.20 |
| 1 | 83-A | 24 | LEU | CB-CG-CD1 | 8.78 | 125.93 | 111.00 |
| 1 | 136-A | 159 | ARG | NE-CZ-NH1 | 8.77 | 124.69 | 120.30 |
| 1 | 108-A | 16 | MET | CG-SD-CE | -8.77 | 86.17 | 100.20 |
| 1 | 141-A | 16 | MET | CA-CB-CG | 8.76 | 128.19 | 113.30 |
| 1 | 204-A | 159 | ARG | NE-CZ-NH2 | -8.74 | 115.93 | 120.30 |
| 1 | 130-A | 20 | MET | CG-SD-CE | 8.73 | 114.16 | 100.20 |
| 1 | 93-A | 159 | ARG | NE-CZ-NH2 | 8.72 | 124.66 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 218-A | 159 | ARG | NE-CZ-NH2 | 8.71 | 124.65 | 120.30 |
| 1 | 164-A | 20 | MET | CG-SD-CE | -8.70 | 86.28 | 100.20 |
| 1 | 85-A | 24 | LEU | CB-CG-CD1 | 8.69 | 125.77 | 111.00 |
| 1 | 137-A | 52 | ARG | NE-CZ-NH2 | -8.66 | 115.97 | 120.30 |
| 1 | 38-A | 44 | ARG | NE-CZ-NH1 | 8.66 | 124.63 | 120.30 |
| 1 | 106-A | 20 | MET | CG-SD-CE | -8.60 | 86.44 | 100.20 |
| 1 | 29-A | 20 | MET | CA-CB-CG | 8.60 | 127.91 | 113.30 |
| 1 | 203-A | 159 | ARG | NE-CZ-NH2 | -8.59 | 116.01 | 120.30 |
| 1 | 56-A | 44 | ARG | NE-CZ-NH1 | 8.57 | 124.59 | 120.30 |
| 1 | 79-A | 159 | ARG | NE-CZ-NH2 | -8.57 | 116.02 | 120.30 |
| 1 | 24-A | 119 | VAL | CB-CA-C | -8.56 | 95.13 | 111.40 |
| 1 | 174-A | 152 | CYS | CA-CB-SG | 8.56 | 129.41 | 114.00 |
| 1 | 223-A | 152 | CYS | CA-CB-SG | 8.56 | 129.40 | 114.00 |
| 1 | 23-A | 52 | ARG | NE-CZ-NH2 | -8.54 | 116.03 | 120.30 |
| 1 | 149-A | 159 | ARG | NE-CZ-NH1 | 8.50 | 124.55 | 120.30 |
| 1 | 244-A | 1 | MET | CG-SD-CE | 8.48 | 113.77 | 100.20 |
| 1 | 53-A | 1 | MET | N-CA-C | -8.47 | 88.13 | 111.00 |
| 1 | 179-A | 52 | ARG | NE-CZ-NH2 | -8.44 | 116.08 | 120.30 |
| 1 | 145-A | 20 | MET | N-CA-CB | 8.42 | 125.76 | 110.60 |
| 1 | 105-A | 36 | LEU | CA-CB-CG | 8.42 | 134.66 | 115.30 |
| 1 | 121-A | 159 | ARG | NE-CZ-NH1 | 8.41 | 124.51 | 120.30 |
| 1 | 106-A | 87 | ASP | CB-CG-OD2 | 8.41 | 125.87 | 118.30 |
| 1 | 245-A | 1 | MET | CG-SD-CE | 8.39 | 113.62 | 100.20 |
| 1 | 78-A | 127 | ASP | CB-CG-OD1 | -8.38 | 110.75 | 118.30 |
| 1 | 75-A | 20 | MET | CG-SD-CE | 8.38 | 113.61 | 100.20 |
| 1 | 217-A | 16 | MET | CG-SD-CE | 8.37 | 113.60 | 100.20 |
| 1 | 94-A | 159 | ARG | NE-CZ-NH1 | 8.37 | 124.48 | 120.30 |
| 1 | 217-A | 12 | ARG | NE-CZ-NH2 | -8.36 | 116.12 | 120.30 |
| 1 | 19-A | 156 | LEU | CA-CB-CG | 8.35 | 134.49 | 115.30 |
| 1 | 232-A | 79 | ASP | CB-CG-OD1 | 8.35 | 125.81 | 118.30 |
| 1 | 103-A | 1 | MET | CG-SD-CE | 8.33 | 113.53 | 100.20 |
| 1 | 234-A | 159 | ARG | NE-CZ-NH1 | 8.33 | 124.46 | 120.30 |
| 1 | 150-A | 157 | GLU | OE1-CD-OE2 | -8.31 | 113.33 | 123.30 |
| 1 | 101-A | 33 | ARG | NE-CZ-NH2 | -8.30 | 116.15 | 120.30 |
| 1 | 234-A | 4 | LEU | CB-CG-CD1 | 8.30 | 125.11 | 111.00 |
| 1 | 162-A | 1 | MET | CG-SD-CE | 8.30 | 113.48 | 100.20 |
| 1 | 101-A | 20 | MET | N-CA-C | -8.28 | 88.65 | 111.00 |
| 1 | 67-A | 159 | ARG | NE-CZ-NH1 | 8.27 | 124.44 | 120.30 |
| 1 | 113-A | 36 | LEU | CA-CB-CG | 8.27 | 134.32 | 115.30 |
| 1 | 175-A | 20 | MET | N-CA-C | -8.26 | 88.70 | 111.00 |
| 1 | 81-A | 16 | MET | CG-SD-CE | -8.25 | 87.00 | 100.20 |
| 1 | 49-A | 52 | ARG | NE-CZ-NH1 | -8.24 | 116.18 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 193-A | 52 | ARG | NE-CZ-NH2 | -8.23 | 116.18 | 120.30 |
| 1 | 66-A | 20 | MET | CA-CB-CG | 8.22 | 127.27 | 113.30 |
| 1 | 120-A | 79 | ASP | CB-CG-OD2 | 8.21 | 125.69 | 118.30 |
| 1 | 174-A | 142 | ASP | CB-CG-OD2 | 8.19 | 125.67 | 118.30 |
| 1 | 185-A | 87 | ASP | CB-CG-OD2 | 8.18 | 125.66 | 118.30 |
| 1 | 237-A | 159 | ARG | NE-CZ-NH2 | -8.17 | 116.21 | 120.30 |
| 1 | 185-A | 152 | CYS | CA-CB-SG | 8.16 | 128.69 | 114.00 |
| 1 | 203-A | 159 | ARG | NE-CZ-NH1 | 8.16 | 124.38 | 120.30 |
| 1 | 136-A | 20 | MET | N-CA-CB | 8.14 | 125.26 | 110.60 |
| 1 | 225-A | 12 | ARG | NE-CZ-NH2 | -8.14 | 116.23 | 120.30 |
| 1 | 66-A | 19 | ALA | O-C-N | 8.12 | 135.69 | 122.70 |
| 1 | 214-A | 159 | ARG | NE-CZ-NH1 | 8.09 | 124.34 | 120.30 |
| 1 | 195-A | 52 | ARG | CD-NE-CZ | 8.08 | 134.91 | 123.60 |
| 1 | 66-A | 16 | MET | CB-CG-SD | 8.06 | 136.59 | 112.40 |
| 1 | 26-A | 44 | ARG | NE-CZ-NH1 | 8.06 | 124.33 | 120.30 |
| 1 | 172-A | 142 | ASP | CB-CG-OD2 | 8.05 | 125.55 | 118.30 |
| 1 | 131-A | 1 | MET | CG-SD-CE | 8.05 | 113.08 | 100.20 |
| 1 | 148-A | 28 | LEU | CB-CG-CD1 | 8.05 | 124.68 | 111.00 |
| 1 | 132-A | 20 | MET | CG-SD-CE | -8.05 | 87.32 | 100.20 |
| 1 | 63-A | 52 | ARG | NE-CZ-NH1 | 8.04 | 124.32 | 120.30 |
| 1 | 69-A | 44 | ARG | CG-CD-NE | -8.04 | 94.92 | 111.80 |
| 1 | 26-A | 52 | ARG | NE-CZ-NH1 | 8.04 | 124.32 | 120.30 |
| 1 | 178-A | 52 | ARG | NE-CZ-NH1 | 8.03 | 124.31 | 120.30 |
| 1 | 150-A | 19 | ALA | N-CA-C | 8.03 | 132.67 | 111.00 |
| 1 | 22-A | 52 | ARG | NE-CZ-NH2 | -8.02 | 116.29 | 120.30 |
| 1 | 84-A | 20 | MET | C-N-CD | -8.02 | 102.96 | 120.60 |
| 1 | 38-A | 44 | ARG | NE-CZ-NH2 | -8.02 | 116.29 | 120.30 |
| 1 | 35-A | 132 | ASP | CB-CG-OD2 | 8.01 | 125.51 | 118.30 |
| 1 | 121-A | 87 | ASP | CB-CG-OD1 | 7.98 | 125.49 | 118.30 |
| 1 | 166-A | 1 | MET | CB-CG-SD | -7.98 | 88.46 | 112.40 |
| 1 | 189-A | 52 | ARG | NE-CZ-NH1 | -7.98 | 116.31 | 120.30 |
| 1 | 110-A | 104 | LEU | CB-CG-CD2 | 7.98 | 124.56 | 111.00 |
| 1 | 67-A | 159 | ARG | NE-CZ-NH2 | -7.96 | 116.32 | 120.30 |
| 1 | 87-A | 20 | MET | CB-CG-SD | -7.96 | 88.51 | 112.40 |
| 1 | 47-A | 44 | ARG | CG-CD-NE | 7.93 | 128.46 | 111.80 |
| 1 | 127-A | 20 | MET | CG-SD-CE | 7.93 | 112.89 | 100.20 |
| 1 | 100-A | 104 | LEU | CB-CG-CD2 | 7.93 | 124.48 | 111.00 |
| 1 | 14-A | 18 | ASN | CB-CA-C | 7.92 | 126.24 | 110.40 |
| 1 | 31-A | 33 | ARG | NE-CZ-NH2 | -7.92 | 116.34 | 120.30 |
| 1 | 56-A | 44 | ARG | CG-CD-NE | -7.91 | 95.19 | 111.80 |
| 1 | 35-A | 52 | ARG | NE-CZ-NH1 | 7.91 | 124.25 | 120.30 |
| 1 | 140-A | 16 | MET | CA-CB-CG | 7.90 | 126.73 | 113.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 133-A | 52 | ARG | NE-CZ-NH2 | -7.90 | 116.35 | 120.30 |
| 1 | 194-A | 127 | ASP | N-CA-C | -7.90 | 89.68 | 111.00 |
| 1 | 89-A | 33 | ARG | NE-CZ-NH1 | 7.88 | 124.24 | 120.30 |
| 1 | 40-A | 142 | ASP | CB-CG-OD1 | -7.87 | 111.22 | 118.30 |
| 1 | 69-A | 76 | LYS | CD-CE-NZ | 7.86 | 129.78 | 111.70 |
| 1 | 59-A | 44 | ARG | CD-NE-CZ | 7.84 | 134.57 | 123.60 |
| 1 | 155-A | 120 | GLU | N-CA-CB | -7.82 | 96.53 | 110.60 |
| 1 | 19-A | 79 | ASP | CB-CG-OD1 | 7.80 | 125.32 | 118.30 |
| 1 | 178-A | 132 | ASP | CB-CG-OD1 | 7.79 | 125.31 | 118.30 |
| 1 | 137-A | 20 | MET | CB-CG-SD | -7.79 | 89.03 | 112.40 |
| 1 | 195-A | 152 | CYS | CA-CB-SG | 7.79 | 128.01 | 114.00 |
| 1 | 21-A | 119 | VAL | CB-CA-C | -7.78 | 96.63 | 111.40 |
| 1 | 144-A | 52 | ARG | NE-CZ-NH2 | -7.77 | 116.41 | 120.30 |
| 1 | 237-A | 52 | ARG | NE-CZ-NH2 | -7.76 | 116.42 | 120.30 |
| 1 | 83-A | 20 | MET | CG-SD-CE | 7.76 | 112.61 | 100.20 |
| 1 | 97-A | 109 | LYS | CD-CE-NZ | 7.75 | 129.53 | 111.70 |
| 1 | 8-A | 157 | GLU | OE1-CD-OE2 | -7.75 | 114.00 | 123.30 |
| 1 | 58-A | 24 | LEU | CB-CG-CD1 | -7.75 | 97.83 | 111.00 |
| 1 | 106-A | 36 | LEU | CA-CB-CG | 7.74 | 133.10 | 115.30 |
| 1 | 127-A | 52 | ARG | NE-CZ-NH1 | 7.73 | 124.17 | 120.30 |
| 1 | 188-A | 159 | ARG | NE-CZ-NH2 | -7.72 | 116.44 | 120.30 |
| 1 | 111-A | 36 | LEU | CA-CB-CG | 7.71 | 133.03 | 115.30 |
| 1 | 213-A | 152 | CYS | CA-CB-SG | -7.71 | 100.12 | 114.00 |
| 1 | 211-A | 142 | ASP | CB-CG-OD2 | 7.69 | 125.22 | 118.30 |
| 1 | 226-A | 19 | ALA | N-CA-C | 7.68 | 131.75 | 111.00 |
| 1 | 65-A | 24 | LEU | CB-CG-CD2 | 7.68 | 124.05 | 111.00 |
| 1 | 136-A | 20 | MET | CB-CG-SD | 7.67 | 135.42 | 112.40 |
| 1 | 183-A | 52 | ARG | CG-CD-NE | 7.66 | 127.89 | 111.80 |
| 1 | 36-A | 44 | ARG | CG-CD-NE | 7.66 | 127.88 | 111.80 |
| 1 | 152-A | 79 | ASP | CB-CG-OD2 | 7.65 | 125.19 | 118.30 |
| 1 | 75-A | 159 | ARG | CG-CD-NE | -7.64 | 95.75 | 111.80 |
| 1 | 110-A | 16 | MET | CG-SD-CE | -7.64 | 87.98 | 100.20 |
| 1 | 44-A | 120 | GLU | CB-CA-C | 7.63 | 125.66 | 110.40 |
| 1 | 160-A | 52 | ARG | NE-CZ-NH2 | -7.63 | 116.49 | 120.30 |
| 1 | 133-A | 52 | ARG | NE-CZ-NH1 | 7.61 | 124.10 | 120.30 |
| 1 | 160-A | 1 | MET | CG-SD-CE | 7.61 | 112.37 | 100.20 |
| 1 | 143-A | 52 | ARG | NE-CZ-NH1 | 7.60 | 124.10 | 120.30 |
| 1 | 226-A | 127 | ASP | N-CA-C | -7.60 | 90.48 | 111.00 |
| 1 | 70-A | 44 | ARG | NE-CZ-NH2 | -7.59 | 116.50 | 120.30 |
| 1 | 73-A | 76 | LYS | CD-CE-NZ | 7.59 | 129.16 | 111.70 |
| 1 | 150-A | 159 | ARG | NE-CZ-NH2 | -7.59 | 116.50 | 120.30 |
| 1 | 160-A | 142 | ASP | CB-CG-OD1 | 7.59 | 125.13 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 226-A | 154 | GLU | OE1-CD-OE2 | -7.58 | 114.20 | 123.30 |
| 1 | 39-A | 87 | ASP | CB-CG-OD2 | 7.57 | 125.11 | 118.30 |
| 1 | 69-A | 159 | ARG | NE-CZ-NH1 | 7.54 | 124.07 | 120.30 |
| 1 | 8-A | 79 | ASP | CB-CG-OD1 | -7.54 | 111.52 | 118.30 |
| 1 | 249-A | 159 | ARG | NE-CZ-NH2 | -7.52 | 116.54 | 120.30 |
| 1 | 4-A | 20 | MET | CG-SD-CE | -7.51 | 88.18 | 100.20 |
| 1 | 106-A | 24 | LEU | CB-CG-CD1 | -7.51 | 98.24 | 111.00 |
| 1 | 110-A | 20 | MET | CB-CG-SD | -7.49 | 89.92 | 112.40 |
| 1 | 170-A | 87 | ASP | CB-CG-OD2 | 7.49 | 125.04 | 118.30 |
| 1 | 63-A | 79 | ASP | CB-CG-OD1 | -7.48 | 111.57 | 118.30 |
| 1 | 137-A | 127 | ASP | CB-CG-OD1 | 7.48 | 125.03 | 118.30 |
| 1 | 10-A | 1 | MET | CB-CA-C | 7.48 | 125.35 | 110.40 |
| 1 | 2-A | 142 | ASP | CB-CG-OD1 | 7.47 | 125.03 | 118.30 |
| 1 | 225-A | 159 | ARG | CG-CD-NE | -7.47 | 96.11 | 111.80 |
| 1 | 65-A | 20 | MET | CA-CB-CG | 7.47 | 126.00 | 113.30 |
| 1 | 76-A | 48 | GLU | OE1-CD-OE2 | -7.45 | 114.36 | 123.30 |
| 1 | 184-A | 33 | ARG | NE-CZ-NH2 | -7.45 | 116.58 | 120.30 |
| 1 | 122-A | 22 | TRP | N-CA-C | -7.43 | 90.94 | 111.00 |
| 1 | 249-A | 33 | ARG | NE-CZ-NH2 | -7.43 | 116.58 | 120.30 |
| 1 | 81-A | 1 | MET | CB-CG-SD | 7.42 | 134.68 | 112.40 |
| 1 | 76-A | 33 | ARG | NE-CZ-NH1 | 7.41 | 124.00 | 120.30 |
| 1 | 60-A | 20 | MET | CB-CG-SD | 7.41 | 134.62 | 112.40 |
| 1 | 52-A | 159 | ARG | NE-CZ-NH1 | 7.41 | 124.00 | 120.30 |
| 1 | 113-A | 104 | LEU | CB-CG-CD2 | 7.40 | 123.59 | 111.00 |
| 1 | 161-A | 52 | ARG | NE-CZ-NH1 | 7.40 | 124.00 | 120.30 |
| 1 | 179-A | 98 | ARG | NE-CZ-NH2 | -7.40 | 116.60 | 120.30 |
| 1 | 132-A | 20 | MET | C-N-CD | -7.39 | 104.33 | 120.60 |
| 1 | 72-A | 159 | ARG | NE-CZ-NH2 | -7.39 | 116.61 | 120.30 |
| 1 | 188-A | 79 | ASP | CB-CG-OD2 | 7.38 | 124.94 | 118.30 |
| 1 | 24-A | 44 | ARG | CD-NE-CZ | 7.38 | 133.93 | 123.60 |
| 1 | 22-A | 52 | ARG | NE-CZ-NH1 | 7.38 | 123.99 | 120.30 |
| 1 | 109-A | 87 | ASP | N-CA-C | 7.38 | 130.92 | 111.00 |
| 1 | 36-A | 16 | MET | CG-SD-CE | 7.37 | 112.00 | 100.20 |
| 1 | 184-A | 157 | GLU | CA-CB-CG | 7.37 | 129.62 | 113.40 |
| 1 | 58-A | 44 | ARG | CG-CD-NE | -7.37 | 96.33 | 111.80 |
| 1 | 99-A | 20 | MET | CA-CB-CG | 7.37 | 125.82 | 113.30 |
| 1 | 195-A | 127 | ASP | N-CA-C | -7.37 | 91.11 | 111.00 |
| 1 | 244-A | 159 | ARG | NE-CZ-NH2 | -7.37 | 116.62 | 120.30 |
| 1 | 124-A | 79 | ASP | CB-CG-OD2 | 7.36 | 124.93 | 118.30 |
| 1 | 59-A | 33 | ARG | NE-CZ-NH2 | -7.36 | 116.62 | 120.30 |
| 1 | 154-A | 20 | MET | CB-CG-SD | -7.36 | 90.33 | 112.40 |
| 1 | 49-A | 142 | ASP | CB-CA-C | -7.35 | 95.69 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 127-A | 52 | ARG | NE-CZ-NH2 | -7.35 | 116.62 | 120.30 |
| 1 | 217-A | 104 | LEU | CB-CG-CD1 | -7.35 | 98.51 | 111.00 |
| 1 | 204-A | 159 | ARG | NE-CZ-NH1 | 7.35 | 123.97 | 120.30 |
| 1 | 77-A | 33 | ARG | NE-CZ-NH1 | 7.34 | 123.97 | 120.30 |
| 1 | 45-A | 20 | MET | CB-CG-SD | -7.34 | 90.38 | 112.40 |
| 1 | 180-A | 18 | ASN | CB-CA-C | -7.34 | 95.72 | 110.40 |
| 1 | 47-A | 33 | ARG | NE-CZ-NH1 | 7.34 | 123.97 | 120.30 |
| 1 | 85-A | 159 | ARG | NE-CZ-NH2 | 7.33 | 123.97 | 120.30 |
| 1 | 238-A | 52 | ARG | NE-CZ-NH2 | -7.32 | 116.64 | 120.30 |
| 1 | 137-A | 52 | ARG | NE-CZ-NH1 | 7.31 | 123.96 | 120.30 |
| 1 | 183-A | 152 | CYS | CA-CB-SG | 7.31 | 127.16 | 114.00 |
| 1 | 173-A | 152 | CYS | CB-CA-C | -7.31 | 95.78 | 110.40 |
| 1 | 78-A | 52 | ARG | NE-CZ-NH2 | -7.31 | 116.64 | 120.30 |
| 1 | 218-A | 1 | MET | N-CA-C | 7.30 | 130.72 | 111.00 |
| 1 | 141-A | 21 | PRO | N-CA-C | 7.29 | 131.07 | 112.10 |
| 1 | 227-A | 52 | ARG | NE-CZ-NH1 | 7.29 | 123.94 | 120.30 |
| 1 | 1-A | 98 | ARG | CG-CD-NE | -7.28 | 96.51 | 111.80 |
| 1 | 90-A | 44 | ARG | NE-CZ-NH2 | -7.26 | 116.67 | 120.30 |
| 1 | 85-A | 159 | ARG | NE-CZ-NH1 | -7.25 | 116.67 | 120.30 |
| 1 | 48-A | 52 | ARG | NE-CZ-NH1 | -7.25 | 116.67 | 120.30 |
| 1 | 59-A | 52 | ARG | NE-CZ-NH1 | 7.25 | 123.93 | 120.30 |
| 1 | 208-A | 159 | ARG | NE-CZ-NH2 | -7.25 | 116.67 | 120.30 |
| 1 | 61-A | 159 | ARG | NE-CZ-NH2 | 7.25 | 123.92 | 120.30 |
| 1 | 70-A | 142 | ASP | CB-CG-OD2 | 7.25 | 124.82 | 118.30 |
| 1 | 142-A | 23 | ASN | N-CA-CB | 7.25 | 123.65 | 110.60 |
| 1 | 2-A | 36 | LEU | CB-CG-CD1 | -7.24 | 98.69 | 111.00 |
| 1 | 236-A | 98 | ARG | NE-CZ-NH2 | 7.23 | 123.92 | 120.30 |
| 1 | 195-A | 159 | ARG | NE-CZ-NH2 | -7.21 | 116.69 | 120.30 |
| 1 | 202-A | 159 | ARG | NE-CZ-NH1 | 7.19 | 123.90 | 120.30 |
| 1 | 206-A | 33 | ARG | NE-CZ-NH1 | 7.19 | 123.90 | 120.30 |
| 1 | 186-A | 152 | CYS | CA-CB-SG | 7.18 | 126.93 | 114.00 |
| 1 | 206-A | 1 | MET | CB-CG-SD | 7.18 | 133.94 | 112.40 |
| 1 | 43-A | 44 | ARG | NE-CZ-NH1 | 7.17 | 123.89 | 120.30 |
| 1 | 142-A | 12 | ARG | NE-CZ-NH2 | -7.17 | 116.71 | 120.30 |
| 1 | 89-A | 33 | ARG | NE-CZ-NH2 | -7.16 | 116.72 | 120.30 |
| 1 | 42-A | 159 | ARG | NE-CZ-NH1 | 7.15 | 123.88 | 120.30 |
| 1 | 156-A | 132 | ASP | CB-CG-OD2 | 7.15 | 124.73 | 118.30 |
| 1 | 28-A | 33 | ARG | NE-CZ-NH1 | 7.14 | 123.87 | 120.30 |
| 1 | 36-A | 1 | MET | CB-CG-SD | 7.14 | 133.82 | 112.40 |
| 1 | 82-A | 52 | ARG | NE-CZ-NH1 | 7.14 | 123.87 | 120.30 |
| 1 | 79-A | 159 | ARG | NE-CZ-NH1 | 7.14 | 123.87 | 120.30 |
| 1 | 143-A | 20 | MET | CB-CA-C | 7.13 | 124.66 | 110.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 222-A | 20 | MET | CA-CB-CG | 7.12 | 125.41 | 113.30 |
| 1 | 28-A | 108 | GLN | CA-CB-CG | -7.12 | 97.74 | 113.40 |
| 1 | 195-A | 159 | ARG | NE-CZ-NH1 | 7.12 | 123.86 | 120.30 |
| 1 | 140-A | 156 | LEU | CB-CG-CD1 | -7.11 | 98.91 | 111.00 |
| 1 | 24-A | 127 | ASP | CB-CG-OD2 | 7.10 | 124.69 | 118.30 |
| 1 | 99-A | 104 | LEU | CB-CG-CD2 | 7.10 | 123.07 | 111.00 |
| 1 | 217-A | 159 | ARG | CD-NE-CZ | 7.09 | 133.52 | 123.60 |
| 1 | 47-A | 119 | VAL | CB-CA-C | -7.08 | 97.94 | 111.40 |
| 1 | 141-A | 20 | MET | CG-SD-CE | 7.08 | 111.52 | 100.20 |
| 1 | 248-A | 159 | ARG | NE-CZ-NH1 | 7.08 | 123.84 | 120.30 |
| 1 | 221-A | 52 | ARG | NE-CZ-NH2 | -7.07 | 116.76 | 120.30 |
| 1 | 136-A | 159 | ARG | CA-CB-CG | 7.07 | 128.95 | 113.40 |
| 1 | 178-A | 142 | ASP | CB-CG-OD2 | 7.07 | 124.66 | 118.30 |
| 1 | 190-A | 60 | ILE | CG1-CB-CG2 | -7.07 | 95.85 | 111.40 |
| 1 | 84-A | 16 | MET | CA-CB-CG | 7.07 | 125.31 | 113.30 |
| 1 | 118-A | 52 | ARG | NE-CZ-NH1 | 7.07 | 123.83 | 120.30 |
| 1 | 215-A | 12 | ARG | NE-CZ-NH2 | -7.06 | 116.77 | 120.30 |
| 1 | 64-A | 159 | ARG | CG-CD-NE | -7.06 | 96.97 | 111.80 |
| 1 | 182-A | 101 | GLU | OE1-CD-OE2 | -7.06 | 114.83 | 123.30 |
| 1 | 30-A | 20 | MET | CA-CB-CG | 7.06 | 125.30 | 113.30 |
| 1 | 68-A | 76 | LYS | CD-CE-NZ | 7.06 | 127.93 | 111.70 |
| 1 | 143-A | 20 | MET | N-CA-C | -7.05 | 91.95 | 111.00 |
| 1 | 44-A | 44 | ARG | CG-CD-NE | -7.05 | 97.00 | 111.80 |
| 1 | 151-A | 20 | MET | CB-CG-SD | -7.05 | 91.25 | 112.40 |
| 1 | 102-A | 20 | MET | CA-CB-CG | -7.05 | 101.32 | 113.30 |
| 1 | 111-A | 159 | ARG | NE-CZ-NH2 | 7.05 | 123.82 | 120.30 |
| 1 | 125-A | 12 | ARG | NE-CZ-NH2 | -7.04 | 116.78 | 120.30 |
| 1 | 58-A | 159 | ARG | NE-CZ-NH2 | -7.04 | 116.78 | 120.30 |
| 1 | 46-A | 159 | ARG | NE-CZ-NH1 | -7.04 | 116.78 | 120.30 |
| 1 | 129-A | 157 | GLU | OE1-CD-OE2 | 7.04 | 131.74 | 123.30 |
| 1 | 219-A | 12 | ARG | NE-CZ-NH2 | -7.04 | 116.78 | 120.30 |
| 1 | 224-A | 12 | ARG | NE-CZ-NH1 | 7.04 | 123.82 | 120.30 |
| 1 | 94-A | 20 | MET | N-CA-C | -7.03 | 92.01 | 111.00 |
| 1 | 221-A | 44 | ARG | NE-CZ-NH2 | -7.03 | 116.79 | 120.30 |
| 1 | 222-A | 19 | ALA | N-CA-C | 7.02 | 129.96 | 111.00 |
| 1 | 154-A | 159 | ARG | NE-CZ-NH2 | -7.02 | 116.79 | 120.30 |
| 1 | 63-A | 20 | MET | CA-CB-CG | 7.01 | 125.22 | 113.30 |
| 1 | 225-A | 12 | ARG | NE-CZ-NH1 | 6.99 | 123.79 | 120.30 |
| 1 | 99-A | 142 | ASP | CB-CA-C | -6.98 | 96.45 | 110.40 |
| 1 | 120-A | 79 | ASP | N-CA-CB | 6.98 | 123.16 | 110.60 |
| 1 | 66-A | 22 | TRP | N-CA-C | -6.97 | 92.18 | 111.00 |
| 1 | 139-A | 4 | LEU | CB-CG-CD1 | 6.96 | 122.84 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 220-A | 157 | GLU | OE1-CD-OE2 | -6.96 | 114.95 | 123.30 |
| 1 | 220-A | 159 | ARG | NE-CZ-NH1 | -6.96 | 116.82 | 120.30 |
| 1 | 193-A | 44 | ARG | NE-CZ-NH2 | -6.95 | 116.82 | 120.30 |
| 1 | 231-A | 87 | ASP | CB-CG-OD1 | 6.95 | 124.55 | 118.30 |
| 1 | 215-A | 20 | MET | N-CA-C | 6.94 | 129.75 | 111.00 |
| 1 | 167-A | 1 | MET | CG-SD-CE | -6.94 | 89.10 | 100.20 |
| 1 | 168-A | 52 | ARG | NE-CZ-NH1 | 6.93 | 123.77 | 120.30 |
| 1 | 76-A | 52 | ARG | CG-CD-NE | -6.93 | 97.25 | 111.80 |
| 1 | 110-A | 87 | ASP | N-CA-C | 6.92 | 129.69 | 111.00 |
| 1 | 99-A | 20 | MET | CG-SD-CE | 6.91 | 111.26 | 100.20 |
| 1 | 185-A | 152 | CYS | CB-CA-C | 6.91 | 124.22 | 110.40 |
| 1 | 138-A | 4 | LEU | CB-CG-CD1 | 6.91 | 122.75 | 111.00 |
| 1 | 209-A | 159 | ARG | NE-CZ-NH2 | -6.91 | 116.85 | 120.30 |
| 1 | 2-A | 2 | ILE | N-CA-C | -6.90 | 92.36 | 111.00 |
| 1 | 155-A | 142 | ASP | CB-CG-OD2 | 6.90 | 124.51 | 118.30 |
| 1 | 83-A | 159 | ARG | NE-CZ-NH1 | -6.90 | 116.85 | 120.30 |
| 1 | 116-A | 87 | ASP | CB-CG-OD1 | 6.87 | 124.48 | 118.30 |
| 1 | 32-A | 44 | ARG | CG-CD-NE | 6.86 | 126.22 | 111.80 |
| 1 | 197-A | 33 | ARG | NE-CZ-NH1 | 6.86 | 123.73 | 120.30 |
| 1 | 171-A | 52 | ARG | NE-CZ-NH1 | 6.86 | 123.73 | 120.30 |
| 1 | 94-A | 20 | MET | CG-SD-CE | -6.86 | 89.23 | 100.20 |
| 1 | 154-A | 159 | ARG | NE-CZ-NH1 | 6.85 | 123.73 | 120.30 |
| 1 | 124-A | 159 | ARG | NE-CZ-NH2 | 6.84 | 123.72 | 120.30 |
| 1 | 113-A | 20 | MET | CG-SD-CE | -6.84 | 89.26 | 100.20 |
| 1 | 25-A | 44 | ARG | NE-CZ-NH1 | 6.84 | 123.72 | 120.30 |
| 1 | 93-A | 159 | ARG | NE-CZ-NH1 | -6.83 | 116.88 | 120.30 |
| 1 | 167-A | 142 | ASP | CB-CG-OD2 | 6.83 | 124.45 | 118.30 |
| 1 | 56-A | 20 | MET | CG-SD-CE | 6.82 | 111.11 | 100.20 |
| 1 | 216-A | 1 | MET | CB-CG-SD | 6.82 | 132.86 | 112.40 |
| 1 | 226-A | 52 | ARG | NE-CZ-NH2 | -6.82 | 116.89 | 120.30 |
| 1 | 239-A | 87 | ASP | CB-CG-OD2 | 6.82 | 124.44 | 118.30 |
| 1 | 9-A | 157 | GLU | CA-CB-CG | 6.81 | 128.37 | 113.40 |
| 1 | 111-A | 104 | LEU | CB-CG-CD2 | 6.80 | 122.57 | 111.00 |
| 1 | 141-A | 22 | TRP | CA-CB-CG | -6.80 | 100.78 | 113.70 |
| 1 | 39-A | 20 | MET | CG-SD-CE | 6.79 | 111.07 | 100.20 |
| 1 | 74-A | 156 | LEU | CA-CB-CG | -6.79 | 99.68 | 115.30 |
| 1 | 177-A | 52 | ARG | NE-CZ-NH1 | 6.79 | 123.70 | 120.30 |
| 1 | 10-A | 52 | ARG | NE-CZ-NH1 | 6.79 | 123.69 | 120.30 |
| 1 | 72-A | 142 | ASP | CB-CG-OD2 | 6.78 | 124.41 | 118.30 |
| 1 | 133-A | 21 | PRO | CA-C-N | -6.78 | 102.28 | 117.20 |
| 1 | 199-A | 104 | LEU | CB-CG-CD1 | 6.78 | 122.53 | 111.00 |
| 1 | 111-A | 108 | GLN | N-CA-CB | -6.78 | 98.40 | 110.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 96-A | 1 | MET | CA-CB-CG | 6.77 | 124.81 | 113.30 |
| 1 | 110-A | 4 | LEU | CB-CG-CD2 | 6.77 | 122.50 | 111.00 |
| 1 | 42-A | 1 | MET | CG-SD-CE | -6.76 | 89.38 | 100.20 |
| 1 | 55-A | 156 | LEU | CA-CB-CG | 6.76 | 130.86 | 115.30 |
| 1 | 140-A | 16 | MET | CG-SD-CE | 6.76 | 111.02 | 100.20 |
| 1 | 99-A | 33 | ARG | NE-CZ-NH1 | 6.76 | 123.68 | 120.30 |
| 1 | 234-A | 1 | MET | CG-SD-CE | 6.76 | 111.02 | 100.20 |
| 1 | 194-A | 20 | MET | CA-CB-CG | -6.76 | 101.81 | 113.30 |
| 1 | 24-A | 127 | ASP | N-CA-CB | 6.75 | 122.74 | 110.60 |
| 1 | 149-A | 1 | MET | CA-CB-CG | 6.75 | 124.77 | 113.30 |
| 1 | 192-A | 44 | ARG | NE-CZ-NH2 | -6.74 | 116.93 | 120.30 |
| 1 | 216-A | 1 | MET | CB-CA-C | 6.74 | 123.87 | 110.40 |
| 1 | 140-A | 33 | ARG | NE-CZ-NH1 | 6.73 | 123.66 | 120.30 |
| 1 | 214-A | 142 | ASP | CB-CG-OD2 | -6.73 | 112.25 | 118.30 |
| 1 | 121-A | 87 | ASP | CB-CA-C | 6.72 | 123.85 | 110.40 |
| 1 | 188-A | 44 | ARG | NE-CZ-NH2 | -6.72 | 116.94 | 120.30 |
| 1 | 204-A | 20 | MET | CG-SD-CE | -6.72 | 89.44 | 100.20 |
| 1 | 150-A | 44 | ARG | NE-CZ-NH2 | -6.72 | 116.94 | 120.30 |
| 1 | 50-A | 52 | ARG | NE-CZ-NH2 | -6.71 | 116.94 | 120.30 |
| 1 | 166-A | 52 | ARG | NE-CZ-NH2 | -6.71 | 116.94 | 120.30 |
| 1 | 112-A | 159 | ARG | NE-CZ-NH2 | -6.71 | 116.94 | 120.30 |
| 1 | 25-A | 157 | GLU | OE1-CD-OE2 | -6.70 | 115.26 | 123.30 |
| 1 | 124-A | 52 | ARG | NE-CZ-NH1 | 6.69 | 123.64 | 120.30 |
| 1 | 72-A | 1 | MET | CG-SD-CE | -6.69 | 89.50 | 100.20 |
| 1 | 219-A | 1 | MET | CG-SD-CE | 6.69 | 110.90 | 100.20 |
| 1 | 6-A | 20 | MET | CA-CB-CG | 6.68 | 124.66 | 113.30 |
| 1 | 18-A | 1 | MET | CB-CG-SD | 6.68 | 132.46 | 112.40 |
| 1 | 85-A | 16 | MET | N-CA-CB | -6.68 | 98.57 | 110.60 |
| 1 | 92-A | 52 | ARG | NE-CZ-NH2 | -6.68 | 116.96 | 120.30 |
| 1 | 142-A | 16 | MET | CA-CB-CG | 6.68 | 124.66 | 113.30 |
| 1 | 81-A | 33 | ARG | NE-CZ-NH1 | 6.68 | 123.64 | 120.30 |
| 1 | 78-A | 24 | LEU | CB-CG-CD1 | 6.68 | 122.35 | 111.00 |
| 1 | 165-A | 119 | VAL | CB-CA-C | -6.67 | 98.73 | 111.40 |
| 1 | 186-A | 79 | ASP | CB-CG-OD2 | 6.67 | 124.30 | 118.30 |
| 1 | 84-A | 44 | ARG | NE-CZ-NH2 | -6.66 | 116.97 | 120.30 |
| 1 | 88-A | 44 | ARG | NE-CZ-NH2 | -6.66 | 116.97 | 120.30 |
| 1 | 180-A | 18 | ASN | N-CA-C | 6.65 | 128.96 | 111.00 |
| 1 | 219-A | 12 | ARG | NE-CZ-NH1 | 6.65 | 123.62 | 120.30 |
| 1 | 63-A | 24 | LEU | CB-CG-CD2 | 6.65 | 122.30 | 111.00 |
| 1 | 200-A | 52 | ARG | NE-CZ-NH2 | -6.64 | 116.98 | 120.30 |
| 1 | 80-A | 52 | ARG | NE-CZ-NH2 | 6.64 | 123.62 | 120.30 |
| 1 | 183-A | 52 | ARG | NE-CZ-NH2 | -6.63 | 116.98 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 182-A | 4 | LEU | CB-CG-CD1 | 6.63 | 122.28 | 111.00 |
| 1 | 22-A | 44 | ARG | CG-CD-NE | -6.63 | 97.88 | 111.80 |
| 1 | 216-A | 52 | ARG | NE-CZ-NH2 | -6.63 | 116.99 | 120.30 |
| 1 | 181-A | 152 | CYS | N-CA-CB | -6.62 | 98.68 | 110.60 |
| 1 | 164-A | 1 | MET | CG-SD-CE | 6.62 | 110.79 | 100.20 |
| 1 | 181-A | 44 | ARG | NE-CZ-NH1 | 6.62 | 123.61 | 120.30 |
| 1 | 198-A | 152 | CYS | CA-CB-SG | 6.61 | 125.90 | 114.00 |
| 1 | 239-A | 87 | ASP | CB-CG-OD1 | -6.61 | 112.35 | 118.30 |
| 1 | 149-A | 33 | ARG | NE-CZ-NH1 | 6.60 | 123.60 | 120.30 |
| 1 | 88-A | 159 | ARG | NE-CZ-NH2 | -6.60 | 117.00 | 120.30 |
| 1 | 62-A | 44 | ARG | NE-CZ-NH1 | 6.59 | 123.60 | 120.30 |
| 1 | 174-A | 20 | MET | N-CA-C | -6.59 | 93.19 | 111.00 |
| 1 | 161-A | 33 | ARG | NE-CZ-NH2 | 6.59 | 123.60 | 120.30 |
| 1 | 216-A | 12 | ARG | NE-CZ-NH2 | -6.59 | 117.00 | 120.30 |
| 1 | 130-A | 33 | ARG | NE-CZ-NH1 | 6.58 | 123.59 | 120.30 |
| 1 | 142-A | 52 | ARG | NE-CZ-NH1 | 6.58 | 123.59 | 120.30 |
| 1 | 123-A | 1 | MET | CG-SD-CE | -6.58 | 89.67 | 100.20 |
| 1 | 106-A | 87 | ASP | CB-CG-OD1 | -6.58 | 112.38 | 118.30 |
| 1 | 128-A | 16 | MET | CA-CB-CG | 6.57 | 124.47 | 113.30 |
| 1 | 69-A | 16 | MET | CG-SD-CE | 6.55 | 110.68 | 100.20 |
| 1 | 1-A | 98 | ARG | CD-NE-CZ | 6.55 | 132.76 | 123.60 |
| 1 | 1-A | 1 | MET | CB-CG-SD | -6.54 | 92.77 | 112.40 |
| 1 | 66-A | 20 | MET | CB-CG-SD | 6.54 | 132.02 | 112.40 |
| 1 | 30-A | 44 | ARG | NE-CZ-NH2 | -6.54 | 117.03 | 120.30 |
| 1 | 199-A | 52 | ARG | NE-CZ-NH1 | 6.53 | 123.56 | 120.30 |
| 1 | 140-A | 33 | ARG | NE-CZ-NH2 | -6.53 | 117.04 | 120.30 |
| 1 | 118-A | 52 | ARG | NE-CZ-NH2 | -6.53 | 117.04 | 120.30 |
| 1 | 149-A | 157 | GLU | CG-CD-OE1 | 6.53 | 131.35 | 118.30 |
| 1 | 207-A | 1 | MET | CG-SD-CE | 6.52 | 110.64 | 100.20 |
| 1 | 8-A | 159 | ARG | NE-CZ-NH2 | -6.52 | 117.04 | 120.30 |
| 1 | 154-A | 79 | ASP | CB-CG-OD1 | -6.51 | 112.44 | 118.30 |
| 1 | 177-A | 152 | CYS | CA-CB-SG | 6.51 | 125.72 | 114.00 |
| 1 | 217-A | 12 | ARG | NE-CZ-NH1 | 6.51 | 123.56 | 120.30 |
| 1 | 5-A | 87 | ASP | CB-CA-C | 6.50 | 123.40 | 110.40 |
| 1 | 60-A | 98 | ARG | NE-CZ-NH1 | 6.50 | 123.55 | 120.30 |
| 1 | 33-A | 159 | ARG | NE-CZ-NH2 | -6.50 | 117.05 | 120.30 |
| 1 | 175-A | 44 | ARG | NE-CZ-NH2 | -6.50 | 117.05 | 120.30 |
| 1 | 62-A | 44 | ARG | CG-CD-NE | -6.49 | 98.16 | 111.80 |
| 1 | 78-A | 76 | LYS | CD-CE-NZ | -6.49 | 96.77 | 111.70 |
| 1 | 138-A | 16 | MET | CB-CG-SD | 6.48 | 131.83 | 112.40 |
| 1 | 5-A | 52 | ARG | NE-CZ-NH1 | 6.47 | 123.54 | 120.30 |
| 1 | 90-A | 79 | ASP | CB-CG-OD2 | -6.47 | 112.47 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 110-A | 1 | MET | CA-CB-CG | 6.47 | 124.30 | 113.30 |
| 1 | 67-A | 44 | ARG | CG-CD-NE | -6.46 | 98.22 | 111.80 |
| 1 | 216-A | 33 | ARG | NE-CZ-NH2 | -6.46 | 117.07 | 120.30 |
| 1 | 123-A | 20 | MET | C-N-CD | 6.46 | 141.96 | 128.40 |
| 1 | 244-A | 157 | GLU | CA-CB-CG | 6.46 | 127.61 | 113.40 |
| 1 | 74-A | 159 | ARG | CG-CD-NE | -6.45 | 98.26 | 111.80 |
| 1 | 76-A | 20 | MET | CG-SD-CE | 6.45 | 110.51 | 100.20 |
| 1 | 172-A | 142 | ASP | CB-CG-OD1 | -6.44 | 112.50 | 118.30 |
| 1 | 187-A | 152 | CYS | N-CA-CB | -6.44 | 99.00 | 110.60 |
| 1 | 216-A | 159 | ARG | NE-CZ-NH2 | -6.44 | 117.08 | 120.30 |
| 1 | 141-A | 12 | ARG | NE-CZ-NH2 | -6.44 | 117.08 | 120.30 |
| 1 | 19-A | 157 | GLU | CA-CB-CG | 6.44 | 127.56 | 113.40 |
| 1 | 46-A | 36 | LEU | CB-CG-CD1 | 6.44 | 121.94 | 111.00 |
| 1 | 64-A | 159 | ARG | NE-CZ-NH2 | -6.44 | 117.08 | 120.30 |
| 1 | 178-A | 52 | ARG | CD-NE-CZ | 6.43 | 132.61 | 123.60 |
| 1 | 77-A | 16 | MET | CB-CG-SD | 6.43 | 131.69 | 112.40 |
| 1 | 143-A | 52 | ARG | NE-CZ-NH2 | -6.43 | 117.09 | 120.30 |
| 1 | 182-A | 152 | CYS | CA-CB-SG | -6.42 | 102.45 | 114.00 |
| 1 | 62-A | 20 | MET | CG-SD-CE | 6.41 | 110.46 | 100.20 |
| 1 | 221-A | 19 | ALA | N-CA-C | 6.41 | 128.31 | 111.00 |
| 1 | 201-A | 159 | ARG | NE-CZ-NH1 | -6.41 | 117.10 | 120.30 |
| 1 | 79-A | 128 | TYR | CB-CG-CD1 | 6.41 | 124.84 | 121.00 |
| 1 | 91-A | 20 | MET | CB-CG-SD | 6.40 | 131.59 | 112.40 |
| 1 | 170-A | 21 | PRO | N-CA-C | -6.40 | 95.47 | 112.10 |
| 1 | 98-A | 159 | ARG | NE-CZ-NH1 | -6.39 | 117.10 | 120.30 |
| 1 | 65-A | 132 | ASP | CB-CG-OD2 | 6.39 | 124.05 | 118.30 |
| 1 | 152-A | 120 | GLU | CB-CA-C | 6.39 | 123.18 | 110.40 |
| 1 | 50-A | 159 | ARG | NE-CZ-NH2 | -6.38 | 117.11 | 120.30 |
| 1 | 95-A | 33 | ARG | NE-CZ-NH2 | -6.38 | 117.11 | 120.30 |
| 1 | 103-A | 159 | ARG | NE-CZ-NH1 | 6.38 | 123.49 | 120.30 |
| 1 | 195-A | 33 | ARG | NE-CZ-NH2 | -6.38 | 117.11 | 120.30 |
| 1 | 179-A | 119 | VAL | CB-CA-C | -6.37 | 99.29 | 111.40 |
| 1 | 205-A | 119 | VAL | CB-CA-C | 6.37 | 123.50 | 111.40 |
| 1 | 48-A | 127 | ASP | CB-CG-OD1 | 6.36 | 124.03 | 118.30 |
| 1 | 213-A | 20 | MET | C-N-CD | 6.36 | 141.76 | 128.40 |
| 1 | 76-A | 52 | ARG | NE-CZ-NH1 | 6.36 | 123.48 | 120.30 |
| 1 | 217-A | 152 | CYS | CA-CB-SG | 6.36 | 125.45 | 114.00 |
| 1 | 140-A | 20 | MET | C-N-CD | -6.36 | 106.61 | 120.60 |
| 1 | 31-A | 44 | ARG | CG-CD-NE | 6.36 | 125.15 | 111.80 |
| 1 | 116-A | 132 | ASP | CB-CG-OD2 | 6.35 | 124.02 | 118.30 |
| 1 | 153-A | 98 | ARG | CG-CD-NE | 6.35 | 125.14 | 111.80 |
| 1 | 105-A | 24 | LEU | CB-CG-CD1 | -6.35 | 100.20 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 197-A | 1 | MET | CG-SD-CE | 6.35 | 110.36 | 100.20 |
| 1 | 183-A | 19 | ALA | N-CA-C | 6.34 | 128.13 | 111.00 |
| 1 | 230-A | 4 | LEU | CB-CG-CD2 | -6.34 | 100.22 | 111.00 |
| 1 | 26-A | 158 | ARG | NE-CZ-NH1 | 6.33 | 123.47 | 120.30 |
| 1 | 36-A | 4 | LEU | CB-CG-CD1 | 6.33 | 121.75 | 111.00 |
| 1 | 214-A | 79 | ASP | CB-CG-OD1 | -6.33 | 112.61 | 118.30 |
| 1 | 214-A | 159 | ARG | NE-CZ-NH2 | -6.33 | 117.14 | 120.30 |
| 1 | 66-A | 21 | PRO | N-CA-C | 6.32 | 128.53 | 112.10 |
| 1 | 206-A | 16 | MET | CB-CG-SD | -6.32 | 93.44 | 112.40 |
| 1 | 103-A | 159 | ARG | NE-CZ-NH2 | -6.32 | 117.14 | 120.30 |
| 1 | 59-A | 52 | ARG | NE-CZ-NH2 | -6.31 | 117.14 | 120.30 |
| 1 | 24-A | 12 | ARG | NE-CZ-NH1 | 6.31 | 123.46 | 120.30 |
| 1 | 64-A | 20 | MET | CA-CB-CG | 6.31 | 124.03 | 113.30 |
| 1 | 77-A | 4 | LEU | CB-CG-CD1 | 6.31 | 121.73 | 111.00 |
| 1 | 86-A | 16 | MET | CA-CB-CG | 6.31 | 124.02 | 113.30 |
| 1 | 145-A | 2 | ILE | N-CA-C | 6.31 | 128.03 | 111.00 |
| 1 | 225-A | 20 | MET | N-CA-C | -6.31 | 93.97 | 111.00 |
| 1 | 147-A | 22 | TRP | N-CA-C | -6.30 | 93.98 | 111.00 |
| 1 | 185-A | 44 | ARG | NE-CZ-NH2 | -6.30 | 117.15 | 120.30 |
| 1 | 91-A | 44 | ARG | NE-CZ-NH2 | -6.30 | 117.15 | 120.30 |
| 1 | 64-A | 101 | GLU | CA-CB-CG | 6.30 | 127.25 | 113.40 |
| 1 | 76-A | 76 | LYS | CB-CG-CD | 6.30 | 127.97 | 111.60 |
| 1 | 30-A | 109 | LYS | CD-CE-NZ | 6.29 | 126.16 | 111.70 |
| 1 | 20-A | 52 | ARG | NE-CZ-NH1 | 6.27 | 123.44 | 120.30 |
| 1 | 65-A | 19 | ALA | O-C-N | 6.27 | 132.74 | 122.70 |
| 1 | 54-A | 1 | MET | CA-CB-CG | 6.27 | 123.96 | 113.30 |
| 1 | 216-A | 152 | CYS | CA-CB-SG | 6.27 | 125.28 | 114.00 |
| 1 | 99-A | 159 | ARG | NE-CZ-NH2 | -6.27 | 117.17 | 120.30 |
| 1 | 130-A | 52 | ARG | NE-CZ-NH1 | -6.27 | 117.17 | 120.30 |
| 1 | 57-A | 87 | ASP | CB-CG-OD1 | 6.27 | 123.94 | 118.30 |
| 1 | 169-A | 1 | MET | CA-CB-CG | 6.27 | 123.95 | 113.30 |
| 1 | 189-A | 152 | CYS | CA-CB-SG | 6.26 | 125.27 | 114.00 |
| 1 | 33-A | 1 | MET | CG-SD-CE | -6.26 | 90.19 | 100.20 |
| 1 | 34-A | 17 | GLU | CA-CB-CG | 6.25 | 127.16 | 113.40 |
| 1 | 212-A | 12 | ARG | NE-CZ-NH2 | -6.25 | 117.17 | 120.30 |
| 1 | 178-A | 101 | GLU | CA-CB-CG | 6.25 | 127.15 | 113.40 |
| 1 | 167-A | 52 | ARG | CG-CD-NE | 6.25 | 124.92 | 111.80 |
| 1 | 198-A | 1 | MET | CA-CB-CG | 6.25 | 123.92 | 113.30 |
| 1 | 226-A | 20 | MET | CA-CB-CG | 6.24 | 123.91 | 113.30 |
| 1 | 187-A | 152 | CYS | CA-CB-SG | -6.24 | 102.78 | 114.00 |
| 1 | 216-A | 154 | GLU | OE1-CD-OE2 | -6.24 | 115.82 | 123.30 |
| 1 | 59-A | 33 | ARG | NE-CZ-NH1 | 6.23 | 123.42 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 233-A | 79 | ASP | CB-CG-OD1 | 6.23 | 123.91 | 118.30 |
| 1 | 68-A | 20 | MET | CA-CB-CG | 6.23 | 123.89 | 113.30 |
| 1 | 198-A | 131 | ASP | CB-CG-OD1 | 6.22 | 123.90 | 118.30 |
| 1 | 194-A | 159 | ARG | NE-CZ-NH2 | 6.22 | 123.41 | 120.30 |
| 1 | 131-A | 21 | PRO | CA-C-N | 6.22 | 130.89 | 117.20 |
| 1 | 103-A | 101 | GLU | CG-CD-OE1 | 6.22 | 130.73 | 118.30 |
| 1 | 131-A | 1 | MET | CB-CG-SD | 6.21 | 131.03 | 112.40 |
| 1 | 133-A | 142 | ASP | CB-CG-OD1 | 6.21 | 123.89 | 118.30 |
| 1 | 201-A | 12 | ARG | NE-CZ-NH1 | 6.20 | 123.40 | 120.30 |
| 1 | 46-A | 44 | ARG | CG-CD-NE | 6.19 | 124.80 | 111.80 |
| 1 | 46-A | 118 | GLU | OE1-CD-OE2 | -6.19 | 115.88 | 123.30 |
| 1 | 49-A | 20 | MET | CA-CB-CG | 6.18 | 123.81 | 113.30 |
| 1 | 235-A | 20 | MET | CG-SD-CE | 6.18 | 110.09 | 100.20 |
| 1 | 204-A | 101 | GLU | OE1-CD-OE2 | 6.18 | 130.72 | 123.30 |
| 1 | 70-A | 127 | ASP | N-CA-CB | 6.18 | 121.72 | 110.60 |
| 1 | 176-A | 142 | ASP | CB-CG-OD1 | 6.18 | 123.86 | 118.30 |
| 1 | 21-A | 87 | ASP | CB-CG-OD1 | 6.18 | 123.86 | 118.30 |
| 1 | 89-A | 16 | MET | CB-CG-SD | 6.17 | 130.92 | 112.40 |
| 1 | 134-A | 1 | MET | CB-CA-C | 6.17 | 122.74 | 110.40 |
| 1 | 75-A | 76 | LYS | CD-CE-NZ | 6.17 | 125.89 | 111.70 |
| 1 | 38-A | 16 | MET | CB-CG-SD | -6.17 | 93.90 | 112.40 |
| 1 | 167-A | 1 | MET | CB-CG-SD | 6.17 | 130.90 | 112.40 |
| 1 | 179-A | 142 | ASP | CB-CG-OD1 | 6.17 | 123.85 | 118.30 |
| 1 | 219-A | 159 | ARG | NE-CZ-NH1 | -6.17 | 117.22 | 120.30 |
| 1 | 231-A | 20 | MET | CG-SD-CE | 6.17 | 110.07 | 100.20 |
| 1 | 159-A | 101 | GLU | CA-CB-CG | 6.16 | 126.96 | 113.40 |
| 1 | 153-A | 1 | MET | CB-CG-SD | 6.16 | 130.88 | 112.40 |
| 1 | 23-A | 101 | GLU | CA-CB-CG | 6.16 | 126.95 | 113.40 |
| 1 | 81-A | 16 | MET | CA-CB-CG | 6.16 | 123.76 | 113.30 |
| 1 | 189-A | 91 | ILE | CG1-CB-CG2 | -6.15 | 97.86 | 111.40 |
| 1 | 45-A | 20 | MET | CG-SD-CE | -6.14 | 90.37 | 100.20 |
| 1 | 222-A | 159 | ARG | NE-CZ-NH1 | 6.13 | 123.37 | 120.30 |
| 1 | 66-A | 1 | MET | CG-SD-CE | 6.12 | 110.00 | 100.20 |
| 1 | 35-A | 44 | ARG | NE-CZ-NH2 | -6.12 | 117.24 | 120.30 |
| 1 | 180-A | 142 | ASP | CB-CG-OD2 | -6.12 | 112.79 | 118.30 |
| 1 | 122-A | 159 | ARG | NE-CZ-NH1 | 6.12 | 123.36 | 120.30 |
| 1 | 25-A | 106 | LYS | CD-CE-NZ | 6.11 | 125.76 | 111.70 |
| 1 | 34-A | 44 | ARG | CB-CG-CD | 6.11 | 127.49 | 111.60 |
| 1 | 145-A | 33 | ARG | NE-CZ-NH1 | 6.11 | 123.36 | 120.30 |
| 1 | 101-A | 85 | CYS | CB-CA-C | -6.11 | 98.19 | 110.40 |
| 1 | 144-A | 109 | LYS | CD-CE-NZ | 6.11 | 125.75 | 111.70 |
| 1 | 24-A | 20 | MET | CB-CG-SD | 6.11 | 130.72 | 112.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 174-A | 12 | ARG | NE-CZ-NH2 | -6.11 | 117.25 | 120.30 |
| 1 | 171-A | 12 | ARG | NE-CZ-NH2 | -6.10 | 117.25 | 120.30 |
| 1 | 212-A | 20 | MET | CB-CG-SD | 6.10 | 130.71 | 112.40 |
| 1 | 72-A | 159 | ARG | CG-CD-NE | 6.10 | 124.62 | 111.80 |
| 1 | 16-A | 1 | MET | CB-CA-C | 6.10 | 122.60 | 110.40 |
| 1 | 132-A | 52 | ARG | NE-CZ-NH2 | -6.10 | 117.25 | 120.30 |
| 1 | 181-A | 22 | TRP | N-CA-C | -6.10 | 94.54 | 111.00 |
| 1 | 18-A | 16 | MET | CG-SD-CE | 6.10 | 109.95 | 100.20 |
| 1 | 107-A | 87 | ASP | CB-CG-OD1 | 6.10 | 123.79 | 118.30 |
| 1 | 38-A | 12 | ARG | NE-CZ-NH2 | -6.09 | 117.25 | 120.30 |
| 1 | 177-A | 20 | MET | CG-SD-CE | -6.09 | 90.45 | 100.20 |
| 1 | 136-A | 19 | ALA | C-N-CA | 6.09 | 136.92 | 121.70 |
| 1 | 27-A | 87 | ASP | CB-CG-OD2 | 6.09 | 123.78 | 118.30 |
| 1 | 182-A | 158 | ARG | NE-CZ-NH1 | 6.09 | 123.34 | 120.30 |
| 1 | 145-A | 20 | MET | N-CA-C | -6.08 | 94.57 | 111.00 |
| 1 | 47-A | 159 | ARG | NE-CZ-NH1 | 6.08 | 123.34 | 120.30 |
| 1 | 218-A | 19 | ALA | N-CA-C | 6.08 | 127.42 | 111.00 |
| 1 | 240-A | 12 | ARG | NE-CZ-NH2 | -6.07 | 117.27 | 120.30 |
| 1 | 73-A | 16 | MET | CB-CG-SD | 6.07 | 130.60 | 112.40 |
| 1 | 22-A | 101 | GLU | CA-CB-CG | 6.06 | 126.74 | 113.40 |
| 1 | 134-A | 1 | MET | CB-CG-SD | -6.06 | 94.21 | 112.40 |
| 1 | 206-A | 16 | MET | CG-SD-CE | 6.06 | 109.90 | 100.20 |
| 1 | 2-A | 98 | ARG | NE-CZ-NH2 | 6.06 | 123.33 | 120.30 |
| 1 | 95-A | 24 | LEU | CA-CB-CG | 6.06 | 129.24 | 115.30 |
| 1 | 211-A | 44 | ARG | NE-CZ-NH1 | 6.06 | 123.33 | 120.30 |
| 1 | 137-A | 127 | ASP | N-CA-C | -6.06 | 94.64 | 111.00 |
| 1 | 122-A | 98 | ARG | NE-CZ-NH2 | -6.06 | 117.27 | 120.30 |
| 1 | 124-A | 1 | MET | CG-SD-CE | -6.06 | 90.51 | 100.20 |
| 1 | 175-A | 44 | ARG | NE-CZ-NH1 | 6.05 | 123.33 | 120.30 |
| 1 | 56-A | 156 | LEU | CB-CG-CD2 | 6.05 | 121.29 | 111.00 |
| 1 | 125-A | 12 | ARG | NE-CZ-NH1 | 6.05 | 123.32 | 120.30 |
| 1 | 145-A | 2 | ILE | CB-CA-C | -6.04 | 99.51 | 111.60 |
| 1 | 79-A | 52 | ARG | CG-CD-NE | 6.03 | 124.47 | 111.80 |
| 1 | 124-A | 79 | ASP | CB-CG-OD1 | -6.03 | 112.87 | 118.30 |
| 1 | 174-A | 33 | ARG | NE-CZ-NH2 | -6.03 | 117.28 | 120.30 |
| 1 | 111-A | 12 | ARG | NE-CZ-NH2 | -6.03 | 117.28 | 120.30 |
| 1 | 171-A | 33 | ARG | NE-CZ-NH1 | 6.03 | 123.32 | 120.30 |
| 1 | 84-A | 52 | ARG | NE-CZ-NH2 | -6.02 | 117.29 | 120.30 |
| 1 | 14-A | 20 | MET | CB-CA-C | 6.02 | 122.44 | 110.40 |
| 1 | 97-A | 20 | MET | CA-CB-CG | 6.01 | 123.52 | 113.30 |
| 1 | 210-A | 52 | ARG | CD-NE-CZ | 6.01 | 132.01 | 123.60 |
| 1 | 234-A | 52 | ARG | NE-CZ-NH1 | 6.01 | 123.30 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 6-A | 158 | ARG | NE-CZ-NH1 | 6.00 | 123.30 | 120.30 |
| 1 | 40-A | 120 | GLU | OE1-CD-OE2 | -6.00 | 116.10 | 123.30 |
| 1 | 55-A | 33 | ARG | NE-CZ-NH2 | -6.00 | 117.30 | 120.30 |
| 1 | 73-A | 98 | ARG | CB-CG-CD | 6.00 | 127.20 | 111.60 |
| 1 | 183-A | 148 | SER | CB-CA-C | 6.00 | 121.50 | 110.10 |
| 1 | 226-A | 76 | LYS | CD-CE-NZ | 6.00 | 125.50 | 111.70 |
| 1 | 79-A | 52 | ARG | NE-CZ-NH2 | 6.00 | 123.30 | 120.30 |
| 1 | 80-A | 52 | ARG | CG-CD-NE | 5.99 | 124.39 | 111.80 |
| 1 | 157-A | 33 | ARG | NE-CZ-NH1 | 5.99 | 123.30 | 120.30 |
| 1 | 215-A | 4 | LEU | CB-CG-CD1 | 5.98 | 121.17 | 111.00 |
| 1 | 218-A | 44 | ARG | NE-CZ-NH2 | -5.98 | 117.31 | 120.30 |
| 1 | 43-A | 120 | GLU | CB-CA-C | 5.98 | 122.36 | 110.40 |
| 1 | 140-A | 23 | ASN | N-CA-CB | 5.98 | 121.36 | 110.60 |
| 1 | 144-A | 52 | ARG | NE-CZ-NH1 | 5.98 | 123.29 | 120.30 |
| 1 | 160-A | 109 | LYS | CD-CE-NZ | -5.98 | 97.95 | 111.70 |
| 1 | 82-A | 128 | TYR | CA-CB-CG | 5.97 | 124.75 | 113.40 |
| 1 | 218-A | 44 | ARG | NE-CZ-NH1 | 5.97 | 123.29 | 120.30 |
| 1 | 225-A | 98 | ARG | NE-CZ-NH2 | -5.97 | 117.31 | 120.30 |
| 1 | 73-A | 79 | ASP | CB-CG-OD1 | 5.97 | 123.67 | 118.30 |
| 1 | 6-A | 20 | MET | CB-CG-SD | 5.97 | 130.30 | 112.40 |
| 1 | 213-A | 19 | ALA | N-CA-C | 5.96 | 127.10 | 111.00 |
| 1 | 167-A | 154 | GLU | CG-CD-OE1 | 5.96 | 130.21 | 118.30 |
| 1 | 173-A | 33 | ARG | NE-CZ-NH2 | -5.95 | 117.32 | 120.30 |
| 1 | 48-A | 20 | MET | CB-CG-SD | -5.95 | 94.55 | 112.40 |
| 1 | 132-A | 21 | PRO | CA-C-O | -5.95 | 105.93 | 120.20 |
| 1 | 226-A | 12 | ARG | NE-CZ-NH1 | 5.95 | 123.27 | 120.30 |
| 1 | 245-A | 132 | ASP | CB-CG-OD1 | 5.94 | 123.65 | 118.30 |
| 1 | 134-A | 21 | PRO | CA-C-N | -5.94 | 104.13 | 117.20 |
| 1 | 78-A | 16 | MET | CB-CG-SD | 5.94 | 130.22 | 112.40 |
| 1 | 72-A | 52 | ARG | NE-CZ-NH2 | 5.93 | 123.27 | 120.30 |
| 1 | 65-A | 19 | ALA | CA-C-N | -5.93 | 104.15 | 117.20 |
| 1 | 70-A | 44 | ARG | CD-NE-CZ | 5.93 | 131.90 | 123.60 |
| 1 | 84-A | 16 | MET | CG-SD-CE | 5.93 | 109.68 | 100.20 |
| 1 | 141-A | 1 | MET | CA-CB-CG | 5.93 | 123.37 | 113.30 |
| 1 | 142-A | 20 | MET | C-N-CD | -5.93 | 107.56 | 120.60 |
| 1 | 143-A | 19 | ALA | C-N-CA | -5.92 | 106.89 | 121.70 |
| 1 | 142-A | 12 | ARG | NE-CZ-NH1 | 5.92 | 123.26 | 120.30 |
| 1 | 118-A | 127 | ASP | N-CA-CB | 5.92 | 121.25 | 110.60 |
| 1 | 61-A | 109 | LYS | CD-CE-NZ | 5.91 | 125.30 | 111.70 |
| 1 | 97-A | 157 | GLU | OE1-CD-OE2 | -5.91 | 116.21 | 123.30 |
| 1 | 141-A | 16 | MET | CG-SD-CE | -5.91 | 90.75 | 100.20 |
| 1 | 165-A | 104 | LEU | CB-CG-CD1 | 5.91 | 121.04 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 246-A | 1 | MET | CA-CB-CG | 5.91 | 123.34 | 113.30 |
| 1 | 199-A | 159 | ARG | NE-CZ-NH1 | -5.90 | 117.35 | 120.30 |
| 1 | 149-A | 33 | ARG | NE-CZ-NH2 | -5.90 | 117.35 | 120.30 |
| 1 | 142-A | 21 | PRO | C-N-CA | 5.89 | 136.42 | 121.70 |
| 1 | 120-A | 1 | MET | CB-CG-SD | -5.88 | 94.75 | 112.40 |
| 1 | 177-A | 52 | ARG | NE-CZ-NH2 | -5.88 | 117.36 | 120.30 |
| 1 | 208-A | 16 | MET | CG-SD-CE | -5.88 | 90.78 | 100.20 |
| 1 | 223-A | 87 | ASP | CB-CG-OD2 | 5.88 | 123.60 | 118.30 |
| 1 | 201-A | 132 | ASP | CB-CG-OD2 | 5.88 | 123.59 | 118.30 |
| 1 | 8-A | 159 | ARG | NE-CZ-NH1 | 5.88 | 123.24 | 120.30 |
| 1 | 54-A | 131 | ASP | CB-CG-OD1 | 5.88 | 123.59 | 118.30 |
| 1 | 33-A | 1 | MET | N-CA-C | 5.87 | 126.86 | 111.00 |
| 1 | 183-A | 87 | ASP | CB-CG-OD1 | -5.87 | 113.02 | 118.30 |
| 1 | 213-A | 23 | ASN | CB-CA-C | -5.87 | 98.67 | 110.40 |
| 1 | 103-A | 101 | GLU | CG-CD-OE2 | -5.86 | 106.58 | 118.30 |
| 1 | 216-A | 12 | ARG | NE-CZ-NH1 | 5.86 | 123.23 | 120.30 |
| 1 | 77-A | 48 | GLU | OE1-CD-OE2 | -5.86 | 116.27 | 123.30 |
| 1 | 121-A | 20 | MET | N-CA-C | -5.86 | 95.18 | 111.00 |
| 1 | 71-A | 12 | ARG | NE-CZ-NH2 | -5.86 | 117.37 | 120.30 |
| 1 | 179-A | 17 | GLU | CB-CA-C | 5.86 | 122.11 | 110.40 |
| 1 | 171-A | 101 | GLU | CA-CB-CG | 5.85 | 126.28 | 113.40 |
| 1 | 94-A | 44 | ARG | NE-CZ-NH2 | -5.85 | 117.38 | 120.30 |
| 1 | 207-A | 12 | ARG | NE-CZ-NH2 | -5.85 | 117.38 | 120.30 |
| 1 | 76-A | 108 | GLN | CA-CB-CG | 5.84 | 126.26 | 113.40 |
| 1 | 188-A | 159 | ARG | NE-CZ-NH1 | 5.84 | 123.22 | 120.30 |
| 1 | 82-A | 24 | LEU | CB-CG-CD1 | 5.84 | 120.93 | 111.00 |
| 1 | 23-A | 148 | SER | N-CA-CB | 5.84 | 119.26 | 110.50 |
| 1 | 49-A | 33 | ARG | NE-CZ-NH2 | 5.84 | 123.22 | 120.30 |
| 1 | 166-A | 20 | MET | CB-CG-SD | -5.84 | 94.88 | 112.40 |
| 1 | 103-A | 109 | LYS | CD-CE-NZ | -5.84 | 98.28 | 111.70 |
| 1 | 151-A | 70 | ASP | CB-CG-OD2 | 5.84 | 123.55 | 118.30 |
| 1 | 220-A | 33 | ARG | NE-CZ-NH1 | 5.84 | 123.22 | 120.30 |
| 1 | 137-A | 127 | ASP | CB-CG-OD2 | -5.83 | 113.05 | 118.30 |
| 1 | 13-A | 20 | MET | CA-CB-CG | -5.83 | 103.39 | 113.30 |
| 1 | 215-A | 44 | ARG | NE-CZ-NH1 | 5.83 | 123.22 | 120.30 |
| 1 | 90-A | 20 | MET | CB-CG-SD | 5.83 | 129.88 | 112.40 |
| 1 | 191-A | 127 | ASP | CB-CG-OD1 | 5.83 | 123.54 | 118.30 |
| 1 | 11-A | 120 | GLU | N-CA-CB | 5.83 | 121.09 | 110.60 |
| 1 | 20-A | 156 | LEU | CA-CB-CG | 5.83 | 128.70 | 115.30 |
| 1 | 130-A | 22 | TRP | N-CA-C | -5.83 | 95.27 | 111.00 |
| 1 | 164-A | 109 | LYS | CD-CE-NZ | 5.83 | 125.10 | 111.70 |
| 1 | 86-A | 44 | ARG | NE-CZ-NH2 | -5.82 | 117.39 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 77-A | 24 | LEU | CA-CB-CG | 5.82 | 128.68 | 115.30 |
| 1 | 176-A | 120 | GLU | CB-CA-C | -5.81 | 98.77 | 110.40 |
| 1 | 74-A | 158 | ARG | NE-CZ-NH1 | 5.81 | 123.21 | 120.30 |
| 1 | 76-A | 159 | ARG | NE-CZ-NH1 | 5.81 | 123.21 | 120.30 |
| 1 | 198-A | 32 | LYS | CD-CE-NZ | -5.81 | 98.33 | 111.70 |
| 1 | 8-A | 157 | GLU | CA-CB-CG | 5.81 | 126.18 | 113.40 |
| 1 | 160-A | 139 | GLU | CA-CB-CG | 5.81 | 126.18 | 113.40 |
| 1 | 88-A | 33 | ARG | NE-CZ-NH1 | 5.81 | 123.20 | 120.30 |
| 1 | 122-A | 159 | ARG | NE-CZ-NH2 | -5.81 | 117.40 | 120.30 |
| 1 | 246-A | 157 | GLU | OE1-CD-OE2 | 5.81 | 130.27 | 123.30 |
| 1 | 218-A | 1 | MET | CG-SD-CE | 5.81 | 109.49 | 100.20 |
| 1 | 124-A | 16 | MET | CG-SD-CE | -5.80 | 90.92 | 100.20 |
| 1 | 201-A | 79 | ASP | CB-CG-OD2 | -5.80 | 113.08 | 118.30 |
| 1 | 217-A | 20 | MET | CG-SD-CE | 5.80 | 109.47 | 100.20 |
| 1 | 224-A | 157 | GLU | OE1-CD-OE2 | 5.80 | 130.25 | 123.30 |
| 1 | 248-A | 1 | MET | CB-CA-C | 5.79 | 121.99 | 110.40 |
| 1 | 78-A | 127 | ASP | CB-CG-OD2 | 5.79 | 123.51 | 118.30 |
| 1 | 12-A | 20 | MET | CA-CB-CG | 5.79 | 123.14 | 113.30 |
| 1 | 182-A | 44 | ARG | NE-CZ-NH2 | -5.79 | 117.41 | 120.30 |
| 1 | 197-A | 33 | ARG | NE-CZ-NH2 | -5.79 | 117.41 | 120.30 |
| 1 | 84-A | 159 | ARG | CG-CD-NE | 5.79 | 123.95 | 111.80 |
| 1 | 134-A | 20 | MET | CG-SD-CE | 5.79 | 109.46 | 100.20 |
| 1 | 107-A | 36 | LEU | CA-CB-CG | 5.78 | 128.60 | 115.30 |
| 1 | 203-A | 52 | ARG | NE-CZ-NH1 | 5.78 | 123.19 | 120.30 |
| 1 | 53-A | 1 | MET | CG-SD-CE | 5.78 | 109.45 | 100.20 |
| 1 | 210-A | 12 | ARG | NE-CZ-NH2 | -5.78 | 117.41 | 120.30 |
| 1 | 46-A | 1 | MET | CG-SD-CE | -5.78 | 90.95 | 100.20 |
| 1 | 132-A | 52 | ARG | NE-CZ-NH1 | 5.78 | 123.19 | 120.30 |
| 1 | 162-A | 22 | TRP | N-CA-C | -5.78 | 95.40 | 111.00 |
| 1 | 182-A | 44 | ARG | NE-CZ-NH1 | 5.78 | 123.19 | 120.30 |
| 1 | 158-A | 142 | ASP | CB-CA-C | -5.76 | 98.87 | 110.40 |
| 1 | 123-A | 22 | TRP | N-CA-CB | 5.76 | 120.97 | 110.60 |
| 1 | 73-A | 159 | ARG | CG-CD-NE | -5.76 | 99.71 | 111.80 |
| 1 | 134-A | 20 | MET | N-CA-C | -5.76 | 95.46 | 111.00 |
| 1 | 90-A | 16 | MET | N-CA-CB | 5.75 | 120.95 | 110.60 |
| 1 | 143-A | 21 | PRO | CA-N-CD | -5.75 | 103.44 | 111.50 |
| 1 | 184-A | 139 | GLU | CA-CB-CG | 5.75 | 126.06 | 113.40 |
| 1 | 190-A | 128 | TYR | CB-CG-CD2 | -5.75 | 117.55 | 121.00 |
| 1 | 102-A | 159 | ARG | CG-CD-NE | -5.75 | 99.72 | 111.80 |
| 1 | 137-A | 44 | ARG | NE-CZ-NH2 | -5.75 | 117.43 | 120.30 |
| 1 | 41-A | 4 | LEU | CB-CG-CD2 | 5.74 | 120.76 | 111.00 |
| 1 | 88-A | 20 | MET | CG-SD-CE | -5.74 | 91.01 | 100.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 158-A | 142 | ASP | N-CA-CB | -5.74 | 100.26 | 110.60 |
| 1 | 163-A | 139 | GLU | OE1-CD-OE2 | -5.74 | 116.41 | 123.30 |
| 1 | 242-A | 108 | GLN | CA-CB-CG | 5.74 | 126.03 | 113.40 |
| 1 | 244-A | 119 | VAL | CB-CA-C | -5.74 | 100.49 | 111.40 |
| 1 | 84-A | 16 | MET | N-CA-CB | -5.74 | 100.28 | 110.60 |
| 1 | 30-A | 20 | MET | CG-SD-CE | -5.73 | 91.03 | 100.20 |
| 1 | 226-A | 12 | ARG | NE-CZ-NH2 | -5.73 | 117.43 | 120.30 |
| 1 | 250-A | 21 | PRO | CA-C-N | -5.73 | 104.59 | 117.20 |
| 1 | 66-A | 19 | ALA | CA-C-N | -5.73 | 104.60 | 117.20 |
| 1 | 210-A | 4 | LEU | CB-CG-CD2 | -5.73 | 101.27 | 111.00 |
| 1 | 168-A | 1 | MET | CB-CG-SD | 5.72 | 129.56 | 112.40 |
| 1 | 218-A | 154 | GLU | OE1-CD-OE2 | -5.72 | 116.44 | 123.30 |
| 1 | 68-A | 159 | ARG | CG-CD-NE | 5.72 | 123.80 | 111.80 |
| 1 | 213-A | 12 | ARG | NE-CZ-NH2 | -5.71 | 117.44 | 120.30 |
| 1 | 217-A | 22 | TRP | N-CA-C | -5.71 | 95.57 | 111.00 |
| 1 | 92-A | 52 | ARG | NE-CZ-NH1 | 5.71 | 123.16 | 120.30 |
| 1 | 215-A | 131 | ASP | CB-CG-OD1 | 5.71 | 123.44 | 118.30 |
| 1 | 4-A | 36 | LEU | CB-CG-CD2 | -5.71 | 101.30 | 111.00 |
| 1 | 13-A | 1 | MET | CA-CB-CG | 5.71 | 123.00 | 113.30 |
| 1 | 114-A | 120 | GLU | N-CA-CB | -5.71 | 100.33 | 110.60 |
| 1 | 130-A | 87 | ASP | CB-CG-OD2 | -5.71 | 113.16 | 118.30 |
| 1 | 137-A | 16 | MET | CB-CG-SD | -5.71 | 95.29 | 112.40 |
| 1 | 92-A | 131 | ASP | CB-CG-OD1 | 5.70 | 123.43 | 118.30 |
| 1 | 13-A | 134 | GLU | CB-CA-C | -5.70 | 99.00 | 110.40 |
| 1 | 159-A | 142 | ASP | CB-CG-OD2 | -5.70 | 113.17 | 118.30 |
| 1 | 189-A | 19 | ALA | N-CA-C | 5.70 | 126.39 | 111.00 |
| 1 | 196-A | 20 | MET | N-CA-CB | 5.70 | 120.86 | 110.60 |
| 1 | 107-A | 20 | MET | CB-CG-SD | -5.70 | 95.31 | 112.40 |
| 1 | 63-A | 12 | ARG | NE-CZ-NH2 | -5.70 | 117.45 | 120.30 |
| 1 | 74-A | 24 | LEU | CA-CB-CG | 5.70 | 128.40 | 115.30 |
| 1 | 130-A | 44 | ARG | NE-CZ-NH1 | 5.69 | 123.15 | 120.30 |
| 1 | 215-A | 101 | GLU | N-CA-CB | -5.69 | 100.35 | 110.60 |
| 1 | 115-A | 52 | ARG | CG-CD-NE | 5.69 | 123.75 | 111.80 |
| 1 | 139-A | 12 | ARG | NE-CZ-NH2 | -5.69 | 117.45 | 120.30 |
| 1 | 39-A | 52 | ARG | NE-CZ-NH1 | 5.69 | 123.15 | 120.30 |
| 1 | 62-A | 44 | ARG | CA-CB-CG | 5.69 | 125.91 | 113.40 |
| 1 | 84-A | 52 | ARG | CG-CD-NE | -5.68 | 99.86 | 111.80 |
| 1 | 229-A | 44 | ARG | NE-CZ-NH2 | -5.68 | 117.46 | 120.30 |
| 1 | 91-A | 20 | MET | CA-CB-CG | 5.68 | 122.95 | 113.30 |
| 1 | 200-A | 152 | CYS | CA-CB-SG | 5.68 | 124.22 | 114.00 |
| 1 | 162-A | 20 | MET | CA-CB-CG | 5.67 | 122.94 | 113.30 |
| 1 | 58-A | 49 | SER | N-CA-CB | 5.67 | 119.01 | 110.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 88-A | 159 | ARG | NE-CZ-NH1 | 5.67 | 123.14 | 120.30 |
| 1 | 126-A | 16 | MET | CB-CA-C | -5.67 | 99.06 | 110.40 |
| 1 | 238-A | 132 | ASP | CB-CA-C | 5.67 | 121.74 | 110.40 |
| 1 | 184-A | 12 | ARG | NE-CZ-NH2 | -5.66 | 117.47 | 120.30 |
| 1 | 191-A | 132 | ASP | CB-CG-OD2 | 5.66 | 123.40 | 118.30 |
| 1 | 210-A | 152 | CYS | CA-CB-SG | 5.66 | 124.19 | 114.00 |
| 1 | 82-A | 20 | MET | C-N-CD | 5.66 | 140.29 | 128.40 |
| 1 | 234-A | 52 | ARG | NE-CZ-NH2 | -5.66 | 117.47 | 120.30 |
| 1 | 144-A | 12 | ARG | NE-CZ-NH2 | -5.66 | 117.47 | 120.30 |
| 1 | 52-A | 52 | ARG | NE-CZ-NH1 | 5.65 | 123.13 | 120.30 |
| 1 | 104-A | 154 | GLU | CG-CD-OE2 | 5.65 | 129.60 | 118.30 |
| 1 | 114-A | 127 | ASP | CB-CG-OD1 | 5.65 | 123.39 | 118.30 |
| 1 | 151-A | 101 | GLU | CA-CB-CG | 5.65 | 125.84 | 113.40 |
| 1 | 138-A | 142 | ASP | CB-CA-C | -5.65 | 99.10 | 110.40 |
| 1 | 186-A | 17 | GLU | CB-CA-C | 5.65 | 121.70 | 110.40 |
| 1 | 66-A | 44 | ARG | CG-CD-NE | -5.65 | 99.94 | 111.80 |
| 1 | 188-A | 1 | MET | CA-CB-CG | 5.65 | 122.90 | 113.30 |
| 1 | 217-A | 156 | LEU | CA-CB-CG | 5.65 | 128.29 | 115.30 |
| 1 | 43-A | 33 | ARG | NE-CZ-NH1 | -5.64 | 117.48 | 120.30 |
| 1 | 59-A | 44 | ARG | CG-CD-NE | -5.64 | 99.95 | 111.80 |
| 1 | 50-A | 12 | ARG | NE-CZ-NH1 | 5.64 | 123.12 | 120.30 |
| 1 | 59-A | 24 | LEU | CB-CG-CD1 | 5.64 | 120.58 | 111.00 |
| 1 | 8-A | 4 | LEU | CB-CG-CD1 | 5.63 | 120.58 | 111.00 |
| 1 | 121-A | 119 | VAL | CB-CA-C | -5.63 | 100.70 | 111.40 |
| 1 | 217-A | 79 | ASP | N-CA-CB | 5.63 | 120.73 | 110.60 |
| 1 | 13-A | 142 | ASP | CB-CG-OD1 | 5.63 | 123.37 | 118.30 |
| 1 | 131-A | 21 | PRO | CA-C-O | -5.63 | 106.69 | 120.20 |
| 1 | 47-A | 52 | ARG | NE-CZ-NH1 | 5.63 | 123.11 | 120.30 |
| 1 | 55-A | 159 | ARG | CG-CD-NE | 5.62 | 123.61 | 111.80 |
| 1 | 139-A | 1 | MET | CA-CB-CG | 5.62 | 122.86 | 113.30 |
| 1 | 240-A | 36 | LEU | CB-CG-CD2 | -5.62 | 101.44 | 111.00 |
| 1 | 53-A | 20 | MET | CG-SD-CE | -5.61 | 91.22 | 100.20 |
| 1 | 151-A | 12 | ARG | NE-CZ-NH1 | 5.61 | 123.11 | 120.30 |
| 1 | 231-A | 87 | ASP | CB-CG-OD2 | -5.61 | 113.25 | 118.30 |
| 1 | 205-A | 4 | LEU | CB-CG-CD1 | 5.61 | 120.53 | 111.00 |
| 1 | 205-A | 128 | TYR | CB-CG-CD2 | -5.61 | 117.64 | 121.00 |
| 1 | 89-A | 16 | MET | N-CA-CB | 5.61 | 120.69 | 110.60 |
| 1 | 199-A | 132 | ASP | CB-CG-OD2 | -5.61 | 113.25 | 118.30 |
| 1 | 232-A | 1 | MET | CG-SD-CE | 5.61 | 109.17 | 100.20 |
| 1 | 26-A | 1 | MET | CG-SD-CE | -5.60 | 91.23 | 100.20 |
| 1 | 156-A | 101 | GLU | CG-CD-OE1 | -5.60 | 107.10 | 118.30 |
| 1 | 26-A | 158 | ARG | NE-CZ-NH2 | -5.60 | 117.50 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 41-A | 1 | MET | CG-SD-CE | -5.60 | 91.24 | 100.20 |
| 1 | 124-A | 159 | ARG | CG-CD-NE | 5.60 | 123.56 | 111.80 |
| 1 | 129-A | 101 | GLU | CA-CB-CG | 5.60 | 125.72 | 113.40 |
| 1 | 140-A | 12 | ARG | NE-CZ-NH2 | -5.60 | 117.50 | 120.30 |
| 1 | 71-A | 33 | ARG | N-CA-CB | 5.59 | 120.66 | 110.60 |
| 1 | 120-A | 36 | LEU | CB-CG-CD1 | -5.59 | 101.50 | 111.00 |
| 1 | 242-A | 16 | MET | CG-SD-CE | 5.59 | 109.15 | 100.20 |
| 1 | 85-A | 24 | LEU | CB-CG-CD2 | -5.58 | 101.51 | 111.00 |
| 1 | 190-A | 1 | MET | N-CA-C | 5.58 | 126.08 | 111.00 |
| 1 | 191-A | 128 | TYR | CA-CB-CG | 5.58 | 124.01 | 113.40 |
| 1 | 125-A | 20 | MET | C-N-CA | 5.58 | 145.44 | 122.00 |
| 1 | 150-A | 44 | ARG | NE-CZ-NH1 | 5.58 | 123.09 | 120.30 |
| 1 | 137-A | 119 | VAL | CB-CA-C | -5.58 | 100.80 | 111.40 |
| 1 | 132-A | 21 | PRO | CA-C-N | 5.58 | 129.47 | 117.20 |
| 1 | 206-A | 20 | MET | CA-CB-CG | 5.58 | 122.78 | 113.30 |
| 1 | 224-A | 44 | ARG | NE-CZ-NH2 | -5.58 | 117.51 | 120.30 |
| 1 | 69-A | 44 | ARG | NH1-CZ-NH2 | 5.58 | 125.53 | 119.40 |
| 1 | 249-A | 52 | ARG | NE-CZ-NH1 | 5.58 | 123.09 | 120.30 |
| 1 | 12-A | 1 | MET | N-CA-C | -5.57 | 95.95 | 111.00 |
| 1 | 190-A | 119 | VAL | N-CA-CB | -5.57 | 99.24 | 111.50 |
| 1 | 208-A | 118 | GLU | N-CA-CB | -5.57 | 100.57 | 110.60 |
| 1 | 78-A | 52 | ARG | NE-CZ-NH1 | 5.57 | 123.08 | 120.30 |
| 1 | 184-A | 139 | GLU | CB-CA-C | 5.57 | 121.54 | 110.40 |
| 1 | 232-A | 4 | LEU | CB-CG-CD1 | 5.57 | 120.47 | 111.00 |
| 1 | 173-A | 12 | ARG | NE-CZ-NH2 | -5.57 | 117.52 | 120.30 |
| 1 | 249-A | 159 | ARG | NE-CZ-NH1 | 5.57 | 123.08 | 120.30 |
| 1 | 206-A | 16 | MET | N-CA-CB | -5.56 | 100.59 | 110.60 |
| 1 | 229-A | 1 | MET | CB-CA-C | 5.56 | 121.52 | 110.40 |
| 1 | 202-A | 1 | MET | N-CA-C | 5.56 | 126.01 | 111.00 |
| 1 | 196-A | 20 | MET | CG-SD-CE | -5.56 | 91.31 | 100.20 |
| 1 | 102-A | 104 | LEU | CA-CB-CG | 5.55 | 128.07 | 115.30 |
| 1 | 212-A | 127 | ASP | CB-CG-OD1 | 5.55 | 123.30 | 118.30 |
| 1 | 156-A | 158 | ARG | NE-CZ-NH1 | 5.55 | 123.08 | 120.30 |
| 1 | 180-A | 127 | ASP | CA-C-N | -5.55 | 104.99 | 117.20 |
| 1 | 173-A | 33 | ARG | NE-CZ-NH1 | 5.55 | 123.08 | 120.30 |
| 1 | 102-A | 44 | ARG | NE-CZ-NH2 | -5.55 | 117.53 | 120.30 |
| 1 | 224-A | 12 | ARG | NE-CZ-NH2 | -5.54 | 117.53 | 120.30 |
| 1 | 28-A | 131 | ASP | CB-CG-OD1 | 5.54 | 123.29 | 118.30 |
| 1 | 148-A | 33 | ARG | NE-CZ-NH1 | 5.54 | 123.07 | 120.30 |
| 1 | 104-A | 1 | MET | CG-SD-CE | 5.54 | 109.06 | 100.20 |
| 1 | 195-A | 18 | ASN | N-CA-CB | 5.54 | 120.57 | 110.60 |
| 1 | 60-A | 1 | MET | N-CA-C | 5.54 | 125.96 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 144-A | 16 | MET | CB-CA-C | -5.54 | 99.33 | 110.40 |
| 1 | 157-A | 21 | PRO | N-CA-C | 5.54 | 126.49 | 112.10 |
| 1 | 195-A | 28 | LEU | CA-CB-CG | 5.53 | 128.03 | 115.30 |
| 1 | 66-A | 87 | ASP | CB-CG-OD2 | 5.53 | 123.28 | 118.30 |
| 1 | 20-A | 144 | ASP | CB-CG-OD2 | -5.53 | 113.32 | 118.30 |
| 1 | 216-A | 156 | LEU | CA-CB-CG | 5.53 | 128.01 | 115.30 |
| 1 | 135-A | 142 | ASP | CB-CG-OD1 | -5.53 | 113.33 | 118.30 |
| 1 | 217-A | 79 | ASP | CB-CG-OD1 | 5.53 | 123.27 | 118.30 |
| 1 | 236-A | 4 | LEU | CB-CG-CD2 | -5.53 | 101.61 | 111.00 |
| 1 | 88-A | 44 | ARG | NE-CZ-NH1 | 5.52 | 123.06 | 120.30 |
| 1 | 183-A | 159 | ARG | NE-CZ-NH1 | -5.52 | 117.54 | 120.30 |
| 1 | 85-A | 16 | MET | CB-CG-SD | -5.52 | 95.84 | 112.40 |
| 1 | 2-A | 4 | LEU | CB-CG-CD1 | 5.52 | 120.38 | 111.00 |
| 1 | 58-A | 20 | MET | CG-SD-CE | -5.52 | 91.37 | 100.20 |
| 1 | 101-A | 20 | MET | CG-SD-CE | -5.52 | 91.38 | 100.20 |
| 1 | 175-A | 1 | MET | CG-SD-CE | -5.52 | 91.37 | 100.20 |
| 1 | 240-A | 118 | GLU | CA-CB-CG | 5.52 | 125.53 | 113.40 |
| 1 | 20-A | 122 | ASP | CB-CG-OD2 | -5.51 | 113.34 | 118.30 |
| 1 | 192-A | 134 | GLU | CA-CB-CG | 5.51 | 125.53 | 113.40 |
| 1 | 51-A | 118 | GLU | OE1-CD-OE2 | -5.51 | 116.69 | 123.30 |
| 1 | 94-A | 1 | MET | CA-C-N | -5.51 | 105.08 | 117.20 |
| 1 | 24-A | 44 | ARG | CG-CD-NE | -5.51 | 100.23 | 111.80 |
| 1 | 84-A | 127 | ASP | CB-CG-OD2 | 5.51 | 123.26 | 118.30 |
| 1 | 214-A | 159 | ARG | CD-NE-CZ | 5.51 | 131.31 | 123.60 |
| 1 | 13-A | 142 | ASP | N-CA-CB | -5.51 | 100.69 | 110.60 |
| 1 | 204-A | 20 | MET | CA-CB-CG | 5.51 | 122.66 | 113.30 |
| 1 | 228-A | 79 | ASP | CB-CG-OD1 | -5.51 | 113.34 | 118.30 |
| 1 | 239-A | 159 | ARG | CG-CD-NE | -5.51 | 100.23 | 111.80 |
| 1 | 12-A | 156 | LEU | CB-CG-CD1 | -5.50 | 101.64 | 111.00 |
| 1 | 158-A | 98 | ARG | CG-CD-NE | -5.50 | 100.25 | 111.80 |
| 1 | 36-A | 33 | ARG | NE-CZ-NH2 | -5.50 | 117.55 | 120.30 |
| 1 | 133-A | 19 | ALA | N-CA-C | 5.50 | 125.85 | 111.00 |
| 1 | 223-A | 20 | MET | N-CA-C | -5.50 | 96.16 | 111.00 |
| 1 | 88-A | 33 | ARG | NE-CZ-NH2 | -5.50 | 117.55 | 120.30 |
| 1 | 55-A | 44 | ARG | NE-CZ-NH2 | -5.50 | 117.55 | 120.30 |
| 1 | 129-A | 12 | ARG | NE-CZ-NH2 | -5.49 | 117.55 | 120.30 |
| 1 | 193-A | 44 | ARG | NE-CZ-NH1 | 5.49 | 123.05 | 120.30 |
| 1 | 245-A | 20 | MET | CA-CB-CG | 5.49 | 122.64 | 113.30 |
| 1 | 143-A | 28 | LEU | CB-CG-CD2 | -5.49 | 101.67 | 111.00 |
| 1 | 14-A | 118 | GLU | CA-CB-CG | 5.49 | 125.47 | 113.40 |
| 1 | 56-A | 1 | MET | CB-CG-SD | -5.49 | 95.93 | 112.40 |
| 1 | 76-A | 104 | LEU | CB-CG-CD1 | 5.49 | 120.33 | 111.00 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 96-A | 87 | ASP | CB-CG-OD2 | 5.49 | 123.24 | 118.30 |
| 1 | 229-A | 139 | GLU | CA-CB-CG | 5.49 | 125.47 | 113.40 |
| 1 | 245-A | 132 | ASP | CB-CA-C | -5.49 | 99.42 | 110.40 |
| 1 | 145-A | 20 | MET | C-N-CA | 5.49 | 145.04 | 122.00 |
| 1 | 227-A | 131 | ASP | CB-CG-OD1 | 5.49 | 123.24 | 118.30 |
| 1 | 64-A | 4 | LEU | CB-CG-CD1 | 5.49 | 120.32 | 111.00 |
| 1 | 67-A | 157 | GLU | CA-CB-CG | 5.49 | 125.47 | 113.40 |
| 1 | 78-A | 159 | ARG | CD-NE-CZ | 5.49 | 131.28 | 123.60 |
| 1 | 60-A | 1 | MET | CA-CB-CG | 5.48 | 122.62 | 113.30 |
| 1 | 228-A | 20 | MET | C-N-CD | -5.48 | 108.54 | 120.60 |
| 1 | 50-A | 12 | ARG | NE-CZ-NH2 | -5.48 | 117.56 | 120.30 |
| 1 | 201-A | 159 | ARG | NE-CZ-NH2 | 5.48 | 123.04 | 120.30 |
| 1 | 246-A | 1 | MET | CB-CG-SD | -5.48 | 95.97 | 112.40 |
| 1 | 215-A | 106 | LYS | CD-CE-NZ | 5.48 | 124.30 | 111.70 |
| 1 | 3-A | 79 | ASP | CB-CG-OD1 | -5.47 | 113.37 | 118.30 |
| 1 | 109-A | 4 | LEU | CB-CG-CD2 | 5.47 | 120.31 | 111.00 |
| 1 | 163-A | 33 | ARG | NE-CZ-NH1 | 5.47 | 123.04 | 120.30 |
| 1 | 11-A | 12 | ARG | NE-CZ-NH2 | -5.47 | 117.56 | 120.30 |
| 1 | 60-A | 127 | ASP | N-CA-CB | 5.47 | 120.45 | 110.60 |
| 1 | 212-A | 33 | ARG | NE-CZ-NH2 | -5.47 | 117.56 | 120.30 |
| 1 | 94-A | 1 | MET | CG-SD-CE | 5.47 | 108.95 | 100.20 |
| 1 | 201-A | 12 | ARG | NE-CZ-NH2 | -5.47 | 117.56 | 120.30 |
| 1 | 151-A | 1 | MET | C-N-CA | 5.47 | 135.37 | 121.70 |
| 1 | 14-A | 142 | ASP | N-CA-CB | -5.46 | 100.77 | 110.60 |
| 1 | 120-A | 23 | ASN | CB-CA-C | 5.46 | 121.32 | 110.40 |
| 1 | 157-A | 20 | MET | CB-CG-SD | -5.46 | 96.02 | 112.40 |
| 1 | 121-A | 4 | LEU | CB-CG-CD1 | 5.46 | 120.28 | 111.00 |
| 1 | 101-A | 12 | ARG | NE-CZ-NH2 | -5.46 | 117.57 | 120.30 |
| 1 | 175-A | 28 | LEU | CB-CG-CD1 | 5.46 | 120.28 | 111.00 |
| 1 | 186-A | 52 | ARG | NE-CZ-NH2 | -5.46 | 117.57 | 120.30 |
| 1 | 139-A | 44 | ARG | NE-CZ-NH1 | 5.45 | 123.03 | 120.30 |
| 1 | 224-A | 76 | LYS | CB-CA-C | -5.45 | 99.50 | 110.40 |
| 1 | 213-A | 127 | ASP | CB-CG-OD2 | -5.45 | 113.40 | 118.30 |
| 1 | 13-A | 44 | ARG | NE-CZ-NH1 | 5.45 | 123.02 | 120.30 |
| 1 | 104-A | 36 | LEU | CA-CB-CG | 5.44 | 127.81 | 115.30 |
| 1 | 199-A | 52 | ARG | NE-CZ-NH2 | -5.44 | 117.58 | 120.30 |
| 1 | 71-A | 128 | TYR | CA-CB-CG | 5.43 | 123.72 | 113.40 |
| 1 | 101-A | 20 | MET | CB-CG-SD | 5.43 | 128.69 | 112.40 |
| 1 | 131-A | 21 | PRO | N-CA-C | 5.43 | 126.22 | 112.10 |
| 1 | 11-A | 12 | ARG | NE-CZ-NH1 | 5.42 | 123.01 | 120.30 |
| 1 | 97-A | 24 | LEU | CA-CB-CG | 5.42 | 127.78 | 115.30 |
| 1 | 244-A | 158 | ARG | NE-CZ-NH1 | 5.42 | 123.01 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 26-A | 4 | LEU | CB-CG-CD1 | 5.42 | 120.21 | 111.00 |
| 1 | 68-A | 4 | LEU | CB-CG-CD1 | 5.42 | 120.21 | 111.00 |
| 1 | 94-A | 1 | MET | CB-CG-SD | -5.42 | 96.15 | 112.40 |
| 1 | 130-A | 88 | VAL | C-N-CD | 5.42 | 139.78 | 128.40 |
| 1 | 192-A | 44 | ARG | NE-CZ-NH1 | 5.42 | 123.01 | 120.30 |
| 1 | 41-A | 33 | ARG | NE-CZ-NH1 | 5.41 | 123.00 | 120.30 |
| 1 | 180-A | 12 | ARG | NE-CZ-NH2 | -5.40 | 117.60 | 120.30 |
| 1 | 10-A | 12 | ARG | NE-CZ-NH1 | 5.40 | 123.00 | 120.30 |
| 1 | 110-A | 87 | ASP | N-CA-CB | -5.40 | 100.89 | 110.60 |
| 1 | 90-A | 18 | ASN | CB-CA-C | 5.40 | 121.19 | 110.40 |
| 1 | 90-A | 44 | ARG | NE-CZ-NH1 | 5.39 | 123.00 | 120.30 |
| 1 | 199-A | 12 | ARG | NE-CZ-NH1 | 5.39 | 123.00 | 120.30 |
| 1 | 241-A | 70 | ASP | CB-CG-OD1 | 5.39 | 123.16 | 118.30 |
| 1 | 40-A | 119 | VAL | N-CA-C | -5.39 | 96.44 | 111.00 |
| 1 | 102-A | 109 | LYS | CD-CE-NZ | -5.39 | 99.30 | 111.70 |
| 1 | 143-A | 1 | MET | CG-SD-CE | 5.39 | 108.82 | 100.20 |
| 1 | 193-A | 12 | ARG | NE-CZ-NH2 | -5.39 | 117.61 | 120.30 |
| 1 | 133-A | 21 | PRO | CA-C-O | 5.38 | 133.12 | 120.20 |
| 1 | 105-A | 132 | ASP | CB-CA-C | -5.38 | 99.64 | 110.40 |
| 1 | 46-A | 12 | ARG | NE-CZ-NH2 | -5.38 | 117.61 | 120.30 |
| 1 | 72-A | 12 | ARG | NE-CZ-NH2 | -5.38 | 117.61 | 120.30 |
| 1 | 91-A | 128 | TYR | CA-CB-CG | 5.38 | 123.62 | 113.40 |
| 1 | 179-A | 152 | CYS | CA-CB-SG | -5.38 | 104.32 | 114.00 |
| 1 | 50-A | 33 | ARG | NE-CZ-NH1 | 5.37 | 122.99 | 120.30 |
| 1 | 63-A | 159 | ARG | CA-CB-CG | 5.37 | 125.22 | 113.40 |
| 1 | 78-A | 20 | MET | CB-CG-SD | 5.37 | 128.52 | 112.40 |
| 1 | 42-A | 120 | GLU | N-CA-CB | 5.37 | 120.27 | 110.60 |
| 1 | 62-A | 87 | ASP | CB-CG-OD2 | 5.37 | 123.13 | 118.30 |
| 1 | 153-A | 159 | ARG | CG-CD-NE | -5.37 | 100.53 | 111.80 |
| 1 | 73-A | 157 | GLU | OE1-CD-OE2 | -5.37 | 116.86 | 123.30 |
| 1 | 152-A | 120 | GLU | CA-CB-CG | 5.37 | 125.20 | 113.40 |
| 1 | 4-A | 101 | GLU | CA-CB-CG | 5.36 | 125.20 | 113.40 |
| 1 | 138-A | 12 | ARG | NE-CZ-NH2 | -5.36 | 117.62 | 120.30 |
| 1 | 75-A | 87 | ASP | CB-CG-OD2 | 5.36 | 123.12 | 118.30 |
| 1 | 143-A | 142 | ASP | N-CA-CB | -5.36 | 100.95 | 110.60 |
| 1 | 147-A | 18 | ASN | N-CA-C | 5.36 | 125.47 | 111.00 |
| 1 | 128-A | 1 | MET | CG-SD-CE | 5.36 | 108.77 | 100.20 |
| 1 | 179-A | 1 | MET | CG-SD-CE | -5.36 | 91.63 | 100.20 |
| 1 | 242-A | 131 | ASP | CB-CG-OD1 | 5.36 | 123.12 | 118.30 |
| 1 | 121-A | 52 | ARG | NE-CZ-NH1 | 5.35 | 122.98 | 120.30 |
| 1 | 172-A | 52 | ARG | CG-CD-NE | 5.35 | 123.04 | 111.80 |
| 1 | 245-A | 98 | ARG | NE-CZ-NH1 | 5.35 | 122.98 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 126-A | 12 | ARG | NE-CZ-NH2 | -5.35 | 117.62 | 120.30 |
| 1 | 209-A | 152 | CYS | CA-CB-SG | -5.35 | 104.36 | 114.00 |
| 1 | 115-A | 1 | MET | CA-CB-CG | 5.35 | 122.40 | 113.30 |
| 1 | 197-A | 159 | ARG | NE-CZ-NH2 | -5.35 | 117.62 | 120.30 |
| 1 | 225-A | 19 | ALA | N-CA-C | 5.35 | 125.45 | 111.00 |
| 1 | 155-A | 1 | MET | CG-SD-CE | -5.35 | 91.64 | 100.20 |
| 1 | 217-A | 1 | MET | CA-CB-CG | 5.35 | 122.39 | 113.30 |
| 1 | 219-A | 79 | ASP | CB-CG-OD2 | 5.34 | 123.11 | 118.30 |
| 1 | 24-A | 157 | GLU | CG-CD-OE1 | 5.34 | 128.99 | 118.30 |
| 1 | 223-A | 16 | MET | CB-CG-SD | 5.34 | 128.43 | 112.40 |
| 1 | 62-A | 65 | GLN | N-CA-CB | -5.34 | 100.99 | 110.60 |
| 1 | 140-A | 131 | ASP | CB-CG-OD1 | 5.34 | 123.11 | 118.30 |
| 1 | 164-A | 33 | ARG | CG-CD-NE | 5.34 | 123.02 | 111.80 |
| 1 | 174-A | 1 | MET | CG-SD-CE | -5.34 | 91.66 | 100.20 |
| 1 | 186-A | 101 | GLU | CB-CA-C | -5.34 | 99.72 | 110.40 |
| 1 | 112-A | 106 | LYS | CA-CB-CG | 5.34 | 125.14 | 113.40 |
| 1 | 244-A | 20 | MET | CB-CG-SD | -5.34 | 96.39 | 112.40 |
| 1 | 122-A | 87 | ASP | CB-CG-OD1 | -5.34 | 113.50 | 118.30 |
| 1 | 3-A | 131 | ASP | CB-CG-OD1 | 5.33 | 123.10 | 118.30 |
| 1 | 76-A | 79 | ASP | CB-CG-OD2 | -5.33 | 113.50 | 118.30 |
| 1 | 187-A | 159 | ARG | NE-CZ-NH2 | -5.33 | 117.63 | 120.30 |
| 1 | 22-A | 1 | MET | CG-SD-CE | 5.33 | 108.73 | 100.20 |
| 1 | 132-A | 44 | ARG | NE-CZ-NH2 | -5.33 | 117.64 | 120.30 |
| 1 | 144-A | 28 | LEU | CB-CG-CD1 | 5.33 | 120.05 | 111.00 |
| 1 | 214-A | 101 | GLU | OE1-CD-OE2 | -5.33 | 116.91 | 123.30 |
| 1 | 100-A | 44 | ARG | NE-CZ-NH2 | -5.32 | 117.64 | 120.30 |
| 1 | 101-A | 24 | LEU | CB-CG-CD1 | 5.32 | 120.05 | 111.00 |
| 1 | 182-A | 131 | ASP | CB-CG-OD1 | 5.32 | 123.09 | 118.30 |
| 1 | 174-A | 142 | ASP | N-CA-C | 5.32 | 125.36 | 111.00 |
| 1 | 233-A | 52 | ARG | NE-CZ-NH2 | -5.32 | 117.64 | 120.30 |
| 1 | 95-A | 159 | ARG | NE-CZ-NH2 | -5.32 | 117.64 | 120.30 |
| 1 | 28-A | 4 | LEU | CB-CG-CD1 | 5.32 | 120.04 | 111.00 |
| 1 | 124-A | 20 | MET | N-CA-CB | 5.32 | 120.17 | 110.60 |
| 1 | 217-A | 154 | GLU | CA-CB-CG | -5.32 | 101.70 | 113.40 |
| 1 | 68-A | 159 | ARG | CD-NE-CZ | 5.31 | 131.04 | 123.60 |
| 1 | 184-A | 1 | MET | N-CA-C | -5.31 | 96.65 | 111.00 |
| 1 | 62-A | 20 | MET | C-N-CD | -5.31 | 108.92 | 120.60 |
| 1 | 121-A | 87 | ASP | CB-CG-OD2 | -5.31 | 113.52 | 118.30 |
| 1 | 3-A | 33 | ARG | NE-CZ-NH2 | 5.30 | 122.95 | 120.30 |
| 1 | 111-A | 1 | MET | CB-CG-SD | 5.30 | 128.31 | 112.40 |
| 1 | 196-A | 20 | MET | N-CA-C | -5.30 | 96.68 | 111.00 |
| 1 | 123-A | 79 | ASP | CB-CG-OD1 | 5.30 | 123.07 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 141-A | 12 | ARG | NE-CZ-NH1 | 5.30 | 122.95 | 120.30 |
| 1 | 178-A | 52 | ARG | CG-CD-NE | -5.30 | 100.67 | 111.80 |
| 1 | 162-A | 12 | ARG | NE-CZ-NH1 | 5.30 | 122.95 | 120.30 |
| 1 | 131-A | 44 | ARG | NE-CZ-NH2 | -5.29 | 117.65 | 120.30 |
| 1 | 67-A | 19 | ALA | C-N-CA | 5.29 | 134.93 | 121.70 |
| 1 | 103-A | 1 | MET | CA-CB-CG | 5.29 | 122.29 | 113.30 |
| 1 | 171-A | 4 | LEU | CB-CG-CD1 | 5.29 | 119.99 | 111.00 |
| 1 | 146-A | 2 | ILE | N-CA-C | 5.28 | 125.27 | 111.00 |
| 1 | 23-A | 33 | ARG | NE-CZ-NH1 | 5.28 | 122.94 | 120.30 |
| 1 | 94-A | 159 | ARG | CD-NE-CZ | 5.28 | 131.00 | 123.60 |
| 1 | 149-A | 157 | GLU | CG-CD-OE2 | -5.28 | 107.74 | 118.30 |
| 1 | 79-A | 128 | TYR | CB-CG-CD2 | -5.28 | 117.83 | 121.00 |
| 1 | 129-A | 132 | ASP | CB-CG-OD1 | 5.28 | 123.05 | 118.30 |
| 1 | 86-A | 12 | ARG | NE-CZ-NH2 | -5.28 | 117.66 | 120.30 |
| 1 | 68-A | 44 | ARG | CG-CD-NE | -5.28 | 100.72 | 111.80 |
| 1 | 78-A | 1 | MET | CB-CG-SD | 5.28 | 128.23 | 112.40 |
| 1 | 201-A | 152 | CYS | N-CA-CB | -5.28 | 101.10 | 110.60 |
| 1 | 155-A | 20 | MET | C-N-CD | 5.27 | 139.48 | 128.40 |
| 1 | 200-A | 132 | ASP | CB-CA-C | -5.27 | 99.85 | 110.40 |
| 1 | 180-A | 127 | ASP | N-CA-CB | 5.27 | 120.09 | 110.60 |
| 1 | 245-A | 116 | ASP | CB-CG-OD1 | 5.27 | 123.05 | 118.30 |
| 1 | 132-A | 131 | ASP | CB-CG-OD1 | 5.27 | 123.04 | 118.30 |
| 1 | 156-A | 158 | ARG | NE-CZ-NH2 | -5.27 | 117.67 | 120.30 |
| 1 | 76-A | 20 | MET | CA-CB-CG | 5.27 | 122.25 | 113.30 |
| 1 | 140-A | 1 | MET | CG-SD-CE | -5.26 | 91.78 | 100.20 |
| 1 | 6-A | 158 | ARG | NE-CZ-NH2 | -5.26 | 117.67 | 120.30 |
| 1 | 133-A | 20 | MET | CB-CG-SD | -5.26 | 96.62 | 112.40 |
| 1 | 130-A | 21 | PRO | CA-C-O | 5.26 | 132.82 | 120.20 |
| 1 | 154-A | 131 | ASP | CB-CG-OD1 | 5.26 | 123.03 | 118.30 |
| 1 | 203-A | 159 | ARG | CD-NE-CZ | 5.26 | 130.96 | 123.60 |
| 1 | 230-A | 159 | ARG | CG-CD-NE | 5.25 | 122.84 | 111.80 |
| 1 | 109-A | 101 | GLU | OE1-CD-OE2 | 5.25 | 129.60 | 123.30 |
| 1 | 42-A | 101 | GLU | OE1-CD-OE2 | 5.25 | 129.59 | 123.30 |
| 1 | 138-A | 1 | MET | CG-SD-CE | 5.25 | 108.59 | 100.20 |
| 1 | 171-A | 142 | ASP | CB-CA-C | -5.25 | 99.91 | 110.40 |
| 1 | 129-A | 33 | ARG | NE-CZ-NH1 | 5.24 | 122.92 | 120.30 |
| 1 | 214-A | 4 | LEU | CB-CG-CD1 | 5.24 | 119.91 | 111.00 |
| 1 | 146-A | 12 | ARG | NE-CZ-NH2 | -5.24 | 117.68 | 120.30 |
| 1 | 15-A | 12 | ARG | NE-CZ-NH2 | -5.24 | 117.68 | 120.30 |
| 1 | 40-A | 33 | ARG | NE-CZ-NH1 | 5.24 | 122.92 | 120.30 |
| 1 | 86-A | 16 | MET | CB-CG-SD | -5.24 | 96.69 | 112.40 |
| 1 | 135-A | 16 | MET | CG-SD-CE | 5.24 | 108.58 | 100.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 185-A | 19 | ALA | N-CA-CB | -5.24 | 102.77 | 110.10 |
| 1 | 221-A | 33 | ARG | NE-CZ-NH1 | 5.24 | 122.92 | 120.30 |
| 1 | 132-A | 20 | MET | CB-CG-SD | 5.23 | 128.10 | 112.40 |
| 1 | 127-A | 20 | MET | CA-CB-CG | 5.23 | 122.19 | 113.30 |
| 1 | 128-A | 19 | ALA | C-N-CA | -5.23 | 108.62 | 121.70 |
| 1 | 131-A | 159 | ARG | CB-CG-CD | 5.23 | 125.20 | 111.60 |
| 1 | 173-A | 52 | ARG | CG-CD-NE | 5.23 | 122.78 | 111.80 |
| 1 | 209-A | 152 | CYS | N-CA-CB | -5.22 | 101.20 | 110.60 |
| 1 | 100-A | 159 | ARG | NE-CZ-NH2 | -5.22 | 117.69 | 120.30 |
| 1 | 184-A | 119 | VAL | CG1-CB-CG2 | -5.22 | 102.54 | 110.90 |
| 1 | 196-A | 20 | MET | CB-CA-C | -5.22 | 99.95 | 110.40 |
| 1 | 230-A | 20 | MET | N-CA-C | -5.22 | 96.90 | 111.00 |
| 1 | 250-A | 158 | ARG | NE-CZ-NH1 | 5.22 | 122.91 | 120.30 |
| 1 | 70-A | 52 | ARG | NE-CZ-NH1 | 5.22 | 122.91 | 120.30 |
| 1 | 142-A | 104 | LEU | CB-CG-CD1 | -5.22 | 102.13 | 111.00 |
| 1 | 152-A | 12 | ARG | NE-CZ-NH1 | 5.22 | 122.91 | 120.30 |
| 1 | 219-A | 159 | ARG | CG-CD-NE | 5.22 | 122.76 | 111.80 |
| 1 | 5-A | 108 | GLN | CB-CA-C | -5.22 | 99.97 | 110.40 |
| 1 | 53-A | 52 | ARG | NE-CZ-NH2 | -5.22 | 117.69 | 120.30 |
| 1 | 62-A | 16 | MET | CG-SD-CE | 5.21 | 108.54 | 100.20 |
| 1 | 28-A | 12 | ARG | NE-CZ-NH2 | -5.21 | 117.69 | 120.30 |
| 1 | 36-A | 12 | ARG | NE-CZ-NH2 | -5.21 | 117.69 | 120.30 |
| 1 | 23-A | 20 | MET | CG-SD-CE | -5.21 | 91.86 | 100.20 |
| 1 | 95-A | 52 | ARG | NE-CZ-NH1 | 5.21 | 122.91 | 120.30 |
| 1 | 13-A | 33 | ARG | NE-CZ-NH1 | 5.21 | 122.90 | 120.30 |
| 1 | 47-A | 20 | MET | C-N-CD | -5.21 | 109.15 | 120.60 |
| 1 | 58-A | 20 | MET | CB-CG-SD | 5.21 | 128.02 | 112.40 |
| 1 | 151-A | 79 | ASP | CB-CG-OD1 | 5.21 | 122.99 | 118.30 |
| 1 | 200-A | 139 | GLU | CA-CB-CG | 5.21 | 124.86 | 113.40 |
| 1 | 196-A | 4 | LEU | CB-CG-CD1 | 5.21 | 119.85 | 111.00 |
| 1 | 220-A | 159 | ARG | NE-CZ-NH2 | 5.21 | 122.90 | 120.30 |
| 1 | 129-A | 44 | ARG | NE-CZ-NH2 | -5.20 | 117.70 | 120.30 |
| 1 | 229-A | 52 | ARG | NE-CZ-NH1 | 5.20 | 122.90 | 120.30 |
| 1 | 34-A | 44 | ARG | NE-CZ-NH1 | -5.20 | 117.70 | 120.30 |
| 1 | 194-A | 70 | ASP | CB-CG-OD1 | 5.20 | 122.98 | 118.30 |
| 1 | 136-A | 159 | ARG | CD-NE-CZ | 5.20 | 130.88 | 123.60 |
| 1 | 151-A | 1 | MET | CG-SD-CE | 5.20 | 108.52 | 100.20 |
| 1 | 181-A | 44 | ARG | NE-CZ-NH2 | -5.20 | 117.70 | 120.30 |
| 1 | 59-A | 109 | LYS | CD-CE-NZ | 5.20 | 123.65 | 111.70 |
| 1 | 107-A | 12 | ARG | NE-CZ-NH2 | -5.19 | 117.70 | 120.30 |
| 1 | 238-A | 118 | GLU | OE1-CD-OE2 | -5.19 | 117.07 | 123.30 |
| 1 | 51-A | 159 | ARG | NE-CZ-NH2 | -5.19 | 117.70 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 238-A | 87 | ASP | CB-CG-OD2 | 5.19 | 122.97 | 118.30 |
| 1 | 113-A | 22 | TRP | N-CA-CB | -5.19 | 101.26 | 110.60 |
| 1 | 123-A | 158 | ARG | NE-CZ-NH1 | 5.19 | 122.89 | 120.30 |
| 1 | 5-A | 132 | ASP | CB-CG-OD2 | -5.19 | 113.63 | 118.30 |
| 1 | 125-A | 33 | ARG | CG-CD-NE | 5.19 | 122.69 | 111.80 |
| 1 | 162-A | 158 | ARG | NE-CZ-NH1 | 5.18 | 122.89 | 120.30 |
| 1 | 3-A | 2 | ILE | N-CA-C | -5.18 | 97.01 | 111.00 |
| 1 | 130-A | 12 | ARG | NE-CZ-NH2 | -5.18 | 117.71 | 120.30 |
| 1 | 196-A | 159 | ARG | NE-CZ-NH1 | 5.18 | 122.89 | 120.30 |
| 1 | 27-A | 4 | LEU | CB-CG-CD1 | 5.18 | 119.81 | 111.00 |
| 1 | 177-A | 4 | LEU | CB-CG-CD1 | 5.18 | 119.81 | 111.00 |
| 1 | 63-A | 4 | LEU | CB-CG-CD1 | 5.18 | 119.81 | 111.00 |
| 1 | 157-A | 20 | MET | CA-CB-CG | 5.18 | 122.10 | 113.30 |
| 1 | 157-A | 142 | ASP | N-CA-CB | -5.18 | 101.28 | 110.60 |
| 1 | 35-A | 132 | ASP | CB-CG-OD1 | -5.17 | 113.64 | 118.30 |
| 1 | 61-A | 12 | ARG | NE-CZ-NH2 | -5.17 | 117.71 | 120.30 |
| 1 | 28-A | 22 | TRP | N-CA-C | -5.17 | 97.03 | 111.00 |
| 1 | 122-A | 159 | ARG | CG-CD-NE | -5.17 | 100.94 | 111.80 |
| 1 | 203-A | 12 | ARG | NE-CZ-NH2 | -5.17 | 117.72 | 120.30 |
| 1 | 61-A | 20 | MET | CA-CB-CG | 5.17 | 122.09 | 113.30 |
| 1 | 134-A | 4 | LEU | CB-CG-CD1 | 5.17 | 119.79 | 111.00 |
| 1 | 215-A | 152 | CYS | CA-CB-SG | 5.17 | 123.30 | 114.00 |
| 1 | 73-A | 79 | ASP | CB-CG-OD2 | -5.17 | 113.65 | 118.30 |
| 1 | 79-A | 159 | ARG | CD-NE-CZ | 5.17 | 130.83 | 123.60 |
| 1 | 238-A | 12 | ARG | NE-CZ-NH2 | -5.17 | 117.72 | 120.30 |
| 1 | 160-A | 12 | ARG | NE-CZ-NH2 | -5.16 | 117.72 | 120.30 |
| 1 | 169-A | 22 | TRP | N-CA-C | -5.16 | 97.06 | 111.00 |
| 1 | 212-A | 98 | ARG | NE-CZ-NH1 | 5.16 | 122.88 | 120.30 |
| 1 | 91-A | 1 | MET | CG-SD-CE | -5.16 | 91.94 | 100.20 |
| 1 | 92-A | 24 | LEU | CB-CG-CD2 | 5.16 | 119.77 | 111.00 |
| 1 | 63-A | 44 | ARG | CA-CB-CG | 5.16 | 124.75 | 113.40 |
| 1 | 183-A | 87 | ASP | CB-CG-OD2 | 5.16 | 122.94 | 118.30 |
| 1 | 93-A | 52 | ARG | CG-CD-NE | -5.16 | 100.97 | 111.80 |
| 1 | 189-A | 98 | ARG | NE-CZ-NH2 | -5.16 | 117.72 | 120.30 |
| 1 | 190-A | 118 | GLU | C-N-CA | 5.16 | 134.59 | 121.70 |
| 1 | 161-A | 33 | ARG | NE-CZ-NH1 | -5.15 | 117.72 | 120.30 |
| 1 | 1-A | 52 | ARG | NE-CZ-NH2 | -5.15 | 117.72 | 120.30 |
| 1 | 165-A | 132 | ASP | CB-CG-OD2 | 5.15 | 122.94 | 118.30 |
| 1 | 46-A | 1 | MET | CA-CB-CG | 5.15 | 122.06 | 113.30 |
| 1 | 139-A | 102 | GLN | CA-CB-CG | -5.15 | 102.07 | 113.40 |
| 1 | 216-A | 44 | ARG | NE-CZ-NH2 | -5.15 | 117.73 | 120.30 |
| 1 | 47-A | 44 | ARG | NE-CZ-NH2 | -5.15 | 117.73 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1 | 36-A | 101 | GLU | N-CA-CB | 5.14 | 119.86 | 110.60 |
| 1 | 145-A | 20 | MET | CB-CG-SD | 5.14 | 127.83 | 112.40 |
| 1 | 102-A | 109 | LYS | CB-CA-C | -5.14 | 100.11 | 110.40 |
| 1 | 144-A | 109 | LYS | CB-CA-C | -5.14 | 100.11 | 110.40 |
| 1 | 90-A | 65 | GLN | CA-CB-CG | 5.14 | 124.71 | 113.40 |
| 1 | 130-A | 159 | ARG | CA-CB-CG | -5.14 | 102.10 | 113.40 |
| 1 | 52-A | 16 | MET | CG-SD-CE | 5.13 | 108.41 | 100.20 |
| 1 | 73-A | 106 | LYS | CB-CA-C | 5.13 | 120.66 | 110.40 |
| 1 | 169-A | 159 | ARG | NE-CZ-NH2 | 5.13 | 122.86 | 120.30 |
| 1 | 231-A | 132 | ASP | CB-CA-C | -5.13 | 100.14 | 110.40 |
| 1 | 3-A | 87 | ASP | CB-CG-OD1 | 5.13 | 122.91 | 118.30 |
| 1 | 5-A | 12 | ARG | NE-CZ-NH2 | -5.13 | 117.74 | 120.30 |
| 1 | 28-A | 156 | LEU | CA-CB-CG | -5.13 | 103.51 | 115.30 |
| 1 | 215-A | 1 | MET | CA-CB-CG | 5.12 | 122.01 | 113.30 |
| 1 | 31-A | 1 | MET | CB-CG-SD | 5.12 | 127.77 | 112.40 |
| 1 | 138-A | 33 | ARG | NE-CZ-NH2 | -5.12 | 117.74 | 120.30 |
| 1 | 167-A | 52 | ARG | CB-CG-CD | 5.12 | 124.92 | 111.60 |
| 1 | 212-A | 20 | MET | CA-CB-CG | 5.12 | 122.01 | 113.30 |
| 1 | 212-A | 33 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 1 | 121-A | 36 | LEU | CB-CG-CD2 | -5.12 | 102.30 | 111.00 |
| 1 | 216-A | 44 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 1 | 111-A | 12 | ARG | NE-CZ-NH1 | 5.12 | 122.86 | 120.30 |
| 1 | 153-A | 98 | ARG | CA-CB-CG | 5.12 | 124.65 | 113.40 |
| 1 | 71-A | 12 | ARG | NE-CZ-NH1 | 5.11 | 122.86 | 120.30 |
| 1 | 142-A | 98 | ARG | NE-CZ-NH2 | -5.11 | 117.74 | 120.30 |
| 1 | 187-A | 1 | MET | CG-SD-CE | 5.11 | 108.38 | 100.20 |
| 1 | 213-A | 1 | MET | CA-CB-CG | 5.11 | 121.99 | 113.30 |
| 1 | 86-A | 1 | MET | CB-CG-SD | 5.11 | 127.74 | 112.40 |
| 1 | 65-A | 44 | ARG | NE-CZ-NH2 | -5.11 | 117.75 | 120.30 |
| 1 | 222-A | 1 | MET | N-CA-C | 5.11 | 124.79 | 111.00 |
| 1 | 7-A | 16 | MET | CG-SD-CE | -5.11 | 92.03 | 100.20 |
| 1 | 7-A | 1 | MET | CA-CB-CG | 5.10 | 121.98 | 113.30 |
| 1 | 71-A | 52 | ARG | CG-CD-NE | 5.10 | 122.52 | 111.80 |
| 1 | 97-A | 138 | SER | CB-CA-C | -5.10 | 100.40 | 110.10 |
| 1 | 49-A | 22 | TRP | N-CA-CB | 5.10 | 119.78 | 110.60 |
| 1 | 145-A | 19 | ALA | O-C-N | -5.10 | 114.54 | 122.70 |
| 1 | 218-A | 33 | ARG | NE-CZ-NH2 | -5.10 | 117.75 | 120.30 |
| 1 | 90-A | 52 | ARG | NE-CZ-NH1 | 5.10 | 122.85 | 120.30 |
| 1 | 204-A | 159 | ARG | CD-NE-CZ | 5.10 | 130.74 | 123.60 |
| 1 | 223-A | 21 | PRO | N-CA-C | 5.10 | 125.35 | 112.10 |
| 1 | 62-A | 12 | ARG | NE-CZ-NH2 | -5.09 | 117.75 | 120.30 |
| 1 | 63-A | 20 | MET | CG-SD-CE | 5.09 | 108.35 | 100.20 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 168-A | 87 | ASP | CB-CG-OD2 | 5.09 | 122.88 | 118.30 |
| 1 | 208-A | 98 | ARG | NE-CZ-NH2 | -5.09 | 117.75 | 120.30 |
| 1 | 225-A | 154 | GLU | OE1-CD-OE2 | -5.09 | 117.19 | 123.30 |
| 1 | 70-A | 2 | ILE | N-CA-C | -5.09 | 97.25 | 111.00 |
| 1 | 84-A | 20 | MET | N-CA-C | 5.09 | 124.75 | 111.00 |
| 1 | 182-A | 152 | CYS | N-CA-CB | -5.09 | 101.44 | 110.60 |
| 1 | 215-A | 20 | MET | CB-CA-C | -5.09 | 100.22 | 110.40 |
| 1 | 175-A | 33 | ARG | NE-CZ-NH2 | -5.09 | 117.75 | 120.30 |
| 1 | 123-A | 70 | ASP | CB-CG-OD2 | 5.09 | 122.88 | 118.30 |
| 1 | 197-A | 20 | MET | N-CA-C | -5.08 | 97.27 | 111.00 |
| 1 | 163-A | 70 | ASP | CB-CG-OD1 | 5.08 | 122.88 | 118.30 |
| 1 | 219-A | 148 | SER | N-CA-CB | 5.08 | 118.12 | 110.50 |
| 1 | 210-A | 142 | ASP | CB-CA-C | -5.08 | 100.24 | 110.40 |
| 1 | 110-A | 159 | ARG | NE-CZ-NH2 | 5.08 | 122.84 | 120.30 |
| 1 | 150-A | 157 | GLU | CG-CD-OE1 | 5.08 | 128.46 | 118.30 |
| 1 | 46-A | 142 | ASP | N-CA-CB | -5.08 | 101.46 | 110.60 |
| 1 | 53-A | 87 | ASP | CB-CA-C | 5.08 | 120.55 | 110.40 |
| 1 | 156-A | 142 | ASP | CB-CG-OD1 | -5.08 | 113.73 | 118.30 |
| 1 | 192-A | 98 | ARG | NE-CZ-NH2 | -5.08 | 117.76 | 120.30 |
| 1 | 208-A | 4 | LEU | CB-CG-CD1 | 5.08 | 119.63 | 111.00 |
| 1 | 52-A | 101 | GLU | OE1-CD-OE2 | -5.07 | 117.21 | 123.30 |
| 1 | 96-A | 158 | ARG | NE-CZ-NH2 | -5.07 | 117.76 | 120.30 |
| 1 | 180-A | 142 | ASP | CB-CG-OD1 | 5.07 | 122.87 | 118.30 |
| 1 | 75-A | 24 | LEU | CA-CB-CG | 5.07 | 126.97 | 115.30 |
| 1 | 195-A | 28 | LEU | CB-CG-CD1 | 5.07 | 119.62 | 111.00 |
| 1 | 3-A | 52 | ARG | NE-CZ-NH2 | -5.07 | 117.77 | 120.30 |
| 1 | 41-A | 120 | GLU | CB-CA-C | 5.07 | 120.54 | 110.40 |
| 1 | 205-A | 20 | MET | CB-CG-SD | -5.07 | 97.19 | 112.40 |
| 1 | 2-A | 20 | MET | C-N-CD | -5.07 | 109.45 | 120.60 |
| 1 | 108-A | 20 | MET | N-CA-C | -5.07 | 97.32 | 111.00 |
| 1 | 123-A | 20 | MET | CB-CG-SD | 5.07 | 127.60 | 112.40 |
| 1 | 163-A | 12 | ARG | NE-CZ-NH2 | -5.07 | 117.77 | 120.30 |
| 1 | 59-A | 20 | MET | C-N-CD | -5.06 | 109.46 | 120.60 |
| 1 | 214-A | 158 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 1 | 125-A | 21 | PRO | CA-C-N | -5.06 | 106.06 | 117.20 |
| 1 | 185-A | 20 | MET | CA-CB-CG | 5.06 | 121.91 | 113.30 |
| 1 | 42-A | 4 | LEU | CB-CG-CD1 | 5.06 | 119.60 | 111.00 |
| 1 | 131-A | 4 | LEU | CB-CG-CD1 | 5.06 | 119.60 | 111.00 |
| 1 | 147-A | 12 | ARG | NE-CZ-NH2 | -5.06 | 117.77 | 120.30 |
| 1 | 148-A | 19 | ALA | N-CA-C | 5.06 | 124.66 | 111.00 |
| 1 | 239-A | 12 | ARG | NE-CZ-NH1 | 5.06 | 122.83 | 120.30 |
| 1 | 57-A | 79 | ASP | CB-CG-OD1 | -5.06 | 113.75 | 118.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 153-A | 1 | MET | CG-SD-CE | -5.06 | 92.11 | 100.20 |
| 1 | 12-A | 33 | ARG | CA-CB-CG | 5.05 | 124.52 | 113.40 |
| 1 | 56-A | 22 | TRP | CB-CA-C | 5.05 | 120.51 | 110.40 |
| 1 | 225-A | 157 | GLU | CG-CD-OE1 | -5.05 | 108.19 | 118.30 |
| 1 | 38-A | 120 | GLU | OE1-CD-OE2 | -5.05 | 117.24 | 123.30 |
| 1 | 191-A | 4 | LEU | CB-CG-CD1 | 5.05 | 119.59 | 111.00 |
| 1 | 211-A | 20 | MET | N-CA-C | 5.05 | 124.64 | 111.00 |
| 1 | 163-A | 118 | GLU | OE1-CD-OE2 | -5.05 | 117.24 | 123.30 |
| 1 | 243-A | 157 | GLU | CA-CB-CG | 5.05 | 124.51 | 113.40 |
| 1 | 173-A | 134 | GLU | CA-CB-CG | 5.05 | 124.50 | 113.40 |
| 1 | 175-A | 142 | ASP | N-CA-CB | -5.05 | 101.51 | 110.60 |
| 1 | 214-A | 21 | PRO | N-CA-C | 5.05 | 125.23 | 112.10 |
| 1 | 8-A | 12 | ARG | NE-CZ-NH1 | 5.05 | 122.82 | 120.30 |
| 1 | 213-A | 33 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 1 | 159-A | 4 | LEU | CB-CG-CD1 | 5.04 | 119.57 | 111.00 |
| 1 | 232-A | 87 | ASP | CB-CG-OD2 | -5.04 | 113.76 | 118.30 |
| 1 | 213-A | 33 | ARG | NE-CZ-NH2 | -5.04 | 117.78 | 120.30 |
| 1 | 67-A | 20 | MET | CA-CB-CG | 5.04 | 121.87 | 113.30 |
| 1 | 136-A | 20 | MET | CG-SD-CE | 5.04 | 108.26 | 100.20 |
| 1 | 183-A | 131 | ASP | CB-CG-OD1 | 5.04 | 122.83 | 118.30 |
| 1 | 141-A | 33 | ARG | NE-CZ-NH1 | 5.04 | 122.82 | 120.30 |
| 1 | 13-A | 4 | LEU | CB-CG-CD1 | 5.03 | 119.56 | 111.00 |
| 1 | 120-A | 4 | LEU | CB-CG-CD1 | 5.03 | 119.56 | 111.00 |
| 1 | 61-A | 20 | MET | CB-CG-SD | 5.03 | 127.50 | 112.40 |
| 1 | 29-A | 12 | ARG | NE-CZ-NH2 | -5.03 | 117.78 | 120.30 |
| 1 | 85-A | 98 | ARG | NE-CZ-NH2 | 5.03 | 122.81 | 120.30 |
| 1 | 199-A | 157 | GLU | OE1-CD-OE2 | 5.03 | 129.34 | 123.30 |
| 1 | 236-A | 1 | MET | CG-SD-CE | 5.03 | 108.25 | 100.20 |
| 1 | 237-A | 12 | ARG | NE-CZ-NH2 | -5.03 | 117.78 | 120.30 |
| 1 | 51-A | 24 | LEU | CA-CB-CG | 5.03 | 126.86 | 115.30 |
| 1 | 124-A | 101 | GLU | OE1-CD-OE2 | -5.03 | 117.27 | 123.30 |
| 1 | 143-A | 16 | MET | CB-CA-C | -5.03 | 100.34 | 110.40 |
| 1 | 95-A | 142 | ASP | CB-CG-OD2 | 5.03 | 122.82 | 118.30 |
| 1 | 124-A | 33 | ARG | NE-CZ-NH2 | 5.03 | 122.81 | 120.30 |
| 1 | 74-A | 76 | LYS | CB-CG-CD | 5.02 | 124.66 | 111.60 |
| 1 | 61-A | 159 | ARG | NE-CZ-NH1 | -5.02 | 117.79 | 120.30 |
| 1 | 183-A | 28 | LEU | CA-CB-CG | -5.02 | 103.75 | 115.30 |
| 1 | 231-A | 20 | MET | C-N-CD | 5.02 | 138.95 | 128.40 |
| 1 | 216-A | 142 | ASP | CB-CA-C | -5.02 | 100.36 | 110.40 |
| 1 | 124-A | 87 | ASP | CB-CA-C | 5.01 | 120.43 | 110.40 |
| 1 | 6-A | 1 | MET | CA-CB-CG | 5.01 | 121.82 | 113.30 |
| 1 | 40-A | 44 | ARG | NE-CZ-NH1 | 5.01 | 122.81 | 120.30 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | 95-A | 127 | ASP | CB-CG-OD2 | 5.01 | 122.81 | 118.30 |
| 1 | 136-A | 4 | LEU | CB-CG-CD1 | 5.01 | 119.52 | 111.00 |
| 1 | 67-A | 65 | GLN | CA-CB-CG | 5.01 | 124.42 | 113.40 |
| 1 | 71-A | 134 | GLU | CB-CA-C | -5.01 | 100.38 | 110.40 |
| 1 | 178-A | 20 | MET | CA-CB-CG | 5.01 | 121.81 | 113.30 |
| 1 | 242-A | 1 | MET | CB-CA-C | 5.01 | 120.42 | 110.40 |
| 1 | 237-A | 131 | ASP | CB-CG-OD1 | -5.01 | 113.79 | 118.30 |
| 1 | 7-A | 2 | ILE | CG1-CB-CG2 | -5.00 | 100.39 | 111.40 |
| 1 | 83-A | 119 | VAL | CB-CA-C | -5.00 | 101.89 | 111.40 |
| 1 | 135-A | 16 | MET | N-CA-CB | -5.00 | 101.59 | 110.60 |
| 1 | 9-A | 44 | ARG | NE-CZ-NH1 | 5.00 | 122.80 | 120.30 |
| 1 | 208-A | 52 | ARG | NE-CZ-NH1 | 5.00 | 122.80 | 120.30 |
| 1 | 95-A | 4 | LEU | CB-CG-CD1 | 5.00 | 119.50 | 111.00 |

There are no chirality outliers.

All (155) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | 1-A | 1 | MET | Peptide |
| 1 | 100-A | 1 | MET | Peptide |
| 1 | 101-A | 20 | MET | Peptide |
| 1 | 109-A | 148 | SER | Peptide |
| 1 | 109-A | 87 | ASP | Peptide |
| 1 | 113-A | 85 | CYS | Peptide |
| 1 | 114-A | 85 | CYS | Peptide |
| 1 | 115-A | 85 | CYS | Mainchain,Peptide |
| 1 | 120-A | 21 | PRO | Peptide |
| 1 | 120-A | 23 | ASN | Mainchain |
| 1 | 121-A | 21 | PRO | Peptide |
| 1 | 121-A | 22 | TRP | Peptide |
| 1 | 122-A | 21 | PRO | Peptide |
| 1 | 122-A | 22 | TRP | Peptide |
| 1 | 122-A | 23 | ASN | Peptide |
| 1 | 123-A | 19 | ALA | Peptide |
| 1 | 124-A | 19 | ALA | Peptide |
| 1 | 124-A | 21 | PRO | Mainchain,Peptide |
| 1 | 125-A | 21 | PRO | Peptide |
| 1 | 126-A | 19 | ALA | Peptide |
| 1 | 126-A | 21 | PRO | Peptide |
| 1 | 127-A | 21 | PRO | Peptide |
| 1 | 128-A | 19 | ALA | Peptide |
| 1 | 128-A | 21 | PRO | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | 129-A | 19 | ALA | Peptide |
| 1 | 129-A | 21 | PRO | Peptide |
| 1 | 13-A | 141 | HIS | Peptide |
| 1 | 130-A | 21 | PRO | Peptide |
| 1 | 131-A | 20 | MET | Peptide |
| 1 | 131-A | 21 | PRO | Peptide |
| 1 | 133-A | 1 | MET | Peptide |
| 1 | 133-A | 21 | PRO | Peptide |
| 1 | 134-A | 1 | MET | Peptide |
| 1 | 134-A | 21 | PRO | Peptide |
| 1 | 138-A | 19 | ALA | Mainchain,Peptide |
| 1 | 140-A | 19 | ALA | Peptide |
| 1 | 140-A | 21 | PRO | Peptide |
| 1 | 141-A | 17 | GLU | Peptide |
| 1 | 142-A | 141 | HIS | Peptide |
| 1 | 142-A | 17 | GLU | Peptide |
| 1 | 143-A | 20 | MET | Peptide |
| 1 | 144-A | 1 | MET | Peptide |
| 1 | 144-A | 20 | MET | Peptide |
| 1 | 146-A | 19 | ALA | Peptide |
| 1 | 147-A | 1 | MET | Peptide |
| 1 | 148-A | 1 | MET | Peptide |
| 1 | 149-A | 1 | MET | Peptide |
| 1 | 151-A | 1 | MET | Peptide |
| 1 | 152-A | 1 | MET | Peptide |
| 1 | 154-A | 22 | TRP | Peptide |
| 1 | 155-A | 119 | VAL | Peptide |
| 1 | 157-A | 141 | HIS | Peptide |
| 1 | 158-A | 141 | HIS | Peptide |
| 1 | 160-A | 87 | ASP | Peptide |
| 1 | 164-A | 1 | MET | Peptide |
| 1 | 173-A | 19 | ALA | Peptide |
| 1 | 174-A | 141 | HIS | Peptide |
| 1 | 175-A | 141 | HIS | Peptide |
| 1 | 175-A | 21 | PRO | Peptide |
| 1 | 176-A | 17 | GLU | Peptide |
| 1 | 177-A | 19 | ALA | Peptide |
| 1 | 178-A | 18 | ASN | Peptide |
| 1 | 178-A | 21 | PRO | Peptide |
| 1 | 180-A | 18 | ASN | Peptide |
| 1 | 181-A | 18 | ASN | Peptide |
| 1 | 182-A | 18 | ASN | Peptide |

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| Mol | Chain | Res | Type | Group |
|------------|--------------|------------|-------------|-------------------|
| 1 | 182-A | 22 | TRP | Peptide |
| 1 | 183-A | 1 | MET | Peptide |
| 1 | 184-A | 19 | ALA | Peptide |
| 1 | 185-A | 18 | ASN | Peptide |
| 1 | 185-A | 19 | ALA | Peptide |
| 1 | 186-A | 18 | ASN | Peptide |
| 1 | 187-A | 17 | GLU | Peptide |
| 1 | 187-A | 18 | ASN | Mainchain,Peptide |
| 1 | 188-A | 17 | GLU | Peptide |
| 1 | 188-A | 18 | ASN | Peptide |
| 1 | 190-A | 18 | ASN | Peptide |
| 1 | 191-A | 18 | ASN | Peptide |
| 1 | 192-A | 18 | ASN | Peptide |
| 1 | 193-A | 18 | ASN | Peptide |
| 1 | 194-A | 17 | GLU | Peptide |
| 1 | 194-A | 18 | ASN | Peptide |
| 1 | 195-A | 18 | ASN | Peptide |
| 1 | 197-A | 19 | ALA | Peptide |
| 1 | 205-A | 1 | MET | Peptide |
| 1 | 209-A | 118 | GLU | Peptide |
| 1 | 210-A | 19 | ALA | Peptide |
| 1 | 210-A | 20 | MET | Peptide |
| 1 | 212-A | 20 | MET | Peptide |
| 1 | 213-A | 19 | ALA | Peptide |
| 1 | 213-A | 20 | MET | Mainchain |
| 1 | 214-A | 19 | ALA | Peptide |
| 1 | 214-A | 87 | ASP | Peptide |
| 1 | 215-A | 18 | ASN | Peptide |
| 1 | 216-A | 18 | ASN | Peptide |
| 1 | 217-A | 19 | ALA | Peptide |
| 1 | 217-A | 86 | GLY | Peptide |
| 1 | 218-A | 18 | ASN | Peptide |
| 1 | 219-A | 18 | ASN | Peptide |
| 1 | 22-A | 148 | SER | Peptide |
| 1 | 220-A | 18 | ASN | Peptide |
| 1 | 221-A | 18 | ASN | Peptide |
| 1 | 222-A | 21 | PRO | Peptide |
| 1 | 223-A | 18 | ASN | Peptide |
| 1 | 223-A | 20 | MET | Peptide |
| 1 | 224-A | 1 | MET | Peptide |
| 1 | 224-A | 20 | MET | Peptide |
| 1 | 224-A | 21 | PRO | Peptide |

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| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-------------------|
| 1 | 225-A | 19 | ALA | Peptide |
| 1 | 226-A | 128 | TYR | Peptide |
| 1 | 226-A | 19 | ALA | Peptide |
| 1 | 229-A | 21 | PRO | Peptide |
| 1 | 247-A | 1 | MET | Peptide |
| 1 | 25-A | 19 | ALA | Peptide |
| 1 | 3-A | 1 | MET | Peptide |
| 1 | 34-A | 21 | PRO | Peptide |
| 1 | 35-A | 21 | PRO | Peptide |
| 1 | 4-A | 1 | MET | Peptide |
| 1 | 41-A | 1 | MET | Peptide |
| 1 | 46-A | 86 | GLY | Peptide |
| 1 | 47-A | 1 | MET | Peptide |
| 1 | 48-A | 65 | GLN | Peptide |
| 1 | 5-A | 1 | MET | Peptide |
| 1 | 53-A | 19 | ALA | Peptide |
| 1 | 57-A | 19 | ALA | Peptide |
| 1 | 57-A | 44 | ARG | Sidechain |
| 1 | 58-A | 118 | GLU | Peptide |
| 1 | 59-A | 119 | VAL | Peptide |
| 1 | 62-A | 20 | MET | Peptide |
| 1 | 65-A | 19 | ALA | Peptide |
| 1 | 65-A | 20 | MET | Peptide |
| 1 | 66-A | 19 | ALA | Mainchain,Peptide |
| 1 | 66-A | 20 | MET | Peptide |
| 1 | 67-A | 19 | ALA | Mainchain,Peptide |
| 1 | 67-A | 20 | MET | Peptide |
| 1 | 68-A | 19 | ALA | Mainchain,Peptide |
| 1 | 69-A | 1 | MET | Peptide |
| 1 | 70-A | 1 | MET | Peptide |
| 1 | 71-A | 1 | MET | Peptide |
| 1 | 78-A | 19 | ALA | Peptide |
| 1 | 8-A | 1 | MET | Peptide |
| 1 | 82-A | 1 | MET | Peptide |
| 1 | 83-A | 19 | ALA | Peptide |
| 1 | 84-A | 20 | MET | Peptide |
| 1 | 85-A | 21 | PRO | Peptide |
| 1 | 94-A | 1 | MET | Peptide |
| 1 | 96-A | 1 | MET | Peptide |
| 1 | 96-A | 118 | GLU | 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 | 1224 | 1223 | 0 | 0 |
| 1 | 2-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 3-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 4-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 5-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 6-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 7-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 8-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 9-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 10-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 11-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 12-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 13-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 14-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 15-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 16-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 17-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 18-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 19-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 20-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 21-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 22-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 23-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 24-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 25-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 26-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 27-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 28-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 29-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 30-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 31-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 32-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 33-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 34-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 35-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 36-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 37-A | 1268 | 1224 | 1223 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 38-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 39-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 40-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 41-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 42-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 43-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 44-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 45-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 46-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 47-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 48-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 49-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 50-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 51-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 52-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 53-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 54-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 55-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 56-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 57-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 58-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 59-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 60-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 61-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 62-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 63-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 64-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 65-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 66-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 67-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 68-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 69-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 70-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 71-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 72-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 73-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 74-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 75-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 76-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 77-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 78-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 79-A | 1268 | 1224 | 1223 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 80-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 81-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 82-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 83-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 84-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 85-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 86-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 87-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 88-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 89-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 90-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 91-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 92-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 93-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 94-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 95-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 96-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 97-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 98-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 99-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 100-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 101-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 102-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 103-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 104-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 105-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 106-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 107-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 108-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 109-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 110-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 111-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 112-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 113-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 114-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 115-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 116-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 117-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 118-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 119-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 120-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 121-A | 1268 | 1224 | 1223 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 122-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 123-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 124-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 125-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 126-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 127-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 128-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 129-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 130-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 131-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 132-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 133-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 134-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 135-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 136-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 137-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 138-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 139-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 140-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 141-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 142-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 143-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 144-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 145-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 146-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 147-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 148-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 149-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 150-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 151-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 152-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 153-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 154-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 155-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 156-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 157-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 158-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 159-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 160-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 161-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 162-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 163-A | 1268 | 1224 | 1223 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 164-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 165-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 166-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 167-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 168-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 169-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 170-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 171-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 172-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 173-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 174-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 175-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 176-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 177-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 178-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 179-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 180-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 181-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 182-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 183-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 184-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 185-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 186-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 187-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 188-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 189-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 190-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 191-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 192-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 193-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 194-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 195-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 196-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 197-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 198-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 199-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 200-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 201-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 202-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 203-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 204-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 205-A | 1268 | 1224 | 1223 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 206-A | 1268 | 1224 | 1222 | 0 | 0 |
| 1 | 207-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 208-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 209-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 210-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 211-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 212-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 213-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 214-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 215-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 216-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 217-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 218-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 219-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 220-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 221-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 222-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 223-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 224-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 225-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 226-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 227-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 228-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 229-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 230-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 231-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 232-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 233-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 234-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 235-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 236-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 237-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 238-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 239-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 240-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 241-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 242-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 243-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 244-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 245-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 246-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 247-A | 1268 | 1224 | 1223 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | 248-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 249-A | 1268 | 1224 | 1223 | 0 | 0 |
| 1 | 250-A | 1268 | 1224 | 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 |
| 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 | 16 | 0 | 0 |
| 2 | 38-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 39-A | 32 | 17 | 17 | 0 | 0 |

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

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

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

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | 166-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 167-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 168-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 169-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 170-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 171-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 172-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 173-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 174-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 175-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 176-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 177-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 178-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 179-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 180-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 181-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 182-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 183-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 184-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 185-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 186-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 187-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 188-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 189-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 190-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 191-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 192-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 193-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 194-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 195-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 196-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 197-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 198-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 199-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 200-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 201-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 202-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 203-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 204-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 205-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 206-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 207-A | 32 | 17 | 17 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | 208-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 209-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 210-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 211-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 212-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 213-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 214-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 215-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 216-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 217-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 218-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 219-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 220-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 221-A | 32 | 17 | 16 | 0 | 0 |
| 2 | 222-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 223-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 224-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 225-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 226-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 227-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 228-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 229-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 230-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 231-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 232-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 233-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 234-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 235-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 236-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 237-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 238-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 239-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 240-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 241-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 242-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 243-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 244-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 245-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 246-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 247-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 248-A | 32 | 17 | 17 | 0 | 0 |
| 2 | 249-A | 32 | 17 | 17 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 2 | 250-A | 32 | 17 | 17 | 0 | 0 |
| 3 | 1-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 2-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 3-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 4-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 5-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 6-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 7-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 8-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 9-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 10-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 11-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 12-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 13-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 14-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 15-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 16-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 17-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 18-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 19-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 20-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 21-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 22-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 23-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 24-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 25-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 26-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 27-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 28-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 29-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 30-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 31-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 32-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 33-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 34-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 35-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 36-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 37-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 38-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 39-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 40-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 41-A | 48 | 21 | 23 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | 42-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 43-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 44-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 45-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 46-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 47-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 48-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 49-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 50-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 51-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 52-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 53-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 54-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 55-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 56-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 57-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 58-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 59-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 60-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 61-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 62-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 63-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 64-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 65-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 66-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 67-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 68-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 69-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 70-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 71-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 72-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 73-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 74-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 75-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 76-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 77-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 78-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 79-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 80-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 81-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 82-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 83-A | 48 | 21 | 23 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | 84-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 85-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 86-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 87-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 88-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 89-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 90-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 91-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 92-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 93-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 94-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 95-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 96-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 97-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 98-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 99-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 100-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 101-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 102-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 103-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 104-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 105-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 106-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 107-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 108-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 109-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 110-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 111-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 112-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 113-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 114-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 115-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 116-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 117-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 118-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 119-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 120-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 121-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 122-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 123-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 124-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 125-A | 48 | 21 | 23 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | 126-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 127-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 128-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 129-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 130-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 131-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 132-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 133-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 134-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 135-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 136-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 137-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 138-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 139-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 140-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 141-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 142-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 143-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 144-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 145-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 146-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 147-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 148-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 149-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 150-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 151-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 152-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 153-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 154-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 155-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 156-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 157-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 158-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 159-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 160-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 161-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 162-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 163-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 164-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 165-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 166-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 167-A | 48 | 21 | 23 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | 168-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 169-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 170-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 171-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 172-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 173-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 174-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 175-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 176-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 177-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 178-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 179-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 180-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 181-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 182-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 183-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 184-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 185-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 186-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 187-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 188-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 189-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 190-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 191-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 192-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 193-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 194-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 195-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 196-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 197-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 198-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 199-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 200-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 201-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 202-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 203-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 204-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 205-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 206-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 207-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 208-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 209-A | 48 | 21 | 23 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | 210-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 211-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 212-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 213-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 214-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 215-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 216-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 217-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 218-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 219-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 220-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 221-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 222-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 223-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 224-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 225-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 226-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 227-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 228-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 229-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 230-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 231-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 232-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 233-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 234-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 235-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 236-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 237-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 238-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 239-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 240-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 241-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 242-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 243-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 244-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 245-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 246-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 247-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 248-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 249-A | 48 | 21 | 23 | 0 | 0 |
| 3 | 250-A | 48 | 21 | 23 | 0 | 0 |
| 4 | 1-A | 200 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | 2-A | 206 | 0 | 0 | 0 | 0 |
| 4 | 3-A | 185 | 0 | 0 | 0 | 0 |
| 4 | 4-A | 175 | 0 | 0 | 0 | 0 |
| 4 | 5-A | 186 | 0 | 0 | 0 | 0 |
| 4 | 6-A | 185 | 0 | 0 | 0 | 0 |
| 4 | 7-A | 202 | 0 | 0 | 0 | 0 |
| 4 | 8-A | 200 | 0 | 0 | 0 | 0 |
| 4 | 9-A | 201 | 0 | 0 | 0 | 0 |
| 4 | 10-A | 204 | 0 | 0 | 0 | 0 |
| 4 | 11-A | 205 | 0 | 0 | 0 | 0 |
| 4 | 12-A | 197 | 0 | 0 | 0 | 0 |
| 4 | 13-A | 192 | 0 | 0 | 0 | 0 |
| 4 | 14-A | 189 | 0 | 0 | 0 | 0 |
| 4 | 15-A | 173 | 0 | 0 | 0 | 0 |
| 4 | 16-A | 176 | 0 | 0 | 0 | 0 |
| 4 | 17-A | 188 | 0 | 0 | 0 | 0 |
| 4 | 18-A | 195 | 0 | 0 | 0 | 0 |
| 4 | 19-A | 196 | 0 | 0 | 0 | 0 |
| 4 | 20-A | 211 | 0 | 0 | 0 | 0 |
| 4 | 21-A | 189 | 0 | 0 | 0 | 0 |
| 4 | 22-A | 191 | 0 | 0 | 0 | 0 |
| 4 | 23-A | 173 | 0 | 0 | 0 | 0 |
| 4 | 24-A | 183 | 0 | 0 | 0 | 0 |
| 4 | 25-A | 174 | 0 | 0 | 0 | 0 |
| 4 | 26-A | 195 | 0 | 0 | 0 | 0 |
| 4 | 27-A | 188 | 0 | 0 | 0 | 0 |
| 4 | 28-A | 181 | 0 | 0 | 0 | 0 |
| 4 | 29-A | 183 | 0 | 0 | 0 | 0 |
| 4 | 30-A | 186 | 0 | 0 | 0 | 0 |
| 4 | 31-A | 191 | 0 | 0 | 0 | 0 |
| 4 | 32-A | 187 | 0 | 0 | 0 | 0 |
| 4 | 33-A | 190 | 0 | 0 | 0 | 0 |
| 4 | 34-A | 194 | 0 | 0 | 0 | 0 |
| 4 | 35-A | 201 | 0 | 0 | 0 | 0 |
| 4 | 36-A | 197 | 0 | 0 | 0 | 0 |
| 4 | 37-A | 196 | 0 | 0 | 0 | 0 |
| 4 | 38-A | 203 | 0 | 0 | 0 | 0 |
| 4 | 39-A | 181 | 0 | 0 | 0 | 0 |
| 4 | 40-A | 171 | 0 | 0 | 0 | 0 |
| 4 | 41-A | 179 | 0 | 0 | 0 | 0 |
| 4 | 42-A | 176 | 0 | 0 | 0 | 0 |
| 4 | 43-A | 176 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | 44-A | 183 | 0 | 0 | 0 | 0 |
| 4 | 45-A | 187 | 0 | 0 | 0 | 0 |
| 4 | 46-A | 197 | 0 | 0 | 0 | 0 |
| 4 | 47-A | 191 | 0 | 0 | 0 | 0 |
| 4 | 48-A | 184 | 0 | 0 | 0 | 0 |
| 4 | 49-A | 195 | 0 | 0 | 0 | 0 |
| 4 | 50-A | 189 | 0 | 0 | 0 | 0 |
| 4 | 51-A | 198 | 0 | 0 | 0 | 0 |
| 4 | 52-A | 190 | 0 | 0 | 0 | 0 |
| 4 | 53-A | 182 | 0 | 0 | 0 | 0 |
| 4 | 54-A | 180 | 0 | 0 | 0 | 0 |
| 4 | 55-A | 185 | 0 | 0 | 0 | 0 |
| 4 | 56-A | 184 | 0 | 0 | 0 | 0 |
| 4 | 57-A | 191 | 0 | 0 | 0 | 0 |
| 4 | 58-A | 187 | 0 | 0 | 0 | 0 |
| 4 | 59-A | 192 | 0 | 0 | 0 | 0 |
| 4 | 60-A | 173 | 0 | 0 | 0 | 0 |
| 4 | 61-A | 186 | 0 | 0 | 0 | 0 |
| 4 | 62-A | 201 | 0 | 0 | 0 | 0 |
| 4 | 63-A | 201 | 0 | 0 | 0 | 0 |
| 4 | 64-A | 188 | 0 | 0 | 0 | 0 |
| 4 | 65-A | 187 | 0 | 0 | 0 | 0 |
| 4 | 66-A | 174 | 0 | 0 | 0 | 0 |
| 4 | 67-A | 184 | 0 | 0 | 0 | 0 |
| 4 | 68-A | 178 | 0 | 0 | 0 | 0 |
| 4 | 69-A | 173 | 0 | 0 | 0 | 0 |
| 4 | 70-A | 171 | 0 | 0 | 0 | 0 |
| 4 | 71-A | 171 | 0 | 0 | 0 | 0 |
| 4 | 72-A | 196 | 0 | 0 | 0 | 0 |
| 4 | 73-A | 207 | 0 | 0 | 0 | 0 |
| 4 | 74-A | 191 | 0 | 0 | 0 | 0 |
| 4 | 75-A | 193 | 0 | 0 | 0 | 0 |
| 4 | 76-A | 182 | 0 | 0 | 0 | 0 |
| 4 | 77-A | 176 | 0 | 0 | 0 | 0 |
| 4 | 78-A | 184 | 0 | 0 | 0 | 0 |
| 4 | 79-A | 193 | 0 | 0 | 0 | 0 |
| 4 | 80-A | 201 | 0 | 0 | 0 | 0 |
| 4 | 81-A | 187 | 0 | 0 | 0 | 0 |
| 4 | 82-A | 175 | 0 | 0 | 0 | 0 |
| 4 | 83-A | 175 | 0 | 0 | 0 | 0 |
| 4 | 84-A | 172 | 0 | 0 | 0 | 0 |
| 4 | 85-A | 186 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | 86-A | 199 | 0 | 0 | 0 | 0 |
| 4 | 87-A | 200 | 0 | 0 | 0 | 0 |
| 4 | 88-A | 191 | 0 | 0 | 0 | 0 |
| 4 | 89-A | 189 | 0 | 0 | 0 | 0 |
| 4 | 90-A | 180 | 0 | 0 | 0 | 0 |
| 4 | 91-A | 190 | 0 | 0 | 0 | 0 |
| 4 | 92-A | 181 | 0 | 0 | 0 | 0 |
| 4 | 93-A | 177 | 0 | 0 | 0 | 0 |
| 4 | 94-A | 189 | 0 | 0 | 0 | 0 |
| 4 | 95-A | 173 | 0 | 0 | 0 | 0 |
| 4 | 96-A | 182 | 0 | 0 | 0 | 0 |
| 4 | 97-A | 188 | 0 | 0 | 0 | 0 |
| 4 | 98-A | 191 | 0 | 0 | 0 | 0 |
| 4 | 99-A | 198 | 0 | 0 | 0 | 0 |
| 4 | 100-A | 200 | 0 | 0 | 0 | 0 |
| 4 | 101-A | 204 | 0 | 0 | 0 | 0 |
| 4 | 102-A | 189 | 0 | 0 | 0 | 0 |
| 4 | 103-A | 211 | 0 | 0 | 0 | 0 |
| 4 | 104-A | 202 | 0 | 0 | 0 | 0 |
| 4 | 105-A | 196 | 0 | 0 | 0 | 0 |
| 4 | 106-A | 189 | 0 | 0 | 0 | 0 |
| 4 | 107-A | 179 | 0 | 0 | 0 | 0 |
| 4 | 108-A | 185 | 0 | 0 | 0 | 0 |
| 4 | 109-A | 186 | 0 | 0 | 0 | 0 |
| 4 | 110-A | 186 | 0 | 0 | 0 | 0 |
| 4 | 111-A | 181 | 0 | 0 | 0 | 0 |
| 4 | 112-A | 175 | 0 | 0 | 0 | 0 |
| 4 | 113-A | 183 | 0 | 0 | 0 | 0 |
| 4 | 114-A | 189 | 0 | 0 | 0 | 0 |
| 4 | 115-A | 183 | 0 | 0 | 0 | 0 |
| 4 | 116-A | 194 | 0 | 0 | 0 | 0 |
| 4 | 117-A | 190 | 0 | 0 | 0 | 0 |
| 4 | 118-A | 194 | 0 | 0 | 0 | 0 |
| 4 | 119-A | 194 | 0 | 0 | 0 | 0 |
| 4 | 120-A | 204 | 0 | 0 | 0 | 0 |
| 4 | 121-A | 191 | 0 | 0 | 0 | 0 |
| 4 | 122-A | 192 | 0 | 0 | 0 | 0 |
| 4 | 123-A | 195 | 0 | 0 | 0 | 0 |
| 4 | 124-A | 186 | 0 | 0 | 0 | 0 |
| 4 | 125-A | 185 | 0 | 0 | 0 | 0 |
| 4 | 126-A | 178 | 0 | 0 | 0 | 0 |
| 4 | 127-A | 185 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | 128-A | 175 | 0 | 0 | 0 | 0 |
| 4 | 129-A | 180 | 0 | 0 | 0 | 0 |
| 4 | 130-A | 186 | 0 | 0 | 0 | 0 |
| 4 | 131-A | 201 | 0 | 0 | 0 | 0 |
| 4 | 132-A | 205 | 0 | 0 | 0 | 0 |
| 4 | 133-A | 205 | 0 | 0 | 0 | 0 |
| 4 | 134-A | 209 | 0 | 0 | 0 | 0 |
| 4 | 135-A | 195 | 0 | 0 | 0 | 0 |
| 4 | 136-A | 205 | 0 | 0 | 0 | 0 |
| 4 | 137-A | 190 | 0 | 0 | 0 | 0 |
| 4 | 138-A | 174 | 0 | 0 | 0 | 0 |
| 4 | 139-A | 186 | 0 | 0 | 0 | 0 |
| 4 | 140-A | 186 | 0 | 0 | 0 | 0 |
| 4 | 141-A | 196 | 0 | 0 | 0 | 0 |
| 4 | 142-A | 203 | 0 | 0 | 0 | 0 |
| 4 | 143-A | 192 | 0 | 0 | 0 | 0 |
| 4 | 144-A | 187 | 0 | 0 | 0 | 0 |
| 4 | 145-A | 176 | 0 | 0 | 0 | 0 |
| 4 | 146-A | 176 | 0 | 0 | 0 | 0 |
| 4 | 147-A | 162 | 0 | 0 | 0 | 0 |
| 4 | 148-A | 163 | 0 | 0 | 0 | 0 |
| 4 | 149-A | 178 | 0 | 0 | 0 | 0 |
| 4 | 150-A | 190 | 0 | 0 | 0 | 0 |
| 4 | 151-A | 204 | 0 | 0 | 0 | 0 |
| 4 | 152-A | 187 | 0 | 0 | 0 | 0 |
| 4 | 153-A | 191 | 0 | 0 | 0 | 0 |
| 4 | 154-A | 190 | 0 | 0 | 0 | 0 |
| 4 | 155-A | 187 | 0 | 0 | 0 | 0 |
| 4 | 156-A | 190 | 0 | 0 | 0 | 0 |
| 4 | 157-A | 193 | 0 | 0 | 0 | 0 |
| 4 | 158-A | 181 | 0 | 0 | 0 | 0 |
| 4 | 159-A | 176 | 0 | 0 | 0 | 0 |
| 4 | 160-A | 185 | 0 | 0 | 0 | 0 |
| 4 | 161-A | 187 | 0 | 0 | 0 | 0 |
| 4 | 162-A | 196 | 0 | 0 | 0 | 0 |
| 4 | 163-A | 204 | 0 | 0 | 0 | 0 |
| 4 | 164-A | 198 | 0 | 0 | 0 | 0 |
| 4 | 165-A | 215 | 0 | 0 | 0 | 0 |
| 4 | 166-A | 194 | 0 | 0 | 0 | 0 |
| 4 | 167-A | 175 | 0 | 0 | 0 | 0 |
| 4 | 168-A | 176 | 0 | 0 | 0 | 0 |
| 4 | 169-A | 184 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 4 | 170-A | 190 | 0 | 0 | 0 | 0 |
| 4 | 171-A | 187 | 0 | 0 | 0 | 0 |
| 4 | 172-A | 187 | 0 | 0 | 0 | 0 |
| 4 | 173-A | 191 | 0 | 0 | 0 | 0 |
| 4 | 174-A | 199 | 0 | 0 | 0 | 0 |
| 4 | 175-A | 196 | 0 | 0 | 0 | 0 |
| 4 | 176-A | 194 | 0 | 0 | 0 | 0 |
| 4 | 177-A | 203 | 0 | 0 | 0 | 0 |
| 4 | 178-A | 188 | 0 | 0 | 0 | 0 |
| 4 | 179-A | 175 | 0 | 0 | 0 | 0 |
| 4 | 180-A | 169 | 0 | 0 | 0 | 0 |
| 4 | 181-A | 192 | 0 | 0 | 0 | 0 |
| 4 | 182-A | 187 | 0 | 0 | 0 | 0 |
| 4 | 183-A | 185 | 0 | 0 | 0 | 0 |
| 4 | 184-A | 179 | 0 | 0 | 0 | 0 |
| 4 | 185-A | 197 | 0 | 0 | 0 | 0 |
| 4 | 186-A | 187 | 0 | 0 | 0 | 0 |
| 4 | 187-A | 191 | 0 | 0 | 0 | 0 |
| 4 | 188-A | 203 | 0 | 0 | 0 | 0 |
| 4 | 189-A | 209 | 0 | 0 | 0 | 0 |
| 4 | 190-A | 197 | 0 | 0 | 0 | 0 |
| 4 | 191-A | 179 | 0 | 0 | 0 | 0 |
| 4 | 192-A | 185 | 0 | 0 | 0 | 0 |
| 4 | 193-A | 183 | 0 | 0 | 0 | 0 |
| 4 | 194-A | 182 | 0 | 0 | 0 | 0 |
| 4 | 195-A | 173 | 0 | 0 | 0 | 0 |
| 4 | 196-A | 184 | 0 | 0 | 0 | 0 |
| 4 | 197-A | 181 | 0 | 0 | 0 | 0 |
| 4 | 198-A | 181 | 0 | 0 | 0 | 0 |
| 4 | 199-A | 184 | 0 | 0 | 0 | 0 |
| 4 | 200-A | 192 | 0 | 0 | 0 | 0 |
| 4 | 201-A | 207 | 0 | 0 | 0 | 0 |
| 4 | 202-A | 194 | 0 | 0 | 0 | 0 |
| 4 | 203-A | 184 | 0 | 0 | 0 | 0 |
| 4 | 204-A | 182 | 0 | 0 | 0 | 0 |
| 4 | 205-A | 193 | 0 | 0 | 0 | 0 |
| 4 | 206-A | 190 | 0 | 0 | 0 | 0 |
| 4 | 207-A | 180 | 0 | 0 | 0 | 0 |
| 4 | 208-A | 178 | 0 | 0 | 0 | 0 |
| 4 | 209-A | 185 | 0 | 0 | 0 | 0 |
| 4 | 210-A | 184 | 0 | 0 | 0 | 0 |
| 4 | 211-A | 184 | 0 | 0 | 0 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|--------|----------|----------|---------|--------------|
| 4 | 212-A | 191 | 0 | 0 | 0 | 0 |
| 4 | 213-A | 202 | 0 | 0 | 0 | 0 |
| 4 | 214-A | 190 | 0 | 0 | 0 | 0 |
| 4 | 215-A | 193 | 0 | 0 | 0 | 0 |
| 4 | 216-A | 195 | 0 | 0 | 0 | 0 |
| 4 | 217-A | 197 | 0 | 0 | 0 | 0 |
| 4 | 218-A | 197 | 0 | 0 | 0 | 0 |
| 4 | 219-A | 192 | 0 | 0 | 0 | 0 |
| 4 | 220-A | 177 | 0 | 0 | 0 | 0 |
| 4 | 221-A | 183 | 0 | 0 | 0 | 0 |
| 4 | 222-A | 182 | 0 | 0 | 0 | 0 |
| 4 | 223-A | 181 | 0 | 0 | 0 | 0 |
| 4 | 224-A | 203 | 0 | 0 | 0 | 0 |
| 4 | 225-A | 205 | 0 | 0 | 0 | 0 |
| 4 | 226-A | 202 | 0 | 0 | 0 | 0 |
| 4 | 227-A | 189 | 0 | 0 | 0 | 0 |
| 4 | 228-A | 162 | 0 | 0 | 0 | 0 |
| 4 | 229-A | 180 | 0 | 0 | 0 | 0 |
| 4 | 230-A | 174 | 0 | 0 | 0 | 0 |
| 4 | 231-A | 206 | 0 | 0 | 0 | 0 |
| 4 | 232-A | 211 | 0 | 0 | 0 | 0 |
| 4 | 233-A | 195 | 0 | 0 | 0 | 0 |
| 4 | 234-A | 184 | 0 | 0 | 0 | 0 |
| 4 | 235-A | 167 | 0 | 0 | 0 | 0 |
| 4 | 236-A | 172 | 0 | 0 | 0 | 0 |
| 4 | 237-A | 184 | 0 | 0 | 0 | 0 |
| 4 | 238-A | 198 | 0 | 0 | 0 | 0 |
| 4 | 239-A | 194 | 0 | 0 | 0 | 0 |
| 4 | 240-A | 206 | 0 | 0 | 0 | 0 |
| 4 | 241-A | 208 | 0 | 0 | 0 | 0 |
| 4 | 242-A | 179 | 0 | 0 | 0 | 0 |
| 4 | 243-A | 184 | 0 | 0 | 0 | 0 |
| 4 | 244-A | 181 | 0 | 0 | 0 | 0 |
| 4 | 245-A | 178 | 0 | 0 | 0 | 0 |
| 4 | 246-A | 197 | 0 | 0 | 0 | 0 |
| 4 | 247-A | 186 | 0 | 0 | 0 | 0 |
| 4 | 248-A | 182 | 0 | 0 | 0 | 0 |
| 4 | 249-A | 195 | 0 | 0 | 0 | 0 |
| 4 | 250-A | 202 | 0 | 0 | 0 | 0 |
| All | All | 384153 | 315500 | 315747 | 0 | 0 |

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

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | 1-A | 157/159 (99%) | 154 (98%) | 2 (1%) | 1 (1%) | 25 | 5 |
| 1 | 2-A | 157/159 (99%) | 154 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | 3-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 4-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 5-A | 157/159 (99%) | 154 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | 6-A | 157/159 (99%) | 153 (98%) | 2 (1%) | 2 (1%) | 12 | 0 |
| 1 | 7-A | 157/159 (99%) | 155 (99%) | 1 (1%) | 1 (1%) | 25 | 5 |
| 1 | 8-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 9-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 10-A | 157/159 (99%) | 151 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | 11-A | 157/159 (99%) | 155 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | 12-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 13-A | 157/159 (99%) | 150 (96%) | 6 (4%) | 1 (1%) | 25 | 5 |
| 1 | 14-A | 157/159 (99%) | 149 (95%) | 6 (4%) | 2 (1%) | 12 | 0 |
| 1 | 15-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 16-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 17-A | 157/159 (99%) | 153 (98%) | 2 (1%) | 2 (1%) | 12 | 0 |
| 1 | 18-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 19-A | 157/159 (99%) | 153 (98%) | 2 (1%) | 2 (1%) | 12 | 0 |
| 1 | 20-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 21-A | 157/159 (99%) | 155 (99%) | 1 (1%) | 1 (1%) | 25 | 5 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | 22-A | 157/159 (99%) | 154 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | 23-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 24-A | 157/159 (99%) | 150 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | 25-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 26-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 27-A | 157/159 (99%) | 151 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | 28-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 29-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 30-A | 157/159 (99%) | 153 (98%) | 3 (2%) | 1 (1%) | 25 | 5 |
| 1 | 31-A | 157/159 (99%) | 151 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | 32-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 33-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 34-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 35-A | 157/159 (99%) | 154 (98%) | 2 (1%) | 1 (1%) | 25 | 5 |
| 1 | 36-A | 157/159 (99%) | 151 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | 37-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 38-A | 157/159 (99%) | 151 (96%) | 4 (2%) | 2 (1%) | 12 | 0 |
| 1 | 39-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 40-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 41-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 42-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 43-A | 157/159 (99%) | 149 (95%) | 8 (5%) | 0 | 100 | 100 |
| 1 | 44-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 45-A | 157/159 (99%) | 155 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | 46-A | 157/159 (99%) | 148 (94%) | 7 (4%) | 2 (1%) | 12 | 0 |
| 1 | 47-A | 157/159 (99%) | 150 (96%) | 6 (4%) | 1 (1%) | 25 | 5 |
| 1 | 48-A | 157/159 (99%) | 149 (95%) | 7 (4%) | 1 (1%) | 25 | 5 |
| 1 | 49-A | 157/159 (99%) | 153 (98%) | 3 (2%) | 1 (1%) | 25 | 5 |
| 1 | 50-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 51-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 52-A | 157/159 (99%) | 148 (94%) | 8 (5%) | 1 (1%) | 25 | 5 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | 53-A | 157/159 (99%) | 151 (96%) | 2 (1%) | 4 (2%) | 5 | 0 |
| 1 | 54-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 55-A | 157/159 (99%) | 153 (98%) | 3 (2%) | 1 (1%) | 25 | 5 |
| 1 | 56-A | 157/159 (99%) | 147 (94%) | 8 (5%) | 2 (1%) | 12 | 0 |
| 1 | 57-A | 157/159 (99%) | 151 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | 58-A | 157/159 (99%) | 151 (96%) | 4 (2%) | 2 (1%) | 12 | 0 |
| 1 | 59-A | 157/159 (99%) | 150 (96%) | 5 (3%) | 2 (1%) | 12 | 0 |
| 1 | 60-A | 157/159 (99%) | 154 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | 61-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 62-A | 157/159 (99%) | 148 (94%) | 5 (3%) | 4 (2%) | 5 | 0 |
| 1 | 63-A | 157/159 (99%) | 150 (96%) | 4 (2%) | 3 (2%) | 8 | 0 |
| 1 | 64-A | 157/159 (99%) | 150 (96%) | 6 (4%) | 1 (1%) | 25 | 5 |
| 1 | 65-A | 157/159 (99%) | 152 (97%) | 3 (2%) | 2 (1%) | 12 | 0 |
| 1 | 66-A | 157/159 (99%) | 152 (97%) | 3 (2%) | 2 (1%) | 12 | 0 |
| 1 | 67-A | 157/159 (99%) | 151 (96%) | 3 (2%) | 3 (2%) | 8 | 0 |
| 1 | 68-A | 157/159 (99%) | 149 (95%) | 6 (4%) | 2 (1%) | 12 | 0 |
| 1 | 69-A | 157/159 (99%) | 150 (96%) | 5 (3%) | 2 (1%) | 12 | 0 |
| 1 | 70-A | 157/159 (99%) | 153 (98%) | 3 (2%) | 1 (1%) | 25 | 5 |
| 1 | 71-A | 157/159 (99%) | 155 (99%) | 1 (1%) | 1 (1%) | 25 | 5 |
| 1 | 72-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 73-A | 157/159 (99%) | 154 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | 74-A | 157/159 (99%) | 151 (96%) | 3 (2%) | 3 (2%) | 8 | 0 |
| 1 | 75-A | 157/159 (99%) | 153 (98%) | 3 (2%) | 1 (1%) | 25 | 5 |
| 1 | 76-A | 157/159 (99%) | 146 (93%) | 9 (6%) | 2 (1%) | 12 | 0 |
| 1 | 77-A | 157/159 (99%) | 151 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | 78-A | 157/159 (99%) | 150 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | 79-A | 157/159 (99%) | 153 (98%) | 3 (2%) | 1 (1%) | 25 | 5 |
| 1 | 80-A | 157/159 (99%) | 153 (98%) | 3 (2%) | 1 (1%) | 25 | 5 |
| 1 | 81-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 82-A | 157/159 (99%) | 148 (94%) | 8 (5%) | 1 (1%) | 25 | 5 |
| 1 | 83-A | 157/159 (99%) | 151 (96%) | 4 (2%) | 2 (1%) | 12 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | 84-A | 157/159 (99%) | 145 (92%) | 10 (6%) | 2 (1%) | 12 | 0 |
| 1 | 85-A | 157/159 (99%) | 151 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | 86-A | 157/159 (99%) | 150 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | 87-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 88-A | 157/159 (99%) | 154 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | 89-A | 157/159 (99%) | 150 (96%) | 4 (2%) | 3 (2%) | 8 | 0 |
| 1 | 90-A | 157/159 (99%) | 150 (96%) | 5 (3%) | 2 (1%) | 12 | 0 |
| 1 | 91-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 92-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 93-A | 157/159 (99%) | 149 (95%) | 5 (3%) | 3 (2%) | 8 | 0 |
| 1 | 94-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 95-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 96-A | 157/159 (99%) | 153 (98%) | 3 (2%) | 1 (1%) | 25 | 5 |
| 1 | 97-A | 157/159 (99%) | 154 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | 98-A | 157/159 (99%) | 155 (99%) | 1 (1%) | 1 (1%) | 25 | 5 |
| 1 | 99-A | 157/159 (99%) | 154 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | 100-A | 157/159 (99%) | 151 (96%) | 3 (2%) | 3 (2%) | 8 | 0 |
| 1 | 101-A | 157/159 (99%) | 154 (98%) | 2 (1%) | 1 (1%) | 25 | 5 |
| 1 | 102-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 103-A | 157/159 (99%) | 154 (98%) | 1 (1%) | 2 (1%) | 12 | 0 |
| 1 | 104-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 105-A | 157/159 (99%) | 149 (95%) | 8 (5%) | 0 | 100 | 100 |
| 1 | 106-A | 157/159 (99%) | 151 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | 107-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 108-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 109-A | 157/159 (99%) | 149 (95%) | 7 (4%) | 1 (1%) | 25 | 5 |
| 1 | 110-A | 157/159 (99%) | 150 (96%) | 6 (4%) | 1 (1%) | 25 | 5 |
| 1 | 111-A | 157/159 (99%) | 149 (95%) | 6 (4%) | 2 (1%) | 12 | 0 |
| 1 | 112-A | 157/159 (99%) | 150 (96%) | 5 (3%) | 2 (1%) | 12 | 0 |
| 1 | 113-A | 157/159 (99%) | 149 (95%) | 7 (4%) | 1 (1%) | 25 | 5 |
| 1 | 114-A | 157/159 (99%) | 149 (95%) | 6 (4%) | 2 (1%) | 12 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | 115-A | 157/159 (99%) | 151 (96%) | 4 (2%) | 2 (1%) | 12 | 0 |
| 1 | 116-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 117-A | 157/159 (99%) | 148 (94%) | 9 (6%) | 0 | 100 | 100 |
| 1 | 118-A | 157/159 (99%) | 150 (96%) | 6 (4%) | 1 (1%) | 25 | 5 |
| 1 | 119-A | 157/159 (99%) | 149 (95%) | 6 (4%) | 2 (1%) | 12 | 0 |
| 1 | 120-A | 157/159 (99%) | 153 (98%) | 2 (1%) | 2 (1%) | 12 | 0 |
| 1 | 121-A | 157/159 (99%) | 152 (97%) | 3 (2%) | 2 (1%) | 12 | 0 |
| 1 | 122-A | 157/159 (99%) | 151 (96%) | 4 (2%) | 2 (1%) | 12 | 0 |
| 1 | 123-A | 157/159 (99%) | 149 (95%) | 7 (4%) | 1 (1%) | 25 | 5 |
| 1 | 124-A | 157/159 (99%) | 151 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | 125-A | 157/159 (99%) | 154 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | 126-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 127-A | 157/159 (99%) | 151 (96%) | 3 (2%) | 3 (2%) | 8 | 0 |
| 1 | 128-A | 157/159 (99%) | 153 (98%) | 3 (2%) | 1 (1%) | 25 | 5 |
| 1 | 129-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 130-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 131-A | 157/159 (99%) | 152 (97%) | 3 (2%) | 2 (1%) | 12 | 0 |
| 1 | 132-A | 157/159 (99%) | 144 (92%) | 8 (5%) | 5 (3%) | 4 | 0 |
| 1 | 133-A | 157/159 (99%) | 148 (94%) | 8 (5%) | 1 (1%) | 25 | 5 |
| 1 | 134-A | 157/159 (99%) | 150 (96%) | 5 (3%) | 2 (1%) | 12 | 0 |
| 1 | 135-A | 157/159 (99%) | 150 (96%) | 5 (3%) | 2 (1%) | 12 | 0 |
| 1 | 136-A | 157/159 (99%) | 146 (93%) | 10 (6%) | 1 (1%) | 25 | 5 |
| 1 | 137-A | 157/159 (99%) | 154 (98%) | 2 (1%) | 1 (1%) | 25 | 5 |
| 1 | 138-A | 157/159 (99%) | 149 (95%) | 6 (4%) | 2 (1%) | 12 | 0 |
| 1 | 139-A | 157/159 (99%) | 151 (96%) | 4 (2%) | 2 (1%) | 12 | 0 |
| 1 | 140-A | 157/159 (99%) | 149 (95%) | 6 (4%) | 2 (1%) | 12 | 0 |
| 1 | 141-A | 157/159 (99%) | 149 (95%) | 4 (2%) | 4 (2%) | 5 | 0 |
| 1 | 142-A | 157/159 (99%) | 145 (92%) | 7 (4%) | 5 (3%) | 4 | 0 |
| 1 | 143-A | 157/159 (99%) | 150 (96%) | 4 (2%) | 3 (2%) | 8 | 0 |
| 1 | 144-A | 157/159 (99%) | 148 (94%) | 6 (4%) | 3 (2%) | 8 | 0 |
| 1 | 145-A | 157/159 (99%) | 148 (94%) | 6 (4%) | 3 (2%) | 8 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | 146-A | 157/159 (99%) | 152 (97%) | 3 (2%) | 2 (1%) | 12 | 0 |
| 1 | 147-A | 157/159 (99%) | 151 (96%) | 4 (2%) | 2 (1%) | 12 | 0 |
| 1 | 148-A | 157/159 (99%) | 148 (94%) | 7 (4%) | 2 (1%) | 12 | 0 |
| 1 | 149-A | 157/159 (99%) | 151 (96%) | 4 (2%) | 2 (1%) | 12 | 0 |
| 1 | 150-A | 157/159 (99%) | 148 (94%) | 7 (4%) | 2 (1%) | 12 | 0 |
| 1 | 151-A | 157/159 (99%) | 150 (96%) | 6 (4%) | 1 (1%) | 25 | 5 |
| 1 | 152-A | 157/159 (99%) | 153 (98%) | 3 (2%) | 1 (1%) | 25 | 5 |
| 1 | 153-A | 157/159 (99%) | 151 (96%) | 3 (2%) | 3 (2%) | 8 | 0 |
| 1 | 154-A | 157/159 (99%) | 153 (98%) | 3 (2%) | 1 (1%) | 25 | 5 |
| 1 | 155-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 156-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 157-A | 157/159 (99%) | 154 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | 158-A | 157/159 (99%) | 150 (96%) | 4 (2%) | 3 (2%) | 8 | 0 |
| 1 | 159-A | 157/159 (99%) | 155 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | 160-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 161-A | 157/159 (99%) | 154 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | 162-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 163-A | 157/159 (99%) | 149 (95%) | 7 (4%) | 1 (1%) | 25 | 5 |
| 1 | 164-A | 157/159 (99%) | 155 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | 165-A | 157/159 (99%) | 150 (96%) | 6 (4%) | 1 (1%) | 25 | 5 |
| 1 | 166-A | 157/159 (99%) | 155 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | 167-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 168-A | 157/159 (99%) | 149 (95%) | 4 (2%) | 4 (2%) | 5 | 0 |
| 1 | 169-A | 157/159 (99%) | 154 (98%) | 2 (1%) | 1 (1%) | 25 | 5 |
| 1 | 170-A | 157/159 (99%) | 151 (96%) | 3 (2%) | 3 (2%) | 8 | 0 |
| 1 | 171-A | 157/159 (99%) | 150 (96%) | 5 (3%) | 2 (1%) | 12 | 0 |
| 1 | 172-A | 157/159 (99%) | 151 (96%) | 3 (2%) | 3 (2%) | 8 | 0 |
| 1 | 173-A | 157/159 (99%) | 150 (96%) | 4 (2%) | 3 (2%) | 8 | 0 |
| 1 | 174-A | 157/159 (99%) | 145 (92%) | 6 (4%) | 6 (4%) | 3 | 0 |
| 1 | 175-A | 157/159 (99%) | 149 (95%) | 3 (2%) | 5 (3%) | 4 | 0 |
| 1 | 176-A | 157/159 (99%) | 147 (94%) | 6 (4%) | 4 (2%) | 5 | 0 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | 177-A | 157/159 (99%) | 150 (96%) | 5 (3%) | 2 (1%) | 12 | 0 |
| 1 | 178-A | 157/159 (99%) | 147 (94%) | 8 (5%) | 2 (1%) | 12 | 0 |
| 1 | 179-A | 157/159 (99%) | 150 (96%) | 7 (4%) | 0 | 100 | 100 |
| 1 | 180-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 181-A | 157/159 (99%) | 152 (97%) | 3 (2%) | 2 (1%) | 12 | 0 |
| 1 | 182-A | 157/159 (99%) | 149 (95%) | 7 (4%) | 1 (1%) | 25 | 5 |
| 1 | 183-A | 157/159 (99%) | 146 (93%) | 9 (6%) | 2 (1%) | 12 | 0 |
| 1 | 184-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 185-A | 157/159 (99%) | 149 (95%) | 8 (5%) | 0 | 100 | 100 |
| 1 | 186-A | 157/159 (99%) | 149 (95%) | 8 (5%) | 0 | 100 | 100 |
| 1 | 187-A | 157/159 (99%) | 149 (95%) | 5 (3%) | 3 (2%) | 8 | 0 |
| 1 | 188-A | 157/159 (99%) | 147 (94%) | 8 (5%) | 2 (1%) | 12 | 0 |
| 1 | 189-A | 157/159 (99%) | 149 (95%) | 7 (4%) | 1 (1%) | 25 | 5 |
| 1 | 190-A | 157/159 (99%) | 150 (96%) | 5 (3%) | 2 (1%) | 12 | 0 |
| 1 | 191-A | 157/159 (99%) | 149 (95%) | 6 (4%) | 2 (1%) | 12 | 0 |
| 1 | 192-A | 157/159 (99%) | 151 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | 193-A | 157/159 (99%) | 149 (95%) | 8 (5%) | 0 | 100 | 100 |
| 1 | 194-A | 157/159 (99%) | 154 (98%) | 2 (1%) | 1 (1%) | 25 | 5 |
| 1 | 195-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 196-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 197-A | 157/159 (99%) | 154 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | 198-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 199-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 200-A | 157/159 (99%) | 155 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | 201-A | 157/159 (99%) | 153 (98%) | 3 (2%) | 1 (1%) | 25 | 5 |
| 1 | 202-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 203-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 204-A | 157/159 (99%) | 149 (95%) | 8 (5%) | 0 | 100 | 100 |
| 1 | 205-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 206-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 207-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|---------------|-----------|---------|----------|-------------|-----|
| 1 | 208-A | 157/159 (99%) | 150 (96%) | 6 (4%) | 1 (1%) | 25 | 5 |
| 1 | 209-A | 157/159 (99%) | 152 (97%) | 2 (1%) | 3 (2%) | 8 | 0 |
| 1 | 210-A | 157/159 (99%) | 150 (96%) | 3 (2%) | 4 (2%) | 5 | 0 |
| 1 | 211-A | 157/159 (99%) | 149 (95%) | 7 (4%) | 1 (1%) | 25 | 5 |
| 1 | 212-A | 157/159 (99%) | 150 (96%) | 4 (2%) | 3 (2%) | 8 | 0 |
| 1 | 213-A | 157/159 (99%) | 150 (96%) | 5 (3%) | 2 (1%) | 12 | 0 |
| 1 | 214-A | 157/159 (99%) | 150 (96%) | 5 (3%) | 2 (1%) | 12 | 0 |
| 1 | 215-A | 157/159 (99%) | 147 (94%) | 9 (6%) | 1 (1%) | 25 | 5 |
| 1 | 216-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 217-A | 157/159 (99%) | 148 (94%) | 7 (4%) | 2 (1%) | 12 | 0 |
| 1 | 218-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 219-A | 157/159 (99%) | 149 (95%) | 6 (4%) | 2 (1%) | 12 | 0 |
| 1 | 220-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 221-A | 157/159 (99%) | 151 (96%) | 4 (2%) | 2 (1%) | 12 | 0 |
| 1 | 222-A | 157/159 (99%) | 150 (96%) | 5 (3%) | 2 (1%) | 12 | 0 |
| 1 | 223-A | 157/159 (99%) | 150 (96%) | 4 (2%) | 3 (2%) | 8 | 0 |
| 1 | 224-A | 157/159 (99%) | 149 (95%) | 5 (3%) | 3 (2%) | 8 | 0 |
| 1 | 225-A | 157/159 (99%) | 154 (98%) | 1 (1%) | 2 (1%) | 12 | 0 |
| 1 | 226-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 227-A | 157/159 (99%) | 151 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | 228-A | 157/159 (99%) | 153 (98%) | 3 (2%) | 1 (1%) | 25 | 5 |
| 1 | 229-A | 157/159 (99%) | 154 (98%) | 2 (1%) | 1 (1%) | 25 | 5 |
| 1 | 230-A | 157/159 (99%) | 155 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | 231-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 232-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 233-A | 157/159 (99%) | 151 (96%) | 5 (3%) | 1 (1%) | 25 | 5 |
| 1 | 234-A | 157/159 (99%) | 154 (98%) | 2 (1%) | 1 (1%) | 25 | 5 |
| 1 | 235-A | 157/159 (99%) | 155 (99%) | 2 (1%) | 0 | 100 | 100 |
| 1 | 236-A | 157/159 (99%) | 152 (97%) | 4 (2%) | 1 (1%) | 25 | 5 |
| 1 | 237-A | 157/159 (99%) | 151 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | 238-A | 157/159 (99%) | 151 (96%) | 6 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-------------------|-------------|-----------|----------|-------------|-----|
| 1 | 239-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 240-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 241-A | 157/159 (99%) | 152 (97%) | 5 (3%) | 0 | 100 | 100 |
| 1 | 242-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 243-A | 157/159 (99%) | 154 (98%) | 3 (2%) | 0 | 100 | 100 |
| 1 | 244-A | 157/159 (99%) | 153 (98%) | 4 (2%) | 0 | 100 | 100 |
| 1 | 245-A | 157/159 (99%) | 152 (97%) | 3 (2%) | 2 (1%) | 12 | 0 |
| 1 | 246-A | 157/159 (99%) | 153 (98%) | 3 (2%) | 1 (1%) | 25 | 5 |
| 1 | 247-A | 157/159 (99%) | 152 (97%) | 3 (2%) | 2 (1%) | 12 | 0 |
| 1 | 248-A | 157/159 (99%) | 155 (99%) | 1 (1%) | 1 (1%) | 25 | 5 |
| 1 | 249-A | 157/159 (99%) | 151 (96%) | 6 (4%) | 0 | 100 | 100 |
| 1 | 250-A | 157/159 (99%) | 147 (94%) | 8 (5%) | 2 (1%) | 12 | 0 |
| All | All | 39250/39750 (99%) | 37802 (96%) | 1150 (3%) | 298 (1%) | 19 | 3 |

All (298) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 4-A | 87 | ASP |
| 1 | 6-A | 21 | PRO |
| 1 | 28-A | 22 | TRP |
| 1 | 38-A | 121 | GLY |
| 1 | 48-A | 22 | TRP |
| 1 | 49-A | 22 | TRP |
| 1 | 53-A | 21 | PRO |
| 1 | 56-A | 88 | VAL |
| 1 | 58-A | 21 | PRO |
| 1 | 58-A | 22 | TRP |
| 1 | 62-A | 20 | MET |
| 1 | 62-A | 21 | PRO |
| 1 | 62-A | 22 | TRP |
| 1 | 63-A | 20 | MET |
| 1 | 65-A | 21 | PRO |
| 1 | 65-A | 22 | TRP |
| 1 | 66-A | 21 | PRO |
| 1 | 67-A | 21 | PRO |
| 1 | 69-A | 21 | PRO |
| 1 | 69-A | 22 | TRP |
| 1 | 74-A | 22 | TRP |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 83-A | 17 | GLU |
| 1 | 84-A | 21 | PRO |
| 1 | 90-A | 88 | VAL |
| 1 | 101-A | 87 | ASP |
| 1 | 103-A | 22 | TRP |
| 1 | 109-A | 87 | ASP |
| 1 | 110-A | 87 | ASP |
| 1 | 114-A | 87 | ASP |
| 1 | 115-A | 87 | ASP |
| 1 | 122-A | 24 | LEU |
| 1 | 126-A | 21 | PRO |
| 1 | 127-A | 20 | MET |
| 1 | 131-A | 21 | PRO |
| 1 | 132-A | 20 | MET |
| 1 | 132-A | 21 | PRO |
| 1 | 132-A | 128 | TYR |
| 1 | 133-A | 20 | MET |
| 1 | 135-A | 87 | ASP |
| 1 | 138-A | 21 | PRO |
| 1 | 138-A | 87 | ASP |
| 1 | 140-A | 20 | MET |
| 1 | 141-A | 21 | PRO |
| 1 | 142-A | 18 | ASN |
| 1 | 142-A | 20 | MET |
| 1 | 142-A | 21 | PRO |
| 1 | 142-A | 22 | TRP |
| 1 | 143-A | 20 | MET |
| 1 | 143-A | 21 | PRO |
| 1 | 144-A | 20 | MET |
| 1 | 144-A | 21 | PRO |
| 1 | 144-A | 22 | TRP |
| 1 | 145-A | 20 | MET |
| 1 | 145-A | 21 | PRO |
| 1 | 147-A | 2 | ILE |
| 1 | 147-A | 20 | MET |
| 1 | 148-A | 2 | ILE |
| 1 | 150-A | 2 | ILE |
| 1 | 153-A | 2 | ILE |
| 1 | 154-A | 2 | ILE |
| 1 | 168-A | 18 | ASN |
| 1 | 168-A | 127 | ASP |
| 1 | 169-A | 22 | TRP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 170-A | 22 | TRP |
| 1 | 170-A | 128 | TYR |
| 1 | 171-A | 21 | PRO |
| 1 | 171-A | 22 | TRP |
| 1 | 172-A | 18 | ASN |
| 1 | 174-A | 18 | ASN |
| 1 | 175-A | 18 | ASN |
| 1 | 175-A | 22 | TRP |
| 1 | 176-A | 19 | ALA |
| 1 | 177-A | 18 | ASN |
| 1 | 177-A | 19 | ALA |
| 1 | 178-A | 18 | ASN |
| 1 | 183-A | 18 | ASN |
| 1 | 188-A | 18 | ASN |
| 1 | 189-A | 18 | ASN |
| 1 | 190-A | 18 | ASN |
| 1 | 191-A | 18 | ASN |
| 1 | 209-A | 22 | TRP |
| 1 | 210-A | 20 | MET |
| 1 | 210-A | 22 | TRP |
| 1 | 211-A | 21 | PRO |
| 1 | 212-A | 20 | MET |
| 1 | 212-A | 23 | ASN |
| 1 | 217-A | 21 | PRO |
| 1 | 218-A | 21 | PRO |
| 1 | 219-A | 21 | PRO |
| 1 | 220-A | 21 | PRO |
| 1 | 223-A | 19 | ALA |
| 1 | 223-A | 21 | PRO |
| 1 | 224-A | 21 | PRO |
| 1 | 224-A | 22 | TRP |
| 1 | 224-A | 127 | ASP |
| 1 | 225-A | 20 | MET |
| 1 | 225-A | 21 | PRO |
| 1 | 226-A | 20 | MET |
| 1 | 236-A | 18 | ASN |
| 1 | 245-A | 22 | TRP |
| 1 | 250-A | 128 | TYR |
| 1 | 7-A | 87 | ASP |
| 1 | 14-A | 18 | ASN |
| 1 | 17-A | 21 | PRO |
| 1 | 35-A | 21 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 46-A | 17 | GLU |
| 1 | 46-A | 18 | ASN |
| 1 | 47-A | 21 | PRO |
| 1 | 51-A | 18 | ASN |
| 1 | 54-A | 21 | PRO |
| 1 | 63-A | 21 | PRO |
| 1 | 67-A | 86 | GLY |
| 1 | 74-A | 18 | ASN |
| 1 | 82-A | 22 | TRP |
| 1 | 83-A | 21 | PRO |
| 1 | 89-A | 18 | ASN |
| 1 | 93-A | 22 | TRP |
| 1 | 100-A | 18 | ASN |
| 1 | 112-A | 22 | TRP |
| 1 | 112-A | 85 | CYS |
| 1 | 114-A | 21 | PRO |
| 1 | 121-A | 21 | PRO |
| 1 | 122-A | 21 | PRO |
| 1 | 128-A | 21 | PRO |
| 1 | 131-A | 19 | ALA |
| 1 | 132-A | 18 | ASN |
| 1 | 139-A | 20 | MET |
| 1 | 139-A | 21 | PRO |
| 1 | 141-A | 19 | ALA |
| 1 | 143-A | 22 | TRP |
| 1 | 145-A | 22 | TRP |
| 1 | 146-A | 2 | ILE |
| 1 | 146-A | 20 | MET |
| 1 | 149-A | 2 | ILE |
| 1 | 151-A | 2 | ILE |
| 1 | 152-A | 2 | ILE |
| 1 | 160-A | 143 | ALA |
| 1 | 173-A | 18 | ASN |
| 1 | 174-A | 22 | TRP |
| 1 | 175-A | 17 | GLU |
| 1 | 178-A | 19 | ALA |
| 1 | 187-A | 19 | ALA |
| 1 | 195-A | 18 | ASN |
| 1 | 208-A | 21 | PRO |
| 1 | 209-A | 21 | PRO |
| 1 | 210-A | 21 | PRO |
| 1 | 213-A | 19 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 214-A | 21 | PRO |
| 1 | 221-A | 21 | PRO |
| 1 | 221-A | 139 | GLU |
| 1 | 222-A | 21 | PRO |
| 1 | 223-A | 22 | TRP |
| 1 | 246-A | 21 | PRO |
| 1 | 248-A | 21 | PRO |
| 1 | 3-A | 21 | PRO |
| 1 | 8-A | 17 | GLU |
| 1 | 12-A | 66 | PRO |
| 1 | 13-A | 142 | ASP |
| 1 | 52-A | 21 | PRO |
| 1 | 53-A | 90 | GLU |
| 1 | 56-A | 23 | ASN |
| 1 | 62-A | 18 | ASN |
| 1 | 63-A | 87 | ASP |
| 1 | 67-A | 22 | TRP |
| 1 | 75-A | 69 | ASP |
| 1 | 76-A | 143 | ALA |
| 1 | 79-A | 18 | ASN |
| 1 | 80-A | 18 | ASN |
| 1 | 93-A | 143 | ALA |
| 1 | 98-A | 139 | GLU |
| 1 | 100-A | 87 | ASP |
| 1 | 108-A | 21 | PRO |
| 1 | 119-A | 21 | PRO |
| 1 | 119-A | 24 | LEU |
| 1 | 127-A | 19 | ALA |
| 1 | 127-A | 21 | PRO |
| 1 | 134-A | 18 | ASN |
| 1 | 140-A | 21 | PRO |
| 1 | 141-A | 18 | ASN |
| 1 | 142-A | 142 | ASP |
| 1 | 148-A | 120 | GLU |
| 1 | 149-A | 18 | ASN |
| 1 | 153-A | 17 | GLU |
| 1 | 172-A | 21 | PRO |
| 1 | 172-A | 23 | ASN |
| 1 | 173-A | 22 | TRP |
| 1 | 174-A | 142 | ASP |
| 1 | 187-A | 17 | GLU |
| 1 | 188-A | 19 | ALA |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 194-A | 17 | GLU |
| 1 | 205-A | 21 | PRO |
| 1 | 209-A | 90 | GLU |
| 1 | 212-A | 21 | PRO |
| 1 | 216-A | 19 | ALA |
| 1 | 222-A | 139 | GLU |
| 1 | 247-A | 128 | TYR |
| 1 | 1-A | 21 | PRO |
| 1 | 17-A | 131 | ASP |
| 1 | 19-A | 19 | ALA |
| 1 | 19-A | 21 | PRO |
| 1 | 34-A | 87 | ASP |
| 1 | 53-A | 22 | TRP |
| 1 | 59-A | 21 | PRO |
| 1 | 68-A | 21 | PRO |
| 1 | 70-A | 69 | ASP |
| 1 | 71-A | 66 | PRO |
| 1 | 84-A | 20 | MET |
| 1 | 91-A | 88 | VAL |
| 1 | 129-A | 69 | ASP |
| 1 | 132-A | 87 | ASP |
| 1 | 136-A | 20 | MET |
| 1 | 150-A | 20 | MET |
| 1 | 158-A | 142 | ASP |
| 1 | 162-A | 21 | PRO |
| 1 | 163-A | 18 | ASN |
| 1 | 174-A | 128 | TYR |
| 1 | 175-A | 142 | ASP |
| 1 | 181-A | 21 | PRO |
| 1 | 190-A | 21 | PRO |
| 1 | 191-A | 19 | ALA |
| 1 | 196-A | 21 | PRO |
| 1 | 210-A | 69 | ASP |
| 1 | 217-A | 18 | ASN |
| 1 | 233-A | 88 | VAL |
| 1 | 6-A | 22 | TRP |
| 1 | 14-A | 137 | PHE |
| 1 | 18-A | 90 | GLU |
| 1 | 20-A | 22 | TRP |
| 1 | 21-A | 88 | VAL |
| 1 | 23-A | 128 | TYR |
| 1 | 26-A | 21 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 30-A | 143 | ALA |
| 1 | 41-A | 2 | ILE |
| 1 | 59-A | 145 | ALA |
| 1 | 66-A | 20 | MET |
| 1 | 76-A | 21 | PRO |
| 1 | 81-A | 21 | PRO |
| 1 | 87-A | 21 | PRO |
| 1 | 89-A | 20 | MET |
| 1 | 89-A | 88 | VAL |
| 1 | 90-A | 18 | ASN |
| 1 | 93-A | 21 | PRO |
| 1 | 100-A | 143 | ALA |
| 1 | 111-A | 85 | CYS |
| 1 | 113-A | 21 | PRO |
| 1 | 120-A | 24 | LEU |
| 1 | 121-A | 24 | LEU |
| 1 | 123-A | 21 | PRO |
| 1 | 134-A | 20 | MET |
| 1 | 135-A | 20 | MET |
| 1 | 137-A | 20 | MET |
| 1 | 158-A | 18 | ASN |
| 1 | 158-A | 89 | PRO |
| 1 | 167-A | 21 | PRO |
| 1 | 173-A | 20 | MET |
| 1 | 174-A | 20 | MET |
| 1 | 175-A | 21 | PRO |
| 1 | 176-A | 17 | GLU |
| 1 | 182-A | 24 | LEU |
| 1 | 187-A | 128 | TYR |
| 1 | 199-A | 120 | GLU |
| 1 | 201-A | 21 | PRO |
| 1 | 214-A | 19 | ALA |
| 1 | 215-A | 143 | ALA |
| 1 | 234-A | 21 | PRO |
| 1 | 247-A | 21 | PRO |
| 1 | 250-A | 21 | PRO |
| 1 | 38-A | 120 | GLU |
| 1 | 50-A | 21 | PRO |
| 1 | 74-A | 21 | PRO |
| 1 | 115-A | 85 | CYS |
| 1 | 120-A | 22 | TRP |
| 1 | 141-A | 20 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 153-A | 18 | ASN |
| 1 | 168-A | 17 | GLU |
| 1 | 176-A | 20 | MET |
| 1 | 213-A | 20 | MET |
| 1 | 219-A | 69 | ASP |
| 1 | 55-A | 88 | VAL |
| 1 | 64-A | 20 | MET |
| 1 | 228-A | 21 | PRO |
| 1 | 53-A | 20 | MET |
| 1 | 68-A | 20 | MET |
| 1 | 232-A | 88 | VAL |
| 1 | 245-A | 21 | PRO |
| 1 | 103-A | 21 | PRO |
| 1 | 165-A | 21 | PRO |
| 1 | 170-A | 21 | PRO |
| 1 | 181-A | 24 | LEU |
| 1 | 183-A | 21 | PRO |
| 1 | 33-A | 21 | PRO |
| 1 | 111-A | 86 | GLY |
| 1 | 168-A | 21 | PRO |
| 1 | 96-A | 21 | PRO |
| 1 | 118-A | 21 | PRO |
| 1 | 174-A | 21 | PRO |
| 1 | 176-A | 21 | PRO |
| 1 | 229-A | 21 | PRO |

5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 1-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 2-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 3-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 4-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 5-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 6-A | 136/136 (100%) | 130 (96%) | 6 (4%) | 28 | 3 |
| 1 | 7-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 8-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 9-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 10-A | 136/136 (100%) | 130 (96%) | 6 (4%) | 28 | 3 |
| 1 | 11-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 12-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 13-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 14-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 15-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 16-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 17-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 18-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 19-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 20-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 21-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 22-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 23-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 24-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |
| 1 | 25-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 26-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 27-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 28-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 29-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 30-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 31-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 32-A | 136/136 (100%) | 130 (96%) | 6 (4%) | 28 | 3 |
| 1 | 33-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 34-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 35-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 36-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 37-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 38-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 39-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 40-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 41-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 42-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |
| 1 | 43-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 44-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 45-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 46-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 47-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |
| 1 | 48-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 49-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 50-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 51-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 52-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 5 | 0 |
| 1 | 53-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 54-A | 136/136 (100%) | 119 (88%) | 17 (12%) | 4 | 0 |
| 1 | 55-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 6 | 0 |
| 1 | 56-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 57-A | 136/136 (100%) | 118 (87%) | 18 (13%) | 4 | 0 |
| 1 | 58-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 59-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 60-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 61-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 62-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 63-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 64-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 65-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 66-A | 136/136 (100%) | 116 (85%) | 20 (15%) | 3 | 0 |
| 1 | 67-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 68-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 69-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 70-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 71-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 72-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 73-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 74-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 75-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |
| 1 | 76-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 77-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 78-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 79-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 80-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 81-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 82-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 83-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 84-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 85-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 86-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 87-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 88-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 89-A | 136/136 (100%) | 131 (96%) | 5 (4%) | 34 | 4 |
| 1 | 90-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 91-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 92-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 93-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 94-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |
| 1 | 95-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 96-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 97-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 98-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 99-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 100-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 101-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 102-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 6 | 0 |
| 1 | 103-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 6 | 0 |
| 1 | 104-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 5 | 0 |
| 1 | 105-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 106-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 107-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 108-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 109-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 5 | 0 |
| 1 | 110-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 111-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 112-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 113-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 114-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 115-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 116-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 117-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 118-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 119-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 120-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 121-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 122-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 123-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 124-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 125-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 126-A | 136/136 (100%) | 130 (96%) | 6 (4%) | 28 | 3 |
| 1 | 127-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 128-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 129-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 130-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 131-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 132-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 133-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |
| 1 | 134-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 135-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 136-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 5 | 0 |
| 1 | 137-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 6 | 0 |
| 1 | 138-A | 136/136 (100%) | 131 (96%) | 5 (4%) | 34 | 4 |
| 1 | 139-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 140-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 141-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 142-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 143-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 144-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 145-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 146-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 147-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 148-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 149-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |
| 1 | 150-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 151-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 152-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 153-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 6 | 0 |
| 1 | 154-A | 136/136 (100%) | 122 (90%) | 14 (10%) | 7 | 0 |
| 1 | 155-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 156-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 157-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 158-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 159-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 160-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 161-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 162-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 163-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 164-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 165-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 166-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 167-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 168-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 169-A | 136/136 (100%) | 131 (96%) | 5 (4%) | 34 | 4 |
| 1 | 170-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 171-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 172-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |
| 1 | 173-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 174-A | 136/136 (100%) | 131 (96%) | 5 (4%) | 34 | 4 |
| 1 | 175-A | 136/136 (100%) | 131 (96%) | 5 (4%) | 34 | 4 |
| 1 | 176-A | 136/136 (100%) | 131 (96%) | 5 (4%) | 34 | 4 |
| 1 | 177-A | 136/136 (100%) | 130 (96%) | 6 (4%) | 28 | 3 |
| 1 | 178-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 179-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 180-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 181-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 182-A | 136/136 (100%) | 130 (96%) | 6 (4%) | 28 | 3 |
| 1 | 183-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 184-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 185-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 186-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 187-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |
| 1 | 188-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 189-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 190-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 191-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|----------------|-----------|----------|-------------|---|
| 1 | 192-A | 136/136 (100%) | 130 (96%) | 6 (4%) | 28 | 3 |
| 1 | 193-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |
| 1 | 194-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 195-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 196-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 197-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 198-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 199-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |
| 1 | 200-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 201-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 202-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 203-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 204-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 205-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 206-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 207-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 208-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 209-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 210-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 211-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 212-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 213-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 214-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 215-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |
| 1 | 216-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 217-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 218-A | 136/136 (100%) | 120 (88%) | 16 (12%) | 5 | 0 |
| 1 | 219-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |
| 1 | 220-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |
| 1 | 221-A | 136/136 (100%) | 121 (89%) | 15 (11%) | 6 | 0 |
| 1 | 222-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|-----|-------|--------------------|-------------|-----------|-------------|---|
| 1 | 223-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 224-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 225-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 226-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 227-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 228-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 229-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 230-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 231-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| 1 | 232-A | 136/136 (100%) | 123 (90%) | 13 (10%) | 8 | 0 |
| 1 | 233-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 234-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 235-A | 136/136 (100%) | 131 (96%) | 5 (4%) | 34 | 4 |
| 1 | 236-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 237-A | 136/136 (100%) | 128 (94%) | 8 (6%) | 19 | 1 |
| 1 | 238-A | 136/136 (100%) | 130 (96%) | 6 (4%) | 28 | 3 |
| 1 | 239-A | 136/136 (100%) | 130 (96%) | 6 (4%) | 28 | 3 |
| 1 | 240-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 241-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 242-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 243-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 244-A | 136/136 (100%) | 130 (96%) | 6 (4%) | 28 | 3 |
| 1 | 245-A | 136/136 (100%) | 127 (93%) | 9 (7%) | 16 | 1 |
| 1 | 246-A | 136/136 (100%) | 126 (93%) | 10 (7%) | 13 | 1 |
| 1 | 247-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 248-A | 136/136 (100%) | 129 (95%) | 7 (5%) | 24 | 2 |
| 1 | 249-A | 136/136 (100%) | 124 (91%) | 12 (9%) | 10 | 0 |
| 1 | 250-A | 136/136 (100%) | 125 (92%) | 11 (8%) | 11 | 0 |
| All | All | 34000/34000 (100%) | 31412 (92%) | 2588 (8%) | 13 | 1 |

All (2588) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 1-A | 1 | MET |
| 1 | 1-A | 21 | PRO |
| 1 | 1-A | 33 | ARG |
| 1 | 1-A | 48 | GLU |
| 1 | 1-A | 52 | ARG |
| 1 | 1-A | 59 | ASN |
| 1 | 1-A | 98 | ARG |
| 1 | 1-A | 108 | GLN |
| 1 | 1-A | 118 | GLU |
| 1 | 1-A | 138 | SER |
| 1 | 1-A | 142 | ASP |
| 1 | 1-A | 157 | GLU |
| 1 | 2-A | 1 | MET |
| 1 | 2-A | 33 | ARG |
| 1 | 2-A | 36 | LEU |
| 1 | 2-A | 52 | ARG |
| 1 | 2-A | 59 | ASN |
| 1 | 2-A | 79 | ASP |
| 1 | 2-A | 108 | GLN |
| 1 | 2-A | 142 | ASP |
| 1 | 2-A | 148 | SER |
| 1 | 3-A | 1 | MET |
| 1 | 3-A | 4 | LEU |
| 1 | 3-A | 21 | PRO |
| 1 | 3-A | 23 | ASN |
| 1 | 3-A | 33 | ARG |
| 1 | 3-A | 36 | LEU |
| 1 | 3-A | 52 | ARG |
| 1 | 3-A | 59 | ASN |
| 1 | 3-A | 79 | ASP |
| 1 | 3-A | 104 | LEU |
| 1 | 3-A | 108 | GLN |
| 1 | 3-A | 118 | GLU |
| 1 | 3-A | 142 | ASP |
| 1 | 3-A | 157 | GLU |
| 1 | 4-A | 1 | MET |
| 1 | 4-A | 4 | LEU |
| 1 | 4-A | 20 | MET |
| 1 | 4-A | 33 | ARG |
| 1 | 4-A | 36 | LEU |
| 1 | 4-A | 52 | ARG |
| 1 | 4-A | 59 | ASN |
| 1 | 4-A | 108 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 4-A | 118 | GLU |
| 1 | 4-A | 142 | ASP |
| 1 | 5-A | 1 | MET |
| 1 | 5-A | 52 | ARG |
| 1 | 5-A | 59 | ASN |
| 1 | 5-A | 79 | ASP |
| 1 | 5-A | 87 | ASP |
| 1 | 5-A | 108 | GLN |
| 1 | 5-A | 109 | LYS |
| 1 | 5-A | 128 | TYR |
| 1 | 6-A | 1 | MET |
| 1 | 6-A | 33 | ARG |
| 1 | 6-A | 59 | ASN |
| 1 | 6-A | 106 | LYS |
| 1 | 6-A | 108 | GLN |
| 1 | 6-A | 118 | GLU |
| 1 | 7-A | 1 | MET |
| 1 | 7-A | 2 | ILE |
| 1 | 7-A | 4 | LEU |
| 1 | 7-A | 18 | ASN |
| 1 | 7-A | 20 | MET |
| 1 | 7-A | 59 | ASN |
| 1 | 7-A | 79 | ASP |
| 1 | 7-A | 119 | VAL |
| 1 | 7-A | 142 | ASP |
| 1 | 8-A | 2 | ILE |
| 1 | 8-A | 10 | VAL |
| 1 | 8-A | 33 | ARG |
| 1 | 8-A | 59 | ASN |
| 1 | 8-A | 79 | ASP |
| 1 | 8-A | 137 | PHE |
| 1 | 8-A | 142 | ASP |
| 1 | 8-A | 148 | SER |
| 1 | 8-A | 159 | ARG |
| 1 | 9-A | 1 | MET |
| 1 | 9-A | 4 | LEU |
| 1 | 9-A | 23 | ASN |
| 1 | 9-A | 52 | ARG |
| 1 | 9-A | 59 | ASN |
| 1 | 9-A | 65 | GLN |
| 1 | 9-A | 79 | ASP |
| 1 | 9-A | 108 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 9-A | 120 | GLU |
| 1 | 9-A | 139 | GLU |
| 1 | 9-A | 159 | ARG |
| 1 | 10-A | 1 | MET |
| 1 | 10-A | 59 | ASN |
| 1 | 10-A | 79 | ASP |
| 1 | 10-A | 118 | GLU |
| 1 | 10-A | 120 | GLU |
| 1 | 10-A | 156 | LEU |
| 1 | 11-A | 23 | ASN |
| 1 | 11-A | 52 | ARG |
| 1 | 11-A | 59 | ASN |
| 1 | 11-A | 108 | GLN |
| 1 | 11-A | 109 | LYS |
| 1 | 11-A | 118 | GLU |
| 1 | 11-A | 119 | VAL |
| 1 | 11-A | 134 | GLU |
| 1 | 11-A | 142 | ASP |
| 1 | 12-A | 52 | ARG |
| 1 | 12-A | 59 | ASN |
| 1 | 12-A | 62 | LEU |
| 1 | 12-A | 106 | LYS |
| 1 | 12-A | 109 | LYS |
| 1 | 12-A | 120 | GLU |
| 1 | 12-A | 142 | ASP |
| 1 | 13-A | 16 | MET |
| 1 | 13-A | 18 | ASN |
| 1 | 13-A | 52 | ARG |
| 1 | 13-A | 59 | ASN |
| 1 | 13-A | 111 | TYR |
| 1 | 13-A | 118 | GLU |
| 1 | 13-A | 120 | GLU |
| 1 | 13-A | 142 | ASP |
| 1 | 13-A | 154 | GLU |
| 1 | 13-A | 157 | GLU |
| 1 | 14-A | 1 | MET |
| 1 | 14-A | 4 | LEU |
| 1 | 14-A | 25 | PRO |
| 1 | 14-A | 59 | ASN |
| 1 | 14-A | 65 | GLN |
| 1 | 14-A | 118 | GLU |
| 1 | 14-A | 120 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 14-A | 135 | SER |
| 1 | 14-A | 142 | ASP |
| 1 | 14-A | 157 | GLU |
| 1 | 15-A | 4 | LEU |
| 1 | 15-A | 33 | ARG |
| 1 | 15-A | 59 | ASN |
| 1 | 15-A | 65 | GLN |
| 1 | 15-A | 108 | GLN |
| 1 | 15-A | 118 | GLU |
| 1 | 15-A | 120 | GLU |
| 1 | 15-A | 156 | LEU |
| 1 | 15-A | 157 | GLU |
| 1 | 16-A | 1 | MET |
| 1 | 16-A | 18 | ASN |
| 1 | 16-A | 33 | ARG |
| 1 | 16-A | 52 | ARG |
| 1 | 16-A | 59 | ASN |
| 1 | 16-A | 62 | LEU |
| 1 | 16-A | 65 | GLN |
| 1 | 16-A | 142 | ASP |
| 1 | 16-A | 156 | LEU |
| 1 | 16-A | 157 | GLU |
| 1 | 17-A | 1 | MET |
| 1 | 17-A | 4 | LEU |
| 1 | 17-A | 18 | ASN |
| 1 | 17-A | 33 | ARG |
| 1 | 17-A | 52 | ARG |
| 1 | 17-A | 59 | ASN |
| 1 | 17-A | 65 | GLN |
| 1 | 17-A | 68 | THR |
| 1 | 17-A | 76 | LYS |
| 1 | 17-A | 120 | GLU |
| 1 | 17-A | 142 | ASP |
| 1 | 18-A | 1 | MET |
| 1 | 18-A | 18 | ASN |
| 1 | 18-A | 23 | ASN |
| 1 | 18-A | 49 | SER |
| 1 | 18-A | 52 | ARG |
| 1 | 18-A | 59 | ASN |
| 1 | 18-A | 65 | GLN |
| 1 | 18-A | 120 | GLU |
| 1 | 18-A | 142 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 18-A | 148 | SER |
| 1 | 18-A | 157 | GLU |
| 1 | 19-A | 1 | MET |
| 1 | 19-A | 4 | LEU |
| 1 | 19-A | 17 | GLU |
| 1 | 19-A | 33 | ARG |
| 1 | 19-A | 52 | ARG |
| 1 | 19-A | 59 | ASN |
| 1 | 19-A | 65 | GLN |
| 1 | 19-A | 87 | ASP |
| 1 | 19-A | 108 | GLN |
| 1 | 19-A | 120 | GLU |
| 1 | 19-A | 142 | ASP |
| 1 | 19-A | 148 | SER |
| 1 | 19-A | 156 | LEU |
| 1 | 19-A | 157 | GLU |
| 1 | 20-A | 17 | GLU |
| 1 | 20-A | 18 | ASN |
| 1 | 20-A | 33 | ARG |
| 1 | 20-A | 52 | ARG |
| 1 | 20-A | 59 | ASN |
| 1 | 20-A | 106 | LYS |
| 1 | 20-A | 111 | TYR |
| 1 | 20-A | 118 | GLU |
| 1 | 20-A | 120 | GLU |
| 1 | 20-A | 138 | SER |
| 1 | 20-A | 142 | ASP |
| 1 | 20-A | 156 | LEU |
| 1 | 21-A | 1 | MET |
| 1 | 21-A | 16 | MET |
| 1 | 21-A | 44 | ARG |
| 1 | 21-A | 59 | ASN |
| 1 | 21-A | 68 | THR |
| 1 | 21-A | 118 | GLU |
| 1 | 21-A | 137 | PHE |
| 1 | 21-A | 142 | ASP |
| 1 | 21-A | 156 | LEU |
| 1 | 21-A | 157 | GLU |
| 1 | 22-A | 1 | MET |
| 1 | 22-A | 18 | ASN |
| 1 | 22-A | 52 | ARG |
| 1 | 22-A | 59 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 22-A | 65 | GLN |
| 1 | 22-A | 148 | SER |
| 1 | 22-A | 156 | LEU |
| 1 | 22-A | 157 | GLU |
| 1 | 23-A | 1 | MET |
| 1 | 23-A | 18 | ASN |
| 1 | 23-A | 33 | ARG |
| 1 | 23-A | 52 | ARG |
| 1 | 23-A | 59 | ASN |
| 1 | 23-A | 108 | GLN |
| 1 | 23-A | 118 | GLU |
| 1 | 23-A | 128 | TYR |
| 1 | 23-A | 157 | GLU |
| 1 | 24-A | 12 | ARG |
| 1 | 24-A | 21 | PRO |
| 1 | 24-A | 23 | ASN |
| 1 | 24-A | 33 | ARG |
| 1 | 24-A | 52 | ARG |
| 1 | 24-A | 59 | ASN |
| 1 | 24-A | 68 | THR |
| 1 | 24-A | 108 | GLN |
| 1 | 24-A | 118 | GLU |
| 1 | 24-A | 138 | SER |
| 1 | 24-A | 148 | SER |
| 1 | 24-A | 156 | LEU |
| 1 | 24-A | 157 | GLU |
| 1 | 25-A | 1 | MET |
| 1 | 25-A | 18 | ASN |
| 1 | 25-A | 20 | MET |
| 1 | 25-A | 44 | ARG |
| 1 | 25-A | 49 | SER |
| 1 | 25-A | 52 | ARG |
| 1 | 25-A | 59 | ASN |
| 1 | 25-A | 65 | GLN |
| 1 | 25-A | 68 | THR |
| 1 | 25-A | 118 | GLU |
| 1 | 25-A | 156 | LEU |
| 1 | 25-A | 157 | GLU |
| 1 | 26-A | 4 | LEU |
| 1 | 26-A | 10 | VAL |
| 1 | 26-A | 21 | PRO |
| 1 | 26-A | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 26-A | 59 | ASN |
| 1 | 26-A | 65 | GLN |
| 1 | 26-A | 106 | LYS |
| 1 | 26-A | 108 | GLN |
| 1 | 26-A | 118 | GLU |
| 1 | 26-A | 120 | GLU |
| 1 | 26-A | 156 | LEU |
| 1 | 27-A | 1 | MET |
| 1 | 27-A | 23 | ASN |
| 1 | 27-A | 44 | ARG |
| 1 | 27-A | 52 | ARG |
| 1 | 27-A | 59 | ASN |
| 1 | 27-A | 118 | GLU |
| 1 | 27-A | 159 | ARG |
| 1 | 28-A | 20 | MET |
| 1 | 28-A | 23 | ASN |
| 1 | 28-A | 33 | ARG |
| 1 | 28-A | 44 | ARG |
| 1 | 28-A | 52 | ARG |
| 1 | 28-A | 59 | ASN |
| 1 | 28-A | 65 | GLN |
| 1 | 28-A | 101 | GLU |
| 1 | 28-A | 108 | GLN |
| 1 | 29-A | 1 | MET |
| 1 | 29-A | 4 | LEU |
| 1 | 29-A | 18 | ASN |
| 1 | 29-A | 23 | ASN |
| 1 | 29-A | 33 | ARG |
| 1 | 29-A | 44 | ARG |
| 1 | 29-A | 59 | ASN |
| 1 | 30-A | 18 | ASN |
| 1 | 30-A | 33 | ARG |
| 1 | 30-A | 44 | ARG |
| 1 | 30-A | 49 | SER |
| 1 | 30-A | 52 | ARG |
| 1 | 30-A | 59 | ASN |
| 1 | 30-A | 101 | GLU |
| 1 | 30-A | 159 | ARG |
| 1 | 31-A | 4 | LEU |
| 1 | 31-A | 33 | ARG |
| 1 | 31-A | 44 | ARG |
| 1 | 31-A | 49 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 31-A | 59 | ASN |
| 1 | 31-A | 79 | ASP |
| 1 | 31-A | 101 | GLU |
| 1 | 31-A | 108 | GLN |
| 1 | 31-A | 109 | LYS |
| 1 | 32-A | 1 | MET |
| 1 | 32-A | 20 | MET |
| 1 | 32-A | 44 | ARG |
| 1 | 32-A | 59 | ASN |
| 1 | 32-A | 87 | ASP |
| 1 | 32-A | 119 | VAL |
| 1 | 33-A | 1 | MET |
| 1 | 33-A | 18 | ASN |
| 1 | 33-A | 33 | ARG |
| 1 | 33-A | 44 | ARG |
| 1 | 33-A | 48 | GLU |
| 1 | 33-A | 59 | ASN |
| 1 | 33-A | 79 | ASP |
| 1 | 33-A | 87 | ASP |
| 1 | 33-A | 135 | SER |
| 1 | 34-A | 1 | MET |
| 1 | 34-A | 4 | LEU |
| 1 | 34-A | 18 | ASN |
| 1 | 34-A | 20 | MET |
| 1 | 34-A | 28 | LEU |
| 1 | 34-A | 33 | ARG |
| 1 | 34-A | 44 | ARG |
| 1 | 34-A | 55 | PRO |
| 1 | 34-A | 59 | ASN |
| 1 | 34-A | 79 | ASP |
| 1 | 35-A | 16 | MET |
| 1 | 35-A | 18 | ASN |
| 1 | 35-A | 20 | MET |
| 1 | 35-A | 21 | PRO |
| 1 | 35-A | 23 | ASN |
| 1 | 35-A | 44 | ARG |
| 1 | 35-A | 48 | GLU |
| 1 | 35-A | 49 | SER |
| 1 | 35-A | 59 | ASN |
| 1 | 35-A | 65 | GLN |
| 1 | 35-A | 101 | GLU |
| 1 | 35-A | 118 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 35-A | 128 | TYR |
| 1 | 35-A | 139 | GLU |
| 1 | 36-A | 1 | MET |
| 1 | 36-A | 4 | LEU |
| 1 | 36-A | 18 | ASN |
| 1 | 36-A | 23 | ASN |
| 1 | 36-A | 59 | ASN |
| 1 | 36-A | 87 | ASP |
| 1 | 36-A | 101 | GLU |
| 1 | 36-A | 106 | LYS |
| 1 | 37-A | 1 | MET |
| 1 | 37-A | 4 | LEU |
| 1 | 37-A | 16 | MET |
| 1 | 37-A | 18 | ASN |
| 1 | 37-A | 23 | ASN |
| 1 | 37-A | 52 | ARG |
| 1 | 37-A | 59 | ASN |
| 1 | 37-A | 101 | GLU |
| 1 | 37-A | 142 | ASP |
| 1 | 38-A | 16 | MET |
| 1 | 38-A | 20 | MET |
| 1 | 38-A | 52 | ARG |
| 1 | 38-A | 59 | ASN |
| 1 | 38-A | 65 | GLN |
| 1 | 38-A | 106 | LYS |
| 1 | 38-A | 109 | LYS |
| 1 | 38-A | 119 | VAL |
| 1 | 38-A | 120 | GLU |
| 1 | 38-A | 139 | GLU |
| 1 | 38-A | 156 | LEU |
| 1 | 39-A | 4 | LEU |
| 1 | 39-A | 33 | ARG |
| 1 | 39-A | 52 | ARG |
| 1 | 39-A | 59 | ASN |
| 1 | 39-A | 60 | ILE |
| 1 | 39-A | 65 | GLN |
| 1 | 39-A | 101 | GLU |
| 1 | 39-A | 142 | ASP |
| 1 | 40-A | 1 | MET |
| 1 | 40-A | 33 | ARG |
| 1 | 40-A | 44 | ARG |
| 1 | 40-A | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 40-A | 59 | ASN |
| 1 | 40-A | 79 | ASP |
| 1 | 40-A | 101 | GLU |
| 1 | 40-A | 120 | GLU |
| 1 | 40-A | 142 | ASP |
| 1 | 40-A | 156 | LEU |
| 1 | 41-A | 1 | MET |
| 1 | 41-A | 4 | LEU |
| 1 | 41-A | 49 | SER |
| 1 | 41-A | 52 | ARG |
| 1 | 41-A | 59 | ASN |
| 1 | 41-A | 60 | ILE |
| 1 | 41-A | 65 | GLN |
| 1 | 41-A | 87 | ASP |
| 1 | 41-A | 101 | GLU |
| 1 | 41-A | 108 | GLN |
| 1 | 41-A | 120 | GLU |
| 1 | 41-A | 142 | ASP |
| 1 | 41-A | 148 | SER |
| 1 | 41-A | 156 | LEU |
| 1 | 42-A | 1 | MET |
| 1 | 42-A | 33 | ARG |
| 1 | 42-A | 52 | ARG |
| 1 | 42-A | 59 | ASN |
| 1 | 42-A | 60 | ILE |
| 1 | 42-A | 65 | GLN |
| 1 | 42-A | 66 | PRO |
| 1 | 42-A | 87 | ASP |
| 1 | 42-A | 108 | GLN |
| 1 | 42-A | 120 | GLU |
| 1 | 42-A | 134 | GLU |
| 1 | 42-A | 156 | LEU |
| 1 | 42-A | 159 | ARG |
| 1 | 43-A | 1 | MET |
| 1 | 43-A | 23 | ASN |
| 1 | 43-A | 59 | ASN |
| 1 | 43-A | 65 | GLN |
| 1 | 43-A | 119 | VAL |
| 1 | 43-A | 137 | PHE |
| 1 | 43-A | 142 | ASP |
| 1 | 43-A | 159 | ARG |
| 1 | 44-A | 1 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 44-A | 4 | LEU |
| 1 | 44-A | 18 | ASN |
| 1 | 44-A | 20 | MET |
| 1 | 44-A | 52 | ARG |
| 1 | 44-A | 59 | ASN |
| 1 | 44-A | 65 | GLN |
| 1 | 44-A | 120 | GLU |
| 1 | 44-A | 159 | ARG |
| 1 | 45-A | 4 | LEU |
| 1 | 45-A | 36 | LEU |
| 1 | 45-A | 44 | ARG |
| 1 | 45-A | 59 | ASN |
| 1 | 45-A | 65 | GLN |
| 1 | 45-A | 142 | ASP |
| 1 | 45-A | 148 | SER |
| 1 | 45-A | 159 | ARG |
| 1 | 46-A | 1 | MET |
| 1 | 46-A | 44 | ARG |
| 1 | 46-A | 59 | ASN |
| 1 | 46-A | 65 | GLN |
| 1 | 46-A | 104 | LEU |
| 1 | 46-A | 142 | ASP |
| 1 | 46-A | 159 | ARG |
| 1 | 47-A | 4 | LEU |
| 1 | 47-A | 20 | MET |
| 1 | 47-A | 23 | ASN |
| 1 | 47-A | 44 | ARG |
| 1 | 47-A | 52 | ARG |
| 1 | 47-A | 59 | ASN |
| 1 | 47-A | 65 | GLN |
| 1 | 47-A | 87 | ASP |
| 1 | 47-A | 101 | GLU |
| 1 | 47-A | 106 | LYS |
| 1 | 47-A | 118 | GLU |
| 1 | 47-A | 142 | ASP |
| 1 | 47-A | 159 | ARG |
| 1 | 48-A | 1 | MET |
| 1 | 48-A | 2 | ILE |
| 1 | 48-A | 10 | VAL |
| 1 | 48-A | 16 | MET |
| 1 | 48-A | 20 | MET |
| 1 | 48-A | 44 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 48-A | 49 | SER |
| 1 | 48-A | 52 | ARG |
| 1 | 48-A | 59 | ASN |
| 1 | 48-A | 65 | GLN |
| 1 | 48-A | 128 | TYR |
| 1 | 48-A | 142 | ASP |
| 1 | 48-A | 148 | SER |
| 1 | 48-A | 159 | ARG |
| 1 | 49-A | 1 | MET |
| 1 | 49-A | 23 | ASN |
| 1 | 49-A | 32 | LYS |
| 1 | 49-A | 33 | ARG |
| 1 | 49-A | 44 | ARG |
| 1 | 49-A | 49 | SER |
| 1 | 49-A | 52 | ARG |
| 1 | 49-A | 59 | ASN |
| 1 | 49-A | 65 | GLN |
| 1 | 49-A | 106 | LYS |
| 1 | 49-A | 118 | GLU |
| 1 | 49-A | 119 | VAL |
| 1 | 49-A | 157 | GLU |
| 1 | 49-A | 159 | ARG |
| 1 | 50-A | 1 | MET |
| 1 | 50-A | 4 | LEU |
| 1 | 50-A | 20 | MET |
| 1 | 50-A | 21 | PRO |
| 1 | 50-A | 24 | LEU |
| 1 | 50-A | 33 | ARG |
| 1 | 50-A | 52 | ARG |
| 1 | 50-A | 59 | ASN |
| 1 | 50-A | 65 | GLN |
| 1 | 50-A | 76 | LYS |
| 1 | 50-A | 119 | VAL |
| 1 | 50-A | 132 | ASP |
| 1 | 50-A | 148 | SER |
| 1 | 50-A | 156 | LEU |
| 1 | 51-A | 1 | MET |
| 1 | 51-A | 4 | LEU |
| 1 | 51-A | 20 | MET |
| 1 | 51-A | 24 | LEU |
| 1 | 51-A | 52 | ARG |
| 1 | 51-A | 59 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 51-A | 65 | GLN |
| 1 | 51-A | 76 | LYS |
| 1 | 51-A | 139 | GLU |
| 1 | 51-A | 148 | SER |
| 1 | 51-A | 154 | GLU |
| 1 | 52-A | 1 | MET |
| 1 | 52-A | 17 | GLU |
| 1 | 52-A | 18 | ASN |
| 1 | 52-A | 20 | MET |
| 1 | 52-A | 21 | PRO |
| 1 | 52-A | 23 | ASN |
| 1 | 52-A | 24 | LEU |
| 1 | 52-A | 33 | ARG |
| 1 | 52-A | 44 | ARG |
| 1 | 52-A | 48 | GLU |
| 1 | 52-A | 52 | ARG |
| 1 | 52-A | 59 | ASN |
| 1 | 52-A | 65 | GLN |
| 1 | 52-A | 118 | GLU |
| 1 | 52-A | 148 | SER |
| 1 | 52-A | 157 | GLU |
| 1 | 53-A | 20 | MET |
| 1 | 53-A | 33 | ARG |
| 1 | 53-A | 44 | ARG |
| 1 | 53-A | 48 | GLU |
| 1 | 53-A | 52 | ARG |
| 1 | 53-A | 59 | ASN |
| 1 | 53-A | 76 | LYS |
| 1 | 53-A | 87 | ASP |
| 1 | 53-A | 106 | LYS |
| 1 | 53-A | 118 | GLU |
| 1 | 53-A | 134 | GLU |
| 1 | 53-A | 138 | SER |
| 1 | 53-A | 157 | GLU |
| 1 | 53-A | 159 | ARG |
| 1 | 54-A | 1 | MET |
| 1 | 54-A | 4 | LEU |
| 1 | 54-A | 18 | ASN |
| 1 | 54-A | 23 | ASN |
| 1 | 54-A | 33 | ARG |
| 1 | 54-A | 44 | ARG |
| 1 | 54-A | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 54-A | 59 | ASN |
| 1 | 54-A | 62 | LEU |
| 1 | 54-A | 76 | LYS |
| 1 | 54-A | 87 | ASP |
| 1 | 54-A | 118 | GLU |
| 1 | 54-A | 120 | GLU |
| 1 | 54-A | 134 | GLU |
| 1 | 54-A | 156 | LEU |
| 1 | 54-A | 157 | GLU |
| 1 | 54-A | 159 | ARG |
| 1 | 55-A | 1 | MET |
| 1 | 55-A | 16 | MET |
| 1 | 55-A | 20 | MET |
| 1 | 55-A | 33 | ARG |
| 1 | 55-A | 44 | ARG |
| 1 | 55-A | 48 | GLU |
| 1 | 55-A | 59 | ASN |
| 1 | 55-A | 65 | GLN |
| 1 | 55-A | 76 | LYS |
| 1 | 55-A | 87 | ASP |
| 1 | 55-A | 118 | GLU |
| 1 | 55-A | 119 | VAL |
| 1 | 55-A | 120 | GLU |
| 1 | 55-A | 156 | LEU |
| 1 | 55-A | 159 | ARG |
| 1 | 56-A | 4 | LEU |
| 1 | 56-A | 20 | MET |
| 1 | 56-A | 24 | LEU |
| 1 | 56-A | 33 | ARG |
| 1 | 56-A | 44 | ARG |
| 1 | 56-A | 59 | ASN |
| 1 | 56-A | 76 | LYS |
| 1 | 56-A | 109 | LYS |
| 1 | 56-A | 156 | LEU |
| 1 | 56-A | 159 | ARG |
| 1 | 57-A | 1 | MET |
| 1 | 57-A | 4 | LEU |
| 1 | 57-A | 20 | MET |
| 1 | 57-A | 21 | PRO |
| 1 | 57-A | 23 | ASN |
| 1 | 57-A | 33 | ARG |
| 1 | 57-A | 48 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 57-A | 52 | ARG |
| 1 | 57-A | 59 | ASN |
| 1 | 57-A | 65 | GLN |
| 1 | 57-A | 79 | ASP |
| 1 | 57-A | 87 | ASP |
| 1 | 57-A | 101 | GLU |
| 1 | 57-A | 109 | LYS |
| 1 | 57-A | 111 | TYR |
| 1 | 57-A | 118 | GLU |
| 1 | 57-A | 119 | VAL |
| 1 | 57-A | 159 | ARG |
| 1 | 58-A | 4 | LEU |
| 1 | 58-A | 20 | MET |
| 1 | 58-A | 44 | ARG |
| 1 | 58-A | 48 | GLU |
| 1 | 58-A | 49 | SER |
| 1 | 58-A | 52 | ARG |
| 1 | 58-A | 59 | ASN |
| 1 | 58-A | 65 | GLN |
| 1 | 58-A | 106 | LYS |
| 1 | 58-A | 109 | LYS |
| 1 | 58-A | 134 | GLU |
| 1 | 58-A | 139 | GLU |
| 1 | 59-A | 20 | MET |
| 1 | 59-A | 44 | ARG |
| 1 | 59-A | 52 | ARG |
| 1 | 59-A | 59 | ASN |
| 1 | 59-A | 76 | LYS |
| 1 | 59-A | 118 | GLU |
| 1 | 59-A | 119 | VAL |
| 1 | 59-A | 120 | GLU |
| 1 | 59-A | 128 | TYR |
| 1 | 59-A | 139 | GLU |
| 1 | 59-A | 152 | CYS |
| 1 | 59-A | 159 | ARG |
| 1 | 60-A | 1 | MET |
| 1 | 60-A | 20 | MET |
| 1 | 60-A | 44 | ARG |
| 1 | 60-A | 49 | SER |
| 1 | 60-A | 52 | ARG |
| 1 | 60-A | 59 | ASN |
| 1 | 60-A | 65 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 60-A | 76 | LYS |
| 1 | 60-A | 79 | ASP |
| 1 | 60-A | 87 | ASP |
| 1 | 60-A | 118 | GLU |
| 1 | 60-A | 159 | ARG |
| 1 | 61-A | 1 | MET |
| 1 | 61-A | 16 | MET |
| 1 | 61-A | 20 | MET |
| 1 | 61-A | 24 | LEU |
| 1 | 61-A | 44 | ARG |
| 1 | 61-A | 52 | ARG |
| 1 | 61-A | 59 | ASN |
| 1 | 61-A | 76 | LYS |
| 1 | 61-A | 108 | GLN |
| 1 | 61-A | 156 | LEU |
| 1 | 61-A | 159 | ARG |
| 1 | 62-A | 1 | MET |
| 1 | 62-A | 16 | MET |
| 1 | 62-A | 18 | ASN |
| 1 | 62-A | 25 | PRO |
| 1 | 62-A | 44 | ARG |
| 1 | 62-A | 49 | SER |
| 1 | 62-A | 52 | ARG |
| 1 | 62-A | 59 | ASN |
| 1 | 62-A | 76 | LYS |
| 1 | 62-A | 79 | ASP |
| 1 | 62-A | 101 | GLU |
| 1 | 62-A | 139 | GLU |
| 1 | 62-A | 156 | LEU |
| 1 | 62-A | 159 | ARG |
| 1 | 63-A | 1 | MET |
| 1 | 63-A | 16 | MET |
| 1 | 63-A | 20 | MET |
| 1 | 63-A | 44 | ARG |
| 1 | 63-A | 52 | ARG |
| 1 | 63-A | 59 | ASN |
| 1 | 63-A | 76 | LYS |
| 1 | 63-A | 79 | ASP |
| 1 | 63-A | 106 | LYS |
| 1 | 63-A | 134 | GLU |
| 1 | 63-A | 159 | ARG |
| 1 | 64-A | 1 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 64-A | 16 | MET |
| 1 | 64-A | 20 | MET |
| 1 | 64-A | 33 | ARG |
| 1 | 64-A | 44 | ARG |
| 1 | 64-A | 59 | ASN |
| 1 | 64-A | 65 | GLN |
| 1 | 64-A | 76 | LYS |
| 1 | 64-A | 101 | GLU |
| 1 | 64-A | 106 | LYS |
| 1 | 64-A | 119 | VAL |
| 1 | 64-A | 137 | PHE |
| 1 | 64-A | 152 | CYS |
| 1 | 64-A | 159 | ARG |
| 1 | 65-A | 1 | MET |
| 1 | 65-A | 16 | MET |
| 1 | 65-A | 20 | MET |
| 1 | 65-A | 24 | LEU |
| 1 | 65-A | 59 | ASN |
| 1 | 65-A | 65 | GLN |
| 1 | 65-A | 76 | LYS |
| 1 | 65-A | 106 | LYS |
| 1 | 65-A | 108 | GLN |
| 1 | 66-A | 1 | MET |
| 1 | 66-A | 4 | LEU |
| 1 | 66-A | 16 | MET |
| 1 | 66-A | 17 | GLU |
| 1 | 66-A | 20 | MET |
| 1 | 66-A | 22 | TRP |
| 1 | 66-A | 24 | LEU |
| 1 | 66-A | 33 | ARG |
| 1 | 66-A | 52 | ARG |
| 1 | 66-A | 59 | ASN |
| 1 | 66-A | 65 | GLN |
| 1 | 66-A | 68 | THR |
| 1 | 66-A | 76 | LYS |
| 1 | 66-A | 87 | ASP |
| 1 | 66-A | 104 | LEU |
| 1 | 66-A | 106 | LYS |
| 1 | 66-A | 118 | GLU |
| 1 | 66-A | 138 | SER |
| 1 | 66-A | 154 | GLU |
| 1 | 66-A | 159 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 67-A | 16 | MET |
| 1 | 67-A | 24 | LEU |
| 1 | 67-A | 59 | ASN |
| 1 | 67-A | 65 | GLN |
| 1 | 67-A | 76 | LYS |
| 1 | 67-A | 108 | GLN |
| 1 | 67-A | 109 | LYS |
| 1 | 67-A | 119 | VAL |
| 1 | 67-A | 159 | ARG |
| 1 | 68-A | 1 | MET |
| 1 | 68-A | 4 | LEU |
| 1 | 68-A | 33 | ARG |
| 1 | 68-A | 52 | ARG |
| 1 | 68-A | 59 | ASN |
| 1 | 68-A | 76 | LYS |
| 1 | 68-A | 109 | LYS |
| 1 | 68-A | 118 | GLU |
| 1 | 68-A | 120 | GLU |
| 1 | 68-A | 159 | ARG |
| 1 | 69-A | 1 | MET |
| 1 | 69-A | 4 | LEU |
| 1 | 69-A | 20 | MET |
| 1 | 69-A | 23 | ASN |
| 1 | 69-A | 24 | LEU |
| 1 | 69-A | 48 | GLU |
| 1 | 69-A | 59 | ASN |
| 1 | 69-A | 65 | GLN |
| 1 | 69-A | 76 | LYS |
| 1 | 69-A | 109 | LYS |
| 1 | 69-A | 118 | GLU |
| 1 | 70-A | 1 | MET |
| 1 | 70-A | 2 | ILE |
| 1 | 70-A | 4 | LEU |
| 1 | 70-A | 20 | MET |
| 1 | 70-A | 23 | ASN |
| 1 | 70-A | 24 | LEU |
| 1 | 70-A | 52 | ARG |
| 1 | 70-A | 59 | ASN |
| 1 | 70-A | 65 | GLN |
| 1 | 70-A | 76 | LYS |
| 1 | 70-A | 101 | GLU |
| 1 | 70-A | 137 | PHE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 70-A | 156 | LEU |
| 1 | 70-A | 157 | GLU |
| 1 | 71-A | 1 | MET |
| 1 | 71-A | 2 | ILE |
| 1 | 71-A | 16 | MET |
| 1 | 71-A | 20 | MET |
| 1 | 71-A | 23 | ASN |
| 1 | 71-A | 33 | ARG |
| 1 | 71-A | 52 | ARG |
| 1 | 71-A | 59 | ASN |
| 1 | 71-A | 76 | LYS |
| 1 | 71-A | 119 | VAL |
| 1 | 71-A | 120 | GLU |
| 1 | 71-A | 128 | TYR |
| 1 | 71-A | 142 | ASP |
| 1 | 71-A | 159 | ARG |
| 1 | 72-A | 1 | MET |
| 1 | 72-A | 16 | MET |
| 1 | 72-A | 20 | MET |
| 1 | 72-A | 23 | ASN |
| 1 | 72-A | 52 | ARG |
| 1 | 72-A | 59 | ASN |
| 1 | 72-A | 65 | GLN |
| 1 | 72-A | 76 | LYS |
| 1 | 72-A | 106 | LYS |
| 1 | 72-A | 142 | ASP |
| 1 | 72-A | 159 | ARG |
| 1 | 73-A | 4 | LEU |
| 1 | 73-A | 10 | VAL |
| 1 | 73-A | 16 | MET |
| 1 | 73-A | 20 | MET |
| 1 | 73-A | 24 | LEU |
| 1 | 73-A | 25 | PRO |
| 1 | 73-A | 33 | ARG |
| 1 | 73-A | 59 | ASN |
| 1 | 73-A | 98 | ARG |
| 1 | 73-A | 106 | LYS |
| 1 | 73-A | 118 | GLU |
| 1 | 73-A | 157 | GLU |
| 1 | 74-A | 1 | MET |
| 1 | 74-A | 16 | MET |
| 1 | 74-A | 20 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 74-A | 23 | ASN |
| 1 | 74-A | 24 | LEU |
| 1 | 74-A | 48 | GLU |
| 1 | 74-A | 59 | ASN |
| 1 | 74-A | 98 | ARG |
| 1 | 74-A | 118 | GLU |
| 1 | 74-A | 157 | GLU |
| 1 | 75-A | 1 | MET |
| 1 | 75-A | 4 | LEU |
| 1 | 75-A | 16 | MET |
| 1 | 75-A | 20 | MET |
| 1 | 75-A | 24 | LEU |
| 1 | 75-A | 52 | ARG |
| 1 | 75-A | 59 | ASN |
| 1 | 75-A | 87 | ASP |
| 1 | 75-A | 104 | LEU |
| 1 | 75-A | 106 | LYS |
| 1 | 75-A | 108 | GLN |
| 1 | 75-A | 137 | PHE |
| 1 | 75-A | 159 | ARG |
| 1 | 76-A | 1 | MET |
| 1 | 76-A | 16 | MET |
| 1 | 76-A | 20 | MET |
| 1 | 76-A | 23 | ASN |
| 1 | 76-A | 24 | LEU |
| 1 | 76-A | 33 | ARG |
| 1 | 76-A | 59 | ASN |
| 1 | 76-A | 76 | LYS |
| 1 | 76-A | 104 | LEU |
| 1 | 76-A | 106 | LYS |
| 1 | 76-A | 108 | GLN |
| 1 | 76-A | 118 | GLU |
| 1 | 76-A | 156 | LEU |
| 1 | 76-A | 159 | ARG |
| 1 | 77-A | 1 | MET |
| 1 | 77-A | 16 | MET |
| 1 | 77-A | 20 | MET |
| 1 | 77-A | 24 | LEU |
| 1 | 77-A | 33 | ARG |
| 1 | 77-A | 36 | LEU |
| 1 | 77-A | 48 | GLU |
| 1 | 77-A | 59 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 77-A | 76 | LYS |
| 1 | 77-A | 108 | GLN |
| 1 | 77-A | 138 | SER |
| 1 | 77-A | 156 | LEU |
| 1 | 78-A | 1 | MET |
| 1 | 78-A | 4 | LEU |
| 1 | 78-A | 16 | MET |
| 1 | 78-A | 18 | ASN |
| 1 | 78-A | 33 | ARG |
| 1 | 78-A | 36 | LEU |
| 1 | 78-A | 48 | GLU |
| 1 | 78-A | 59 | ASN |
| 1 | 78-A | 87 | ASP |
| 1 | 78-A | 128 | TYR |
| 1 | 79-A | 4 | LEU |
| 1 | 79-A | 16 | MET |
| 1 | 79-A | 20 | MET |
| 1 | 79-A | 48 | GLU |
| 1 | 79-A | 52 | ARG |
| 1 | 79-A | 59 | ASN |
| 1 | 79-A | 120 | GLU |
| 1 | 80-A | 16 | MET |
| 1 | 80-A | 20 | MET |
| 1 | 80-A | 48 | GLU |
| 1 | 80-A | 49 | SER |
| 1 | 80-A | 59 | ASN |
| 1 | 80-A | 88 | VAL |
| 1 | 80-A | 120 | GLU |
| 1 | 80-A | 138 | SER |
| 1 | 80-A | 148 | SER |
| 1 | 81-A | 1 | MET |
| 1 | 81-A | 16 | MET |
| 1 | 81-A | 20 | MET |
| 1 | 81-A | 33 | ARG |
| 1 | 81-A | 48 | GLU |
| 1 | 81-A | 52 | ARG |
| 1 | 81-A | 59 | ASN |
| 1 | 81-A | 65 | GLN |
| 1 | 81-A | 88 | VAL |
| 1 | 81-A | 101 | GLU |
| 1 | 81-A | 138 | SER |
| 1 | 82-A | 1 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 82-A | 4 | LEU |
| 1 | 82-A | 16 | MET |
| 1 | 82-A | 20 | MET |
| 1 | 82-A | 24 | LEU |
| 1 | 82-A | 52 | ARG |
| 1 | 82-A | 59 | ASN |
| 1 | 82-A | 128 | TYR |
| 1 | 82-A | 134 | GLU |
| 1 | 83-A | 4 | LEU |
| 1 | 83-A | 16 | MET |
| 1 | 83-A | 20 | MET |
| 1 | 83-A | 24 | LEU |
| 1 | 83-A | 33 | ARG |
| 1 | 83-A | 49 | SER |
| 1 | 83-A | 52 | ARG |
| 1 | 83-A | 59 | ASN |
| 1 | 83-A | 70 | ASP |
| 1 | 83-A | 101 | GLU |
| 1 | 83-A | 108 | GLN |
| 1 | 83-A | 111 | TYR |
| 1 | 83-A | 134 | GLU |
| 1 | 83-A | 139 | GLU |
| 1 | 84-A | 1 | MET |
| 1 | 84-A | 4 | LEU |
| 1 | 84-A | 16 | MET |
| 1 | 84-A | 18 | ASN |
| 1 | 84-A | 20 | MET |
| 1 | 84-A | 52 | ARG |
| 1 | 84-A | 59 | ASN |
| 1 | 84-A | 65 | GLN |
| 1 | 84-A | 70 | ASP |
| 1 | 84-A | 101 | GLU |
| 1 | 84-A | 108 | GLN |
| 1 | 84-A | 118 | GLU |
| 1 | 84-A | 119 | VAL |
| 1 | 84-A | 138 | SER |
| 1 | 85-A | 1 | MET |
| 1 | 85-A | 4 | LEU |
| 1 | 85-A | 16 | MET |
| 1 | 85-A | 18 | ASN |
| 1 | 85-A | 20 | MET |
| 1 | 85-A | 48 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 85-A | 52 | ARG |
| 1 | 85-A | 59 | ASN |
| 1 | 85-A | 106 | LYS |
| 1 | 85-A | 118 | GLU |
| 1 | 85-A | 119 | VAL |
| 1 | 85-A | 152 | CYS |
| 1 | 85-A | 154 | GLU |
| 1 | 85-A | 156 | LEU |
| 1 | 86-A | 16 | MET |
| 1 | 86-A | 20 | MET |
| 1 | 86-A | 24 | LEU |
| 1 | 86-A | 28 | LEU |
| 1 | 86-A | 52 | ARG |
| 1 | 86-A | 59 | ASN |
| 1 | 86-A | 106 | LYS |
| 1 | 86-A | 111 | TYR |
| 1 | 86-A | 119 | VAL |
| 1 | 86-A | 156 | LEU |
| 1 | 87-A | 1 | MET |
| 1 | 87-A | 16 | MET |
| 1 | 87-A | 18 | ASN |
| 1 | 87-A | 20 | MET |
| 1 | 87-A | 23 | ASN |
| 1 | 87-A | 59 | ASN |
| 1 | 87-A | 65 | GLN |
| 1 | 87-A | 101 | GLU |
| 1 | 87-A | 119 | VAL |
| 1 | 87-A | 120 | GLU |
| 1 | 87-A | 148 | SER |
| 1 | 87-A | 154 | GLU |
| 1 | 88-A | 1 | MET |
| 1 | 88-A | 4 | LEU |
| 1 | 88-A | 20 | MET |
| 1 | 88-A | 21 | PRO |
| 1 | 88-A | 23 | ASN |
| 1 | 88-A | 48 | GLU |
| 1 | 88-A | 59 | ASN |
| 1 | 88-A | 62 | LEU |
| 1 | 88-A | 101 | GLU |
| 1 | 88-A | 154 | GLU |
| 1 | 89-A | 1 | MET |
| 1 | 89-A | 23 | ASN |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 89-A | 52 | ARG |
| 1 | 89-A | 59 | ASN |
| 1 | 89-A | 148 | SER |
| 1 | 90-A | 1 | MET |
| 1 | 90-A | 4 | LEU |
| 1 | 90-A | 10 | VAL |
| 1 | 90-A | 17 | GLU |
| 1 | 90-A | 18 | ASN |
| 1 | 90-A | 20 | MET |
| 1 | 90-A | 52 | ARG |
| 1 | 90-A | 59 | ASN |
| 1 | 90-A | 79 | ASP |
| 1 | 90-A | 109 | LYS |
| 1 | 90-A | 119 | VAL |
| 1 | 91-A | 4 | LEU |
| 1 | 91-A | 20 | MET |
| 1 | 91-A | 52 | ARG |
| 1 | 91-A | 59 | ASN |
| 1 | 91-A | 79 | ASP |
| 1 | 91-A | 109 | LYS |
| 1 | 91-A | 119 | VAL |
| 1 | 91-A | 148 | SER |
| 1 | 92-A | 1 | MET |
| 1 | 92-A | 20 | MET |
| 1 | 92-A | 24 | LEU |
| 1 | 92-A | 52 | ARG |
| 1 | 92-A | 59 | ASN |
| 1 | 92-A | 79 | ASP |
| 1 | 92-A | 87 | ASP |
| 1 | 92-A | 108 | GLN |
| 1 | 92-A | 109 | LYS |
| 1 | 92-A | 119 | VAL |
| 1 | 92-A | 128 | TYR |
| 1 | 92-A | 138 | SER |
| 1 | 93-A | 1 | MET |
| 1 | 93-A | 18 | ASN |
| 1 | 93-A | 20 | MET |
| 1 | 93-A | 24 | LEU |
| 1 | 93-A | 33 | ARG |
| 1 | 93-A | 52 | ARG |
| 1 | 93-A | 59 | ASN |
| 1 | 93-A | 109 | LYS |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 93-A | 118 | GLU |
| 1 | 93-A | 130 | PRO |
| 1 | 93-A | 156 | LEU |
| 1 | 94-A | 1 | MET |
| 1 | 94-A | 4 | LEU |
| 1 | 94-A | 16 | MET |
| 1 | 94-A | 18 | ASN |
| 1 | 94-A | 20 | MET |
| 1 | 94-A | 24 | LEU |
| 1 | 94-A | 33 | ARG |
| 1 | 94-A | 52 | ARG |
| 1 | 94-A | 59 | ASN |
| 1 | 94-A | 101 | GLU |
| 1 | 94-A | 109 | LYS |
| 1 | 94-A | 118 | GLU |
| 1 | 94-A | 139 | GLU |
| 1 | 95-A | 1 | MET |
| 1 | 95-A | 33 | ARG |
| 1 | 95-A | 52 | ARG |
| 1 | 95-A | 59 | ASN |
| 1 | 95-A | 65 | GLN |
| 1 | 95-A | 109 | LYS |
| 1 | 95-A | 120 | GLU |
| 1 | 95-A | 142 | ASP |
| 1 | 95-A | 148 | SER |
| 1 | 96-A | 1 | MET |
| 1 | 96-A | 24 | LEU |
| 1 | 96-A | 52 | ARG |
| 1 | 96-A | 59 | ASN |
| 1 | 96-A | 65 | GLN |
| 1 | 96-A | 108 | GLN |
| 1 | 96-A | 109 | LYS |
| 1 | 96-A | 118 | GLU |
| 1 | 96-A | 119 | VAL |
| 1 | 96-A | 120 | GLU |
| 1 | 96-A | 148 | SER |
| 1 | 97-A | 1 | MET |
| 1 | 97-A | 4 | LEU |
| 1 | 97-A | 21 | PRO |
| 1 | 97-A | 24 | LEU |
| 1 | 97-A | 52 | ARG |
| 1 | 97-A | 59 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 97-A | 106 | LYS |
| 1 | 97-A | 108 | GLN |
| 1 | 97-A | 118 | GLU |
| 1 | 97-A | 134 | GLU |
| 1 | 97-A | 138 | SER |
| 1 | 97-A | 142 | ASP |
| 1 | 98-A | 1 | MET |
| 1 | 98-A | 18 | ASN |
| 1 | 98-A | 20 | MET |
| 1 | 98-A | 23 | ASN |
| 1 | 98-A | 36 | LEU |
| 1 | 98-A | 59 | ASN |
| 1 | 98-A | 65 | GLN |
| 1 | 98-A | 101 | GLU |
| 1 | 98-A | 104 | LEU |
| 1 | 98-A | 108 | GLN |
| 1 | 98-A | 118 | GLU |
| 1 | 98-A | 142 | ASP |
| 1 | 98-A | 157 | GLU |
| 1 | 99-A | 18 | ASN |
| 1 | 99-A | 20 | MET |
| 1 | 99-A | 23 | ASN |
| 1 | 99-A | 24 | LEU |
| 1 | 99-A | 59 | ASN |
| 1 | 99-A | 101 | GLU |
| 1 | 99-A | 108 | GLN |
| 1 | 99-A | 109 | LYS |
| 1 | 99-A | 148 | SER |
| 1 | 99-A | 157 | GLU |
| 1 | 100-A | 4 | LEU |
| 1 | 100-A | 18 | ASN |
| 1 | 100-A | 49 | SER |
| 1 | 100-A | 59 | ASN |
| 1 | 100-A | 104 | LEU |
| 1 | 100-A | 109 | LYS |
| 1 | 100-A | 148 | SER |
| 1 | 101-A | 1 | MET |
| 1 | 101-A | 4 | LEU |
| 1 | 101-A | 20 | MET |
| 1 | 101-A | 23 | ASN |
| 1 | 101-A | 33 | ARG |
| 1 | 101-A | 49 | SER |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 101-A | 52 | ARG |
| 1 | 101-A | 59 | ASN |
| 1 | 101-A | 104 | LEU |
| 1 | 101-A | 109 | LYS |
| 1 | 101-A | 119 | VAL |
| 1 | 102-A | 1 | MET |
| 1 | 102-A | 17 | GLU |
| 1 | 102-A | 23 | ASN |
| 1 | 102-A | 24 | LEU |
| 1 | 102-A | 33 | ARG |
| 1 | 102-A | 59 | ASN |
| 1 | 102-A | 68 | THR |
| 1 | 102-A | 79 | ASP |
| 1 | 102-A | 104 | LEU |
| 1 | 102-A | 109 | LYS |
| 1 | 102-A | 118 | GLU |
| 1 | 102-A | 120 | GLU |
| 1 | 102-A | 148 | SER |
| 1 | 102-A | 156 | LEU |
| 1 | 102-A | 157 | GLU |
| 1 | 103-A | 1 | MET |
| 1 | 103-A | 4 | LEU |
| 1 | 103-A | 18 | ASN |
| 1 | 103-A | 23 | ASN |
| 1 | 103-A | 24 | LEU |
| 1 | 103-A | 33 | ARG |
| 1 | 103-A | 36 | LEU |
| 1 | 103-A | 52 | ARG |
| 1 | 103-A | 59 | ASN |
| 1 | 103-A | 106 | LYS |
| 1 | 103-A | 108 | GLN |
| 1 | 103-A | 109 | LYS |
| 1 | 103-A | 118 | GLU |
| 1 | 103-A | 120 | GLU |
| 1 | 103-A | 136 | VAL |
| 1 | 104-A | 1 | MET |
| 1 | 104-A | 4 | LEU |
| 1 | 104-A | 17 | GLU |
| 1 | 104-A | 18 | ASN |
| 1 | 104-A | 23 | ASN |
| 1 | 104-A | 24 | LEU |
| 1 | 104-A | 33 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 104-A | 36 | LEU |
| 1 | 104-A | 52 | ARG |
| 1 | 104-A | 59 | ASN |
| 1 | 104-A | 87 | ASP |
| 1 | 104-A | 106 | LYS |
| 1 | 104-A | 111 | TYR |
| 1 | 104-A | 134 | GLU |
| 1 | 104-A | 148 | SER |
| 1 | 104-A | 156 | LEU |
| 1 | 105-A | 1 | MET |
| 1 | 105-A | 2 | ILE |
| 1 | 105-A | 18 | ASN |
| 1 | 105-A | 21 | PRO |
| 1 | 105-A | 23 | ASN |
| 1 | 105-A | 52 | ARG |
| 1 | 105-A | 59 | ASN |
| 1 | 105-A | 106 | LYS |
| 1 | 105-A | 119 | VAL |
| 1 | 105-A | 139 | GLU |
| 1 | 105-A | 157 | GLU |
| 1 | 106-A | 1 | MET |
| 1 | 106-A | 18 | ASN |
| 1 | 106-A | 36 | LEU |
| 1 | 106-A | 52 | ARG |
| 1 | 106-A | 59 | ASN |
| 1 | 106-A | 87 | ASP |
| 1 | 106-A | 104 | LEU |
| 1 | 106-A | 106 | LYS |
| 1 | 106-A | 120 | GLU |
| 1 | 107-A | 4 | LEU |
| 1 | 107-A | 17 | GLU |
| 1 | 107-A | 18 | ASN |
| 1 | 107-A | 23 | ASN |
| 1 | 107-A | 36 | LEU |
| 1 | 107-A | 52 | ARG |
| 1 | 107-A | 59 | ASN |
| 1 | 107-A | 62 | LEU |
| 1 | 107-A | 87 | ASP |
| 1 | 107-A | 104 | LEU |
| 1 | 107-A | 106 | LYS |
| 1 | 107-A | 128 | TYR |
| 1 | 108-A | 1 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 108-A | 4 | LEU |
| 1 | 108-A | 16 | MET |
| 1 | 108-A | 18 | ASN |
| 1 | 108-A | 36 | LEU |
| 1 | 108-A | 52 | ARG |
| 1 | 108-A | 59 | ASN |
| 1 | 108-A | 104 | LEU |
| 1 | 108-A | 138 | SER |
| 1 | 108-A | 156 | LEU |
| 1 | 109-A | 4 | LEU |
| 1 | 109-A | 16 | MET |
| 1 | 109-A | 17 | GLU |
| 1 | 109-A | 18 | ASN |
| 1 | 109-A | 21 | PRO |
| 1 | 109-A | 36 | LEU |
| 1 | 109-A | 52 | ARG |
| 1 | 109-A | 59 | ASN |
| 1 | 109-A | 87 | ASP |
| 1 | 109-A | 104 | LEU |
| 1 | 109-A | 109 | LYS |
| 1 | 109-A | 118 | GLU |
| 1 | 109-A | 119 | VAL |
| 1 | 109-A | 120 | GLU |
| 1 | 109-A | 156 | LEU |
| 1 | 109-A | 158 | ARG |
| 1 | 110-A | 4 | LEU |
| 1 | 110-A | 33 | ARG |
| 1 | 110-A | 36 | LEU |
| 1 | 110-A | 52 | ARG |
| 1 | 110-A | 59 | ASN |
| 1 | 110-A | 76 | LYS |
| 1 | 110-A | 79 | ASP |
| 1 | 110-A | 104 | LEU |
| 1 | 110-A | 119 | VAL |
| 1 | 110-A | 120 | GLU |
| 1 | 110-A | 148 | SER |
| 1 | 110-A | 156 | LEU |
| 1 | 111-A | 2 | ILE |
| 1 | 111-A | 33 | ARG |
| 1 | 111-A | 36 | LEU |
| 1 | 111-A | 59 | ASN |
| 1 | 111-A | 65 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 111-A | 79 | ASP |
| 1 | 111-A | 104 | LEU |
| 1 | 111-A | 106 | LYS |
| 1 | 111-A | 118 | GLU |
| 1 | 111-A | 119 | VAL |
| 1 | 111-A | 120 | GLU |
| 1 | 111-A | 138 | SER |
| 1 | 112-A | 17 | GLU |
| 1 | 112-A | 23 | ASN |
| 1 | 112-A | 33 | ARG |
| 1 | 112-A | 52 | ARG |
| 1 | 112-A | 59 | ASN |
| 1 | 112-A | 106 | LYS |
| 1 | 112-A | 118 | GLU |
| 1 | 112-A | 120 | GLU |
| 1 | 112-A | 128 | TYR |
| 1 | 112-A | 134 | GLU |
| 1 | 112-A | 139 | GLU |
| 1 | 113-A | 16 | MET |
| 1 | 113-A | 24 | LEU |
| 1 | 113-A | 52 | ARG |
| 1 | 113-A | 59 | ASN |
| 1 | 113-A | 79 | ASP |
| 1 | 113-A | 87 | ASP |
| 1 | 113-A | 104 | LEU |
| 1 | 113-A | 108 | GLN |
| 1 | 113-A | 118 | GLU |
| 1 | 113-A | 128 | TYR |
| 1 | 113-A | 134 | GLU |
| 1 | 113-A | 156 | LEU |
| 1 | 114-A | 1 | MET |
| 1 | 114-A | 49 | SER |
| 1 | 114-A | 59 | ASN |
| 1 | 114-A | 65 | GLN |
| 1 | 114-A | 87 | ASP |
| 1 | 114-A | 108 | GLN |
| 1 | 114-A | 118 | GLU |
| 1 | 114-A | 148 | SER |
| 1 | 115-A | 4 | LEU |
| 1 | 115-A | 20 | MET |
| 1 | 115-A | 52 | ARG |
| 1 | 115-A | 59 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 115-A | 87 | ASP |
| 1 | 115-A | 104 | LEU |
| 1 | 115-A | 106 | LYS |
| 1 | 115-A | 111 | TYR |
| 1 | 115-A | 157 | GLU |
| 1 | 116-A | 18 | ASN |
| 1 | 116-A | 36 | LEU |
| 1 | 116-A | 52 | ARG |
| 1 | 116-A | 59 | ASN |
| 1 | 116-A | 65 | GLN |
| 1 | 116-A | 87 | ASP |
| 1 | 116-A | 106 | LYS |
| 1 | 117-A | 1 | MET |
| 1 | 117-A | 20 | MET |
| 1 | 117-A | 52 | ARG |
| 1 | 117-A | 59 | ASN |
| 1 | 117-A | 65 | GLN |
| 1 | 117-A | 76 | LYS |
| 1 | 117-A | 87 | ASP |
| 1 | 117-A | 138 | SER |
| 1 | 117-A | 156 | LEU |
| 1 | 118-A | 1 | MET |
| 1 | 118-A | 4 | LEU |
| 1 | 118-A | 20 | MET |
| 1 | 118-A | 36 | LEU |
| 1 | 118-A | 52 | ARG |
| 1 | 118-A | 59 | ASN |
| 1 | 118-A | 65 | GLN |
| 1 | 118-A | 118 | GLU |
| 1 | 119-A | 1 | MET |
| 1 | 119-A | 52 | ARG |
| 1 | 119-A | 59 | ASN |
| 1 | 119-A | 65 | GLN |
| 1 | 119-A | 76 | LYS |
| 1 | 119-A | 106 | LYS |
| 1 | 119-A | 142 | ASP |
| 1 | 119-A | 157 | GLU |
| 1 | 120-A | 1 | MET |
| 1 | 120-A | 18 | ASN |
| 1 | 120-A | 22 | TRP |
| 1 | 120-A | 36 | LEU |
| 1 | 120-A | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 120-A | 59 | ASN |
| 1 | 120-A | 62 | LEU |
| 1 | 120-A | 76 | LYS |
| 1 | 120-A | 109 | LYS |
| 1 | 120-A | 118 | GLU |
| 1 | 121-A | 1 | MET |
| 1 | 121-A | 4 | LEU |
| 1 | 121-A | 18 | ASN |
| 1 | 121-A | 22 | TRP |
| 1 | 121-A | 52 | ARG |
| 1 | 121-A | 59 | ASN |
| 1 | 121-A | 76 | LYS |
| 1 | 121-A | 111 | TYR |
| 1 | 121-A | 118 | GLU |
| 1 | 121-A | 120 | GLU |
| 1 | 121-A | 126 | PRO |
| 1 | 122-A | 20 | MET |
| 1 | 122-A | 21 | PRO |
| 1 | 122-A | 22 | TRP |
| 1 | 122-A | 48 | GLU |
| 1 | 122-A | 59 | ASN |
| 1 | 122-A | 76 | LYS |
| 1 | 122-A | 108 | GLN |
| 1 | 122-A | 118 | GLU |
| 1 | 123-A | 1 | MET |
| 1 | 123-A | 4 | LEU |
| 1 | 123-A | 20 | MET |
| 1 | 123-A | 22 | TRP |
| 1 | 123-A | 48 | GLU |
| 1 | 123-A | 59 | ASN |
| 1 | 123-A | 76 | LYS |
| 1 | 123-A | 118 | GLU |
| 1 | 123-A | 128 | TYR |
| 1 | 123-A | 138 | SER |
| 1 | 124-A | 4 | LEU |
| 1 | 124-A | 18 | ASN |
| 1 | 124-A | 20 | MET |
| 1 | 124-A | 45 | HIS |
| 1 | 124-A | 52 | ARG |
| 1 | 124-A | 59 | ASN |
| 1 | 124-A | 79 | ASP |
| 1 | 124-A | 108 | GLN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 124-A | 119 | VAL |
| 1 | 124-A | 159 | ARG |
| 1 | 125-A | 16 | MET |
| 1 | 125-A | 21 | PRO |
| 1 | 125-A | 33 | ARG |
| 1 | 125-A | 52 | ARG |
| 1 | 125-A | 59 | ASN |
| 1 | 125-A | 87 | ASP |
| 1 | 125-A | 108 | GLN |
| 1 | 125-A | 137 | PHE |
| 1 | 125-A | 159 | ARG |
| 1 | 126-A | 59 | ASN |
| 1 | 126-A | 65 | GLN |
| 1 | 126-A | 76 | LYS |
| 1 | 126-A | 87 | ASP |
| 1 | 126-A | 118 | GLU |
| 1 | 126-A | 159 | ARG |
| 1 | 127-A | 1 | MET |
| 1 | 127-A | 4 | LEU |
| 1 | 127-A | 20 | MET |
| 1 | 127-A | 49 | SER |
| 1 | 127-A | 52 | ARG |
| 1 | 127-A | 59 | ASN |
| 1 | 127-A | 108 | GLN |
| 1 | 127-A | 118 | GLU |
| 1 | 127-A | 120 | GLU |
| 1 | 127-A | 138 | SER |
| 1 | 127-A | 157 | GLU |
| 1 | 127-A | 159 | ARG |
| 1 | 128-A | 1 | MET |
| 1 | 128-A | 4 | LEU |
| 1 | 128-A | 16 | MET |
| 1 | 128-A | 21 | PRO |
| 1 | 128-A | 23 | ASN |
| 1 | 128-A | 52 | ARG |
| 1 | 128-A | 59 | ASN |
| 1 | 128-A | 118 | GLU |
| 1 | 128-A | 120 | GLU |
| 1 | 128-A | 148 | SER |
| 1 | 128-A | 157 | GLU |
| 1 | 129-A | 1 | MET |
| 1 | 129-A | 4 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 129-A | 52 | ARG |
| 1 | 129-A | 59 | ASN |
| 1 | 129-A | 70 | ASP |
| 1 | 129-A | 108 | GLN |
| 1 | 129-A | 134 | GLU |
| 1 | 129-A | 142 | ASP |
| 1 | 129-A | 159 | ARG |
| 1 | 130-A | 1 | MET |
| 1 | 130-A | 49 | SER |
| 1 | 130-A | 52 | ARG |
| 1 | 130-A | 59 | ASN |
| 1 | 130-A | 65 | GLN |
| 1 | 130-A | 87 | ASP |
| 1 | 130-A | 138 | SER |
| 1 | 131-A | 4 | LEU |
| 1 | 131-A | 16 | MET |
| 1 | 131-A | 17 | GLU |
| 1 | 131-A | 20 | MET |
| 1 | 131-A | 23 | ASN |
| 1 | 131-A | 52 | ARG |
| 1 | 131-A | 59 | ASN |
| 1 | 131-A | 65 | GLN |
| 1 | 131-A | 87 | ASP |
| 1 | 131-A | 101 | GLU |
| 1 | 131-A | 118 | GLU |
| 1 | 131-A | 142 | ASP |
| 1 | 131-A | 156 | LEU |
| 1 | 131-A | 159 | ARG |
| 1 | 132-A | 4 | LEU |
| 1 | 132-A | 16 | MET |
| 1 | 132-A | 17 | GLU |
| 1 | 132-A | 20 | MET |
| 1 | 132-A | 33 | ARG |
| 1 | 132-A | 59 | ASN |
| 1 | 132-A | 62 | LEU |
| 1 | 132-A | 87 | ASP |
| 1 | 132-A | 106 | LYS |
| 1 | 132-A | 118 | GLU |
| 1 | 132-A | 119 | VAL |
| 1 | 132-A | 128 | TYR |
| 1 | 132-A | 156 | LEU |
| 1 | 132-A | 159 | ARG |

Continued on next page...

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 133-A | 1 | MET |
| 1 | 133-A | 16 | MET |
| 1 | 133-A | 20 | MET |
| 1 | 133-A | 33 | ARG |
| 1 | 133-A | 49 | SER |
| 1 | 133-A | 52 | ARG |
| 1 | 133-A | 55 | PRO |
| 1 | 133-A | 59 | ASN |
| 1 | 133-A | 87 | ASP |
| 1 | 133-A | 142 | ASP |
| 1 | 133-A | 148 | SER |
| 1 | 133-A | 156 | LEU |
| 1 | 133-A | 159 | ARG |
| 1 | 134-A | 1 | MET |
| 1 | 134-A | 16 | MET |
| 1 | 134-A | 20 | MET |
| 1 | 134-A | 23 | ASN |
| 1 | 134-A | 52 | ARG |
| 1 | 134-A | 59 | ASN |
| 1 | 134-A | 136 | VAL |
| 1 | 134-A | 142 | ASP |
| 1 | 135-A | 1 | MET |
| 1 | 135-A | 16 | MET |
| 1 | 135-A | 20 | MET |
| 1 | 135-A | 28 | LEU |
| 1 | 135-A | 52 | ARG |
| 1 | 135-A | 59 | ASN |
| 1 | 135-A | 106 | LYS |
| 1 | 135-A | 115 | ILE |
| 1 | 135-A | 138 | SER |
| 1 | 135-A | 142 | ASP |
| 1 | 135-A | 148 | SER |
| 1 | 135-A | 159 | ARG |
| 1 | 136-A | 1 | MET |
| 1 | 136-A | 16 | MET |
| 1 | 136-A | 20 | MET |
| 1 | 136-A | 22 | TRP |
| 1 | 136-A | 24 | LEU |
| 1 | 136-A | 33 | ARG |
| 1 | 136-A | 52 | ARG |
| 1 | 136-A | 59 | ASN |
| 1 | 136-A | 66 | PRO |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 136-A | 79 | ASP |
| 1 | 136-A | 87 | ASP |
| 1 | 136-A | 115 | ILE |
| 1 | 136-A | 118 | GLU |
| 1 | 136-A | 119 | VAL |
| 1 | 136-A | 148 | SER |
| 1 | 136-A | 159 | ARG |
| 1 | 137-A | 4 | LEU |
| 1 | 137-A | 16 | MET |
| 1 | 137-A | 20 | MET |
| 1 | 137-A | 23 | ASN |
| 1 | 137-A | 49 | SER |
| 1 | 137-A | 52 | ARG |
| 1 | 137-A | 59 | ASN |
| 1 | 137-A | 65 | GLN |
| 1 | 137-A | 106 | LYS |
| 1 | 137-A | 118 | GLU |
| 1 | 137-A | 120 | GLU |
| 1 | 137-A | 127 | ASP |
| 1 | 137-A | 139 | GLU |
| 1 | 137-A | 142 | ASP |
| 1 | 137-A | 159 | ARG |
| 1 | 138-A | 20 | MET |
| 1 | 138-A | 23 | ASN |
| 1 | 138-A | 28 | LEU |
| 1 | 138-A | 59 | ASN |
| 1 | 138-A | 65 | GLN |
| 1 | 139-A | 1 | MET |
| 1 | 139-A | 20 | MET |
| 1 | 139-A | 44 | ARG |
| 1 | 139-A | 59 | ASN |
| 1 | 139-A | 60 | ILE |
| 1 | 139-A | 87 | ASP |
| 1 | 139-A | 104 | LEU |
| 1 | 139-A | 142 | ASP |
| 1 | 140-A | 4 | LEU |
| 1 | 140-A | 20 | MET |
| 1 | 140-A | 23 | ASN |
| 1 | 140-A | 36 | LEU |
| 1 | 140-A | 49 | SER |
| 1 | 140-A | 59 | ASN |
| 1 | 140-A | 60 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 140-A | 87 | ASP |
| 1 | 140-A | 108 | GLN |
| 1 | 140-A | 138 | SER |
| 1 | 140-A | 142 | ASP |
| 1 | 140-A | 156 | LEU |
| 1 | 141-A | 16 | MET |
| 1 | 141-A | 20 | MET |
| 1 | 141-A | 21 | PRO |
| 1 | 141-A | 28 | LEU |
| 1 | 141-A | 33 | ARG |
| 1 | 141-A | 49 | SER |
| 1 | 141-A | 59 | ASN |
| 1 | 141-A | 79 | ASP |
| 1 | 141-A | 87 | ASP |
| 1 | 141-A | 101 | GLU |
| 1 | 141-A | 108 | GLN |
| 1 | 141-A | 118 | GLU |
| 1 | 142-A | 1 | MET |
| 1 | 142-A | 21 | PRO |
| 1 | 142-A | 52 | ARG |
| 1 | 142-A | 59 | ASN |
| 1 | 142-A | 79 | ASP |
| 1 | 142-A | 108 | GLN |
| 1 | 142-A | 118 | GLU |
| 1 | 142-A | 142 | ASP |
| 1 | 143-A | 1 | MET |
| 1 | 143-A | 17 | GLU |
| 1 | 143-A | 20 | MET |
| 1 | 143-A | 21 | PRO |
| 1 | 143-A | 28 | LEU |
| 1 | 143-A | 52 | ARG |
| 1 | 143-A | 59 | ASN |
| 1 | 143-A | 60 | ILE |
| 1 | 143-A | 101 | GLU |
| 1 | 143-A | 109 | LYS |
| 1 | 143-A | 120 | GLU |
| 1 | 143-A | 157 | GLU |
| 1 | 144-A | 1 | MET |
| 1 | 144-A | 23 | ASN |
| 1 | 144-A | 25 | PRO |
| 1 | 144-A | 28 | LEU |
| 1 | 144-A | 33 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 144-A | 52 | ARG |
| 1 | 144-A | 59 | ASN |
| 1 | 144-A | 60 | ILE |
| 1 | 144-A | 120 | GLU |
| 1 | 144-A | 138 | SER |
| 1 | 144-A | 157 | GLU |
| 1 | 145-A | 1 | MET |
| 1 | 145-A | 4 | LEU |
| 1 | 145-A | 20 | MET |
| 1 | 145-A | 52 | ARG |
| 1 | 145-A | 59 | ASN |
| 1 | 145-A | 134 | GLU |
| 1 | 145-A | 139 | GLU |
| 1 | 145-A | 142 | ASP |
| 1 | 145-A | 157 | GLU |
| 1 | 146-A | 1 | MET |
| 1 | 146-A | 2 | ILE |
| 1 | 146-A | 23 | ASN |
| 1 | 146-A | 59 | ASN |
| 1 | 146-A | 87 | ASP |
| 1 | 146-A | 138 | SER |
| 1 | 146-A | 158 | ARG |
| 1 | 147-A | 1 | MET |
| 1 | 147-A | 2 | ILE |
| 1 | 147-A | 4 | LEU |
| 1 | 147-A | 33 | ARG |
| 1 | 147-A | 59 | ASN |
| 1 | 147-A | 106 | LYS |
| 1 | 147-A | 157 | GLU |
| 1 | 148-A | 1 | MET |
| 1 | 148-A | 2 | ILE |
| 1 | 148-A | 4 | LEU |
| 1 | 148-A | 59 | ASN |
| 1 | 148-A | 119 | VAL |
| 1 | 148-A | 120 | GLU |
| 1 | 148-A | 142 | ASP |
| 1 | 148-A | 157 | GLU |
| 1 | 149-A | 1 | MET |
| 1 | 149-A | 2 | ILE |
| 1 | 149-A | 4 | LEU |
| 1 | 149-A | 20 | MET |
| 1 | 149-A | 28 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 149-A | 49 | SER |
| 1 | 149-A | 52 | ARG |
| 1 | 149-A | 59 | ASN |
| 1 | 149-A | 60 | ILE |
| 1 | 149-A | 118 | GLU |
| 1 | 149-A | 120 | GLU |
| 1 | 149-A | 138 | SER |
| 1 | 149-A | 159 | ARG |
| 1 | 150-A | 1 | MET |
| 1 | 150-A | 2 | ILE |
| 1 | 150-A | 52 | ARG |
| 1 | 150-A | 59 | ASN |
| 1 | 150-A | 60 | ILE |
| 1 | 150-A | 101 | GLU |
| 1 | 150-A | 118 | GLU |
| 1 | 150-A | 119 | VAL |
| 1 | 150-A | 138 | SER |
| 1 | 150-A | 142 | ASP |
| 1 | 150-A | 159 | ARG |
| 1 | 151-A | 1 | MET |
| 1 | 151-A | 2 | ILE |
| 1 | 151-A | 33 | ARG |
| 1 | 151-A | 49 | SER |
| 1 | 151-A | 52 | ARG |
| 1 | 151-A | 59 | ASN |
| 1 | 151-A | 101 | GLU |
| 1 | 151-A | 106 | LYS |
| 1 | 151-A | 139 | GLU |
| 1 | 151-A | 159 | ARG |
| 1 | 152-A | 2 | ILE |
| 1 | 152-A | 4 | LEU |
| 1 | 152-A | 18 | ASN |
| 1 | 152-A | 33 | ARG |
| 1 | 152-A | 36 | LEU |
| 1 | 152-A | 52 | ARG |
| 1 | 152-A | 59 | ASN |
| 1 | 152-A | 98 | ARG |
| 1 | 152-A | 148 | SER |
| 1 | 152-A | 152 | CYS |
| 1 | 152-A | 159 | ARG |
| 1 | 153-A | 1 | MET |
| 1 | 153-A | 2 | ILE |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 153-A | 4 | LEU |
| 1 | 153-A | 20 | MET |
| 1 | 153-A | 33 | ARG |
| 1 | 153-A | 36 | LEU |
| 1 | 153-A | 52 | ARG |
| 1 | 153-A | 59 | ASN |
| 1 | 153-A | 65 | GLN |
| 1 | 153-A | 79 | ASP |
| 1 | 153-A | 98 | ARG |
| 1 | 153-A | 106 | LYS |
| 1 | 153-A | 118 | GLU |
| 1 | 153-A | 120 | GLU |
| 1 | 153-A | 128 | TYR |
| 1 | 154-A | 1 | MET |
| 1 | 154-A | 4 | LEU |
| 1 | 154-A | 21 | PRO |
| 1 | 154-A | 36 | LEU |
| 1 | 154-A | 52 | ARG |
| 1 | 154-A | 59 | ASN |
| 1 | 154-A | 79 | ASP |
| 1 | 154-A | 87 | ASP |
| 1 | 154-A | 98 | ARG |
| 1 | 154-A | 106 | LYS |
| 1 | 154-A | 118 | GLU |
| 1 | 154-A | 128 | TYR |
| 1 | 154-A | 142 | ASP |
| 1 | 154-A | 156 | LEU |
| 1 | 155-A | 1 | MET |
| 1 | 155-A | 2 | ILE |
| 1 | 155-A | 10 | VAL |
| 1 | 155-A | 20 | MET |
| 1 | 155-A | 23 | ASN |
| 1 | 155-A | 33 | ARG |
| 1 | 155-A | 59 | ASN |
| 1 | 155-A | 98 | ARG |
| 1 | 155-A | 118 | GLU |
| 1 | 156-A | 1 | MET |
| 1 | 156-A | 16 | MET |
| 1 | 156-A | 33 | ARG |
| 1 | 156-A | 59 | ASN |
| 1 | 156-A | 87 | ASP |
| 1 | 156-A | 98 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 156-A | 118 | GLU |
| 1 | 156-A | 148 | SER |
| 1 | 157-A | 1 | MET |
| 1 | 157-A | 4 | LEU |
| 1 | 157-A | 52 | ARG |
| 1 | 157-A | 59 | ASN |
| 1 | 157-A | 76 | LYS |
| 1 | 157-A | 87 | ASP |
| 1 | 157-A | 98 | ARG |
| 1 | 157-A | 108 | GLN |
| 1 | 157-A | 118 | GLU |
| 1 | 157-A | 119 | VAL |
| 1 | 157-A | 142 | ASP |
| 1 | 158-A | 1 | MET |
| 1 | 158-A | 59 | ASN |
| 1 | 158-A | 65 | GLN |
| 1 | 158-A | 76 | LYS |
| 1 | 158-A | 98 | ARG |
| 1 | 158-A | 108 | GLN |
| 1 | 158-A | 142 | ASP |
| 1 | 159-A | 1 | MET |
| 1 | 159-A | 33 | ARG |
| 1 | 159-A | 59 | ASN |
| 1 | 159-A | 87 | ASP |
| 1 | 159-A | 98 | ARG |
| 1 | 159-A | 108 | GLN |
| 1 | 159-A | 134 | GLU |
| 1 | 159-A | 142 | ASP |
| 1 | 160-A | 1 | MET |
| 1 | 160-A | 4 | LEU |
| 1 | 160-A | 23 | ASN |
| 1 | 160-A | 49 | SER |
| 1 | 160-A | 52 | ARG |
| 1 | 160-A | 59 | ASN |
| 1 | 160-A | 98 | ARG |
| 1 | 160-A | 105 | PRO |
| 1 | 160-A | 108 | GLN |
| 1 | 160-A | 111 | TYR |
| 1 | 160-A | 142 | ASP |
| 1 | 160-A | 156 | LEU |
| 1 | 161-A | 1 | MET |
| 1 | 161-A | 16 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 161-A | 52 | ARG |
| 1 | 161-A | 59 | ASN |
| 1 | 161-A | 65 | GLN |
| 1 | 161-A | 76 | LYS |
| 1 | 161-A | 98 | ARG |
| 1 | 161-A | 118 | GLU |
| 1 | 162-A | 20 | MET |
| 1 | 162-A | 23 | ASN |
| 1 | 162-A | 49 | SER |
| 1 | 162-A | 59 | ASN |
| 1 | 162-A | 76 | LYS |
| 1 | 162-A | 101 | GLU |
| 1 | 162-A | 106 | LYS |
| 1 | 162-A | 142 | ASP |
| 1 | 163-A | 4 | LEU |
| 1 | 163-A | 23 | ASN |
| 1 | 163-A | 52 | ARG |
| 1 | 163-A | 59 | ASN |
| 1 | 163-A | 76 | LYS |
| 1 | 163-A | 105 | PRO |
| 1 | 163-A | 135 | SER |
| 1 | 163-A | 139 | GLU |
| 1 | 163-A | 142 | ASP |
| 1 | 163-A | 148 | SER |
| 1 | 164-A | 18 | ASN |
| 1 | 164-A | 23 | ASN |
| 1 | 164-A | 49 | SER |
| 1 | 164-A | 59 | ASN |
| 1 | 164-A | 65 | GLN |
| 1 | 164-A | 76 | LYS |
| 1 | 164-A | 104 | LEU |
| 1 | 164-A | 118 | GLU |
| 1 | 164-A | 142 | ASP |
| 1 | 165-A | 1 | MET |
| 1 | 165-A | 4 | LEU |
| 1 | 165-A | 23 | ASN |
| 1 | 165-A | 49 | SER |
| 1 | 165-A | 52 | ARG |
| 1 | 165-A | 59 | ASN |
| 1 | 165-A | 87 | ASP |
| 1 | 165-A | 104 | LEU |
| 1 | 165-A | 119 | VAL |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 165-A | 139 | GLU |
| 1 | 165-A | 142 | ASP |
| 1 | 166-A | 1 | MET |
| 1 | 166-A | 4 | LEU |
| 1 | 166-A | 23 | ASN |
| 1 | 166-A | 52 | ARG |
| 1 | 166-A | 59 | ASN |
| 1 | 166-A | 76 | LYS |
| 1 | 166-A | 106 | LYS |
| 1 | 166-A | 118 | GLU |
| 1 | 166-A | 119 | VAL |
| 1 | 167-A | 17 | GLU |
| 1 | 167-A | 52 | ARG |
| 1 | 167-A | 59 | ASN |
| 1 | 167-A | 89 | PRO |
| 1 | 167-A | 118 | GLU |
| 1 | 167-A | 134 | GLU |
| 1 | 167-A | 142 | ASP |
| 1 | 168-A | 4 | LEU |
| 1 | 168-A | 17 | GLU |
| 1 | 168-A | 20 | MET |
| 1 | 168-A | 23 | ASN |
| 1 | 168-A | 52 | ARG |
| 1 | 168-A | 59 | ASN |
| 1 | 168-A | 66 | PRO |
| 1 | 168-A | 101 | GLU |
| 1 | 168-A | 106 | LYS |
| 1 | 168-A | 108 | GLN |
| 1 | 168-A | 142 | ASP |
| 1 | 168-A | 156 | LEU |
| 1 | 169-A | 1 | MET |
| 1 | 169-A | 33 | ARG |
| 1 | 169-A | 59 | ASN |
| 1 | 169-A | 87 | ASP |
| 1 | 169-A | 138 | SER |
| 1 | 170-A | 1 | MET |
| 1 | 170-A | 20 | MET |
| 1 | 170-A | 23 | ASN |
| 1 | 170-A | 59 | ASN |
| 1 | 170-A | 106 | LYS |
| 1 | 170-A | 118 | GLU |
| 1 | 170-A | 139 | GLU |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 171-A | 1 | MET |
| 1 | 171-A | 4 | LEU |
| 1 | 171-A | 33 | ARG |
| 1 | 171-A | 52 | ARG |
| 1 | 171-A | 59 | ASN |
| 1 | 171-A | 106 | LYS |
| 1 | 171-A | 118 | GLU |
| 1 | 171-A | 152 | CYS |
| 1 | 172-A | 1 | MET |
| 1 | 172-A | 20 | MET |
| 1 | 172-A | 23 | ASN |
| 1 | 172-A | 33 | ARG |
| 1 | 172-A | 52 | ARG |
| 1 | 172-A | 59 | ASN |
| 1 | 172-A | 65 | GLN |
| 1 | 172-A | 79 | ASP |
| 1 | 172-A | 106 | LYS |
| 1 | 172-A | 118 | GLU |
| 1 | 172-A | 120 | GLU |
| 1 | 172-A | 148 | SER |
| 1 | 172-A | 152 | CYS |
| 1 | 173-A | 1 | MET |
| 1 | 173-A | 4 | LEU |
| 1 | 173-A | 23 | ASN |
| 1 | 173-A | 33 | ARG |
| 1 | 173-A | 52 | ARG |
| 1 | 173-A | 59 | ASN |
| 1 | 173-A | 108 | GLN |
| 1 | 173-A | 118 | GLU |
| 1 | 173-A | 138 | SER |
| 1 | 173-A | 142 | ASP |
| 1 | 173-A | 152 | CYS |
| 1 | 174-A | 1 | MET |
| 1 | 174-A | 4 | LEU |
| 1 | 174-A | 59 | ASN |
| 1 | 174-A | 108 | GLN |
| 1 | 174-A | 120 | GLU |
| 1 | 175-A | 18 | ASN |
| 1 | 175-A | 52 | ARG |
| 1 | 175-A | 59 | ASN |
| 1 | 175-A | 148 | SER |
| 1 | 175-A | 154 | GLU |

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Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 176-A | 1 | MET |
| 1 | 176-A | 18 | ASN |
| 1 | 176-A | 52 | ARG |
| 1 | 176-A | 59 | ASN |
| 1 | 176-A | 156 | LEU |
| 1 | 177-A | 1 | MET |
| 1 | 177-A | 4 | LEU |
| 1 | 177-A | 49 | SER |
| 1 | 177-A | 52 | ARG |
| 1 | 177-A | 59 | ASN |
| 1 | 177-A | 65 | GLN |
| 1 | 178-A | 1 | MET |
| 1 | 178-A | 20 | MET |
| 1 | 178-A | 36 | LEU |
| 1 | 178-A | 52 | ARG |
| 1 | 178-A | 59 | ASN |
| 1 | 178-A | 65 | GLN |
| 1 | 178-A | 118 | GLU |
| 1 | 178-A | 142 | ASP |
| 1 | 178-A | 148 | SER |
| 1 | 179-A | 1 | MET |
| 1 | 179-A | 18 | ASN |
| 1 | 179-A | 52 | ARG |
| 1 | 179-A | 59 | ASN |
| 1 | 179-A | 65 | GLN |
| 1 | 179-A | 120 | GLU |
| 1 | 179-A | 128 | TYR |
| 1 | 179-A | 142 | ASP |
| 1 | 180-A | 1 | MET |
| 1 | 180-A | 4 | LEU |
| 1 | 180-A | 33 | ARG |
| 1 | 180-A | 52 | ARG |
| 1 | 180-A | 59 | ASN |
| 1 | 180-A | 65 | GLN |
| 1 | 180-A | 79 | ASP |
| 1 | 180-A | 104 | LEU |
| 1 | 180-A | 106 | LYS |
| 1 | 180-A | 111 | TYR |
| 1 | 180-A | 152 | CYS |
| 1 | 181-A | 1 | MET |
| 1 | 181-A | 4 | LEU |
| 1 | 181-A | 20 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 181-A | 21 | PRO |
| 1 | 181-A | 49 | SER |
| 1 | 181-A | 52 | ARG |
| 1 | 181-A | 59 | ASN |
| 1 | 181-A | 106 | LYS |
| 1 | 181-A | 139 | GLU |
| 1 | 181-A | 148 | SER |
| 1 | 181-A | 152 | CYS |
| 1 | 182-A | 23 | ASN |
| 1 | 182-A | 52 | ARG |
| 1 | 182-A | 59 | ASN |
| 1 | 182-A | 106 | LYS |
| 1 | 182-A | 148 | SER |
| 1 | 182-A | 152 | CYS |
| 1 | 183-A | 1 | MET |
| 1 | 183-A | 4 | LEU |
| 1 | 183-A | 16 | MET |
| 1 | 183-A | 33 | ARG |
| 1 | 183-A | 52 | ARG |
| 1 | 183-A | 59 | ASN |
| 1 | 183-A | 108 | GLN |
| 1 | 183-A | 118 | GLU |
| 1 | 183-A | 148 | SER |
| 1 | 183-A | 152 | CYS |
| 1 | 183-A | 156 | LEU |
| 1 | 184-A | 1 | MET |
| 1 | 184-A | 16 | MET |
| 1 | 184-A | 49 | SER |
| 1 | 184-A | 52 | ARG |
| 1 | 184-A | 59 | ASN |
| 1 | 184-A | 65 | GLN |
| 1 | 184-A | 79 | ASP |
| 1 | 184-A | 118 | GLU |
| 1 | 184-A | 119 | VAL |
| 1 | 184-A | 138 | SER |
| 1 | 184-A | 139 | GLU |
| 1 | 184-A | 152 | CYS |
| 1 | 185-A | 1 | MET |
| 1 | 185-A | 16 | MET |
| 1 | 185-A | 33 | ARG |
| 1 | 185-A | 59 | ASN |
| 1 | 185-A | 79 | ASP |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 185-A | 119 | VAL |
| 1 | 185-A | 132 | ASP |
| 1 | 185-A | 148 | SER |
| 1 | 186-A | 1 | MET |
| 1 | 186-A | 33 | ARG |
| 1 | 186-A | 52 | ARG |
| 1 | 186-A | 59 | ASN |
| 1 | 186-A | 79 | ASP |
| 1 | 186-A | 118 | GLU |
| 1 | 186-A | 138 | SER |
| 1 | 186-A | 152 | CYS |
| 1 | 186-A | 157 | GLU |
| 1 | 187-A | 1 | MET |
| 1 | 187-A | 4 | LEU |
| 1 | 187-A | 33 | ARG |
| 1 | 187-A | 52 | ARG |
| 1 | 187-A | 59 | ASN |
| 1 | 187-A | 108 | GLN |
| 1 | 187-A | 118 | GLU |
| 1 | 187-A | 120 | GLU |
| 1 | 187-A | 134 | GLU |
| 1 | 187-A | 152 | CYS |
| 1 | 187-A | 156 | LEU |
| 1 | 187-A | 157 | GLU |
| 1 | 187-A | 159 | ARG |
| 1 | 188-A | 1 | MET |
| 1 | 188-A | 49 | SER |
| 1 | 188-A | 52 | ARG |
| 1 | 188-A | 59 | ASN |
| 1 | 188-A | 108 | GLN |
| 1 | 188-A | 118 | GLU |
| 1 | 188-A | 120 | GLU |
| 1 | 188-A | 148 | SER |
| 1 | 188-A | 152 | CYS |
| 1 | 188-A | 156 | LEU |
| 1 | 188-A | 157 | GLU |
| 1 | 189-A | 1 | MET |
| 1 | 189-A | 4 | LEU |
| 1 | 189-A | 52 | ARG |
| 1 | 189-A | 59 | ASN |
| 1 | 189-A | 79 | ASP |
| 1 | 189-A | 108 | GLN |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 189-A | 118 | GLU |
| 1 | 189-A | 120 | GLU |
| 1 | 189-A | 152 | CYS |
| 1 | 190-A | 1 | MET |
| 1 | 190-A | 59 | ASN |
| 1 | 190-A | 60 | ILE |
| 1 | 190-A | 62 | LEU |
| 1 | 190-A | 65 | GLN |
| 1 | 190-A | 79 | ASP |
| 1 | 190-A | 106 | LYS |
| 1 | 190-A | 108 | GLN |
| 1 | 190-A | 118 | GLU |
| 1 | 190-A | 134 | GLU |
| 1 | 190-A | 152 | CYS |
| 1 | 190-A | 157 | GLU |
| 1 | 191-A | 4 | LEU |
| 1 | 191-A | 10 | VAL |
| 1 | 191-A | 18 | ASN |
| 1 | 191-A | 49 | SER |
| 1 | 191-A | 59 | ASN |
| 1 | 191-A | 106 | LYS |
| 1 | 191-A | 118 | GLU |
| 1 | 191-A | 152 | CYS |
| 1 | 191-A | 157 | GLU |
| 1 | 192-A | 4 | LEU |
| 1 | 192-A | 59 | ASN |
| 1 | 192-A | 66 | PRO |
| 1 | 192-A | 106 | LYS |
| 1 | 192-A | 119 | VAL |
| 1 | 192-A | 134 | GLU |
| 1 | 193-A | 1 | MET |
| 1 | 193-A | 2 | ILE |
| 1 | 193-A | 4 | LEU |
| 1 | 193-A | 16 | MET |
| 1 | 193-A | 17 | GLU |
| 1 | 193-A | 49 | SER |
| 1 | 193-A | 59 | ASN |
| 1 | 193-A | 87 | ASP |
| 1 | 193-A | 108 | GLN |
| 1 | 193-A | 119 | VAL |
| 1 | 193-A | 139 | GLU |
| 1 | 193-A | 152 | CYS |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 193-A | 157 | GLU |
| 1 | 194-A | 1 | MET |
| 1 | 194-A | 18 | ASN |
| 1 | 194-A | 20 | MET |
| 1 | 194-A | 52 | ARG |
| 1 | 194-A | 59 | ASN |
| 1 | 194-A | 87 | ASP |
| 1 | 194-A | 101 | GLU |
| 1 | 194-A | 108 | GLN |
| 1 | 194-A | 118 | GLU |
| 1 | 194-A | 152 | CYS |
| 1 | 194-A | 157 | GLU |
| 1 | 195-A | 1 | MET |
| 1 | 195-A | 16 | MET |
| 1 | 195-A | 20 | MET |
| 1 | 195-A | 52 | ARG |
| 1 | 195-A | 59 | ASN |
| 1 | 195-A | 87 | ASP |
| 1 | 195-A | 119 | VAL |
| 1 | 195-A | 136 | VAL |
| 1 | 195-A | 157 | GLU |
| 1 | 196-A | 4 | LEU |
| 1 | 196-A | 18 | ASN |
| 1 | 196-A | 33 | ARG |
| 1 | 196-A | 49 | SER |
| 1 | 196-A | 52 | ARG |
| 1 | 196-A | 59 | ASN |
| 1 | 196-A | 65 | GLN |
| 1 | 196-A | 68 | THR |
| 1 | 196-A | 108 | GLN |
| 1 | 196-A | 128 | TYR |
| 1 | 196-A | 152 | CYS |
| 1 | 197-A | 10 | VAL |
| 1 | 197-A | 18 | ASN |
| 1 | 197-A | 23 | ASN |
| 1 | 197-A | 33 | ARG |
| 1 | 197-A | 59 | ASN |
| 1 | 197-A | 65 | GLN |
| 1 | 197-A | 118 | GLU |
| 1 | 197-A | 138 | SER |
| 1 | 197-A | 139 | GLU |
| 1 | 197-A | 148 | SER |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 197-A | 152 | CYS |
| 1 | 198-A | 1 | MET |
| 1 | 198-A | 4 | LEU |
| 1 | 198-A | 10 | VAL |
| 1 | 198-A | 18 | ASN |
| 1 | 198-A | 59 | ASN |
| 1 | 198-A | 104 | LEU |
| 1 | 198-A | 108 | GLN |
| 1 | 198-A | 138 | SER |
| 1 | 198-A | 152 | CYS |
| 1 | 199-A | 1 | MET |
| 1 | 199-A | 4 | LEU |
| 1 | 199-A | 18 | ASN |
| 1 | 199-A | 20 | MET |
| 1 | 199-A | 21 | PRO |
| 1 | 199-A | 59 | ASN |
| 1 | 199-A | 76 | LYS |
| 1 | 199-A | 104 | LEU |
| 1 | 199-A | 108 | GLN |
| 1 | 199-A | 118 | GLU |
| 1 | 199-A | 119 | VAL |
| 1 | 199-A | 152 | CYS |
| 1 | 199-A | 159 | ARG |
| 1 | 200-A | 1 | MET |
| 1 | 200-A | 18 | ASN |
| 1 | 200-A | 59 | ASN |
| 1 | 200-A | 108 | GLN |
| 1 | 200-A | 118 | GLU |
| 1 | 200-A | 119 | VAL |
| 1 | 200-A | 139 | GLU |
| 1 | 200-A | 152 | CYS |
| 1 | 200-A | 157 | GLU |
| 1 | 201-A | 1 | MET |
| 1 | 201-A | 18 | ASN |
| 1 | 201-A | 52 | ARG |
| 1 | 201-A | 59 | ASN |
| 1 | 201-A | 68 | THR |
| 1 | 201-A | 79 | ASP |
| 1 | 201-A | 87 | ASP |
| 1 | 201-A | 108 | GLN |
| 1 | 201-A | 119 | VAL |
| 1 | 201-A | 120 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 201-A | 152 | CYS |
| 1 | 202-A | 1 | MET |
| 1 | 202-A | 23 | ASN |
| 1 | 202-A | 52 | ARG |
| 1 | 202-A | 59 | ASN |
| 1 | 202-A | 68 | THR |
| 1 | 202-A | 108 | GLN |
| 1 | 202-A | 119 | VAL |
| 1 | 202-A | 156 | LEU |
| 1 | 203-A | 1 | MET |
| 1 | 203-A | 4 | LEU |
| 1 | 203-A | 52 | ARG |
| 1 | 203-A | 59 | ASN |
| 1 | 203-A | 68 | THR |
| 1 | 203-A | 108 | GLN |
| 1 | 203-A | 118 | GLU |
| 1 | 203-A | 139 | GLU |
| 1 | 203-A | 156 | LEU |
| 1 | 204-A | 16 | MET |
| 1 | 204-A | 18 | ASN |
| 1 | 204-A | 20 | MET |
| 1 | 204-A | 23 | ASN |
| 1 | 204-A | 52 | ARG |
| 1 | 204-A | 59 | ASN |
| 1 | 204-A | 108 | GLN |
| 1 | 204-A | 118 | GLU |
| 1 | 204-A | 152 | CYS |
| 1 | 205-A | 4 | LEU |
| 1 | 205-A | 16 | MET |
| 1 | 205-A | 18 | ASN |
| 1 | 205-A | 23 | ASN |
| 1 | 205-A | 52 | ARG |
| 1 | 205-A | 59 | ASN |
| 1 | 205-A | 62 | LEU |
| 1 | 205-A | 118 | GLU |
| 1 | 205-A | 119 | VAL |
| 1 | 205-A | 120 | GLU |
| 1 | 205-A | 138 | SER |
| 1 | 205-A | 156 | LEU |
| 1 | 206-A | 1 | MET |
| 1 | 206-A | 4 | LEU |
| 1 | 206-A | 16 | MET |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 206-A | 18 | ASN |
| 1 | 206-A | 20 | MET |
| 1 | 206-A | 33 | ARG |
| 1 | 206-A | 52 | ARG |
| 1 | 206-A | 59 | ASN |
| 1 | 206-A | 102 | GLN |
| 1 | 206-A | 108 | GLN |
| 1 | 206-A | 118 | GLU |
| 1 | 206-A | 137 | PHE |
| 1 | 207-A | 16 | MET |
| 1 | 207-A | 18 | ASN |
| 1 | 207-A | 20 | MET |
| 1 | 207-A | 52 | ARG |
| 1 | 207-A | 59 | ASN |
| 1 | 207-A | 79 | ASP |
| 1 | 207-A | 87 | ASP |
| 1 | 207-A | 102 | GLN |
| 1 | 207-A | 118 | GLU |
| 1 | 207-A | 157 | GLU |
| 1 | 208-A | 1 | MET |
| 1 | 208-A | 4 | LEU |
| 1 | 208-A | 16 | MET |
| 1 | 208-A | 20 | MET |
| 1 | 208-A | 33 | ARG |
| 1 | 208-A | 52 | ARG |
| 1 | 208-A | 59 | ASN |
| 1 | 208-A | 65 | GLN |
| 1 | 208-A | 101 | GLU |
| 1 | 208-A | 102 | GLN |
| 1 | 208-A | 142 | ASP |
| 1 | 208-A | 159 | ARG |
| 1 | 209-A | 4 | LEU |
| 1 | 209-A | 18 | ASN |
| 1 | 209-A | 20 | MET |
| 1 | 209-A | 49 | SER |
| 1 | 209-A | 52 | ARG |
| 1 | 209-A | 59 | ASN |
| 1 | 209-A | 102 | GLN |
| 1 | 209-A | 106 | LYS |
| 1 | 209-A | 108 | GLN |
| 1 | 209-A | 118 | GLU |
| 1 | 209-A | 142 | ASP |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 209-A | 152 | CYS |
| 1 | 210-A | 20 | MET |
| 1 | 210-A | 59 | ASN |
| 1 | 210-A | 65 | GLN |
| 1 | 210-A | 87 | ASP |
| 1 | 210-A | 118 | GLU |
| 1 | 210-A | 142 | ASP |
| 1 | 210-A | 152 | CYS |
| 1 | 211-A | 18 | ASN |
| 1 | 211-A | 20 | MET |
| 1 | 211-A | 23 | ASN |
| 1 | 211-A | 33 | ARG |
| 1 | 211-A | 52 | ARG |
| 1 | 211-A | 59 | ASN |
| 1 | 211-A | 65 | GLN |
| 1 | 211-A | 148 | SER |
| 1 | 212-A | 1 | MET |
| 1 | 212-A | 18 | ASN |
| 1 | 212-A | 20 | MET |
| 1 | 212-A | 23 | ASN |
| 1 | 212-A | 33 | ARG |
| 1 | 212-A | 52 | ARG |
| 1 | 212-A | 59 | ASN |
| 1 | 212-A | 87 | ASP |
| 1 | 212-A | 88 | VAL |
| 1 | 212-A | 101 | GLU |
| 1 | 212-A | 156 | LEU |
| 1 | 213-A | 1 | MET |
| 1 | 213-A | 10 | VAL |
| 1 | 213-A | 18 | ASN |
| 1 | 213-A | 33 | ARG |
| 1 | 213-A | 36 | LEU |
| 1 | 213-A | 52 | ARG |
| 1 | 213-A | 55 | PRO |
| 1 | 213-A | 59 | ASN |
| 1 | 213-A | 101 | GLU |
| 1 | 213-A | 106 | LYS |
| 1 | 213-A | 142 | ASP |
| 1 | 213-A | 156 | LEU |
| 1 | 214-A | 20 | MET |
| 1 | 214-A | 33 | ARG |
| 1 | 214-A | 52 | ARG |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 214-A | 59 | ASN |
| 1 | 214-A | 79 | ASP |
| 1 | 214-A | 87 | ASP |
| 1 | 214-A | 88 | VAL |
| 1 | 214-A | 139 | GLU |
| 1 | 214-A | 142 | ASP |
| 1 | 215-A | 1 | MET |
| 1 | 215-A | 4 | LEU |
| 1 | 215-A | 20 | MET |
| 1 | 215-A | 33 | ARG |
| 1 | 215-A | 59 | ASN |
| 1 | 215-A | 87 | ASP |
| 1 | 215-A | 101 | GLU |
| 1 | 215-A | 108 | GLN |
| 1 | 215-A | 118 | GLU |
| 1 | 215-A | 128 | TYR |
| 1 | 215-A | 134 | GLU |
| 1 | 215-A | 142 | ASP |
| 1 | 215-A | 156 | LEU |
| 1 | 216-A | 1 | MET |
| 1 | 216-A | 16 | MET |
| 1 | 216-A | 20 | MET |
| 1 | 216-A | 23 | ASN |
| 1 | 216-A | 24 | LEU |
| 1 | 216-A | 33 | ARG |
| 1 | 216-A | 59 | ASN |
| 1 | 216-A | 108 | GLN |
| 1 | 216-A | 118 | GLU |
| 1 | 216-A | 142 | ASP |
| 1 | 216-A | 152 | CYS |
| 1 | 216-A | 154 | GLU |
| 1 | 217-A | 18 | ASN |
| 1 | 217-A | 20 | MET |
| 1 | 217-A | 21 | PRO |
| 1 | 217-A | 33 | ARG |
| 1 | 217-A | 49 | SER |
| 1 | 217-A | 59 | ASN |
| 1 | 217-A | 108 | GLN |
| 1 | 217-A | 118 | GLU |
| 1 | 217-A | 139 | GLU |
| 1 | 217-A | 156 | LEU |
| 1 | 218-A | 4 | LEU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 218-A | 18 | ASN |
| 1 | 218-A | 20 | MET |
| 1 | 218-A | 21 | PRO |
| 1 | 218-A | 23 | ASN |
| 1 | 218-A | 28 | LEU |
| 1 | 218-A | 52 | ARG |
| 1 | 218-A | 59 | ASN |
| 1 | 218-A | 65 | GLN |
| 1 | 218-A | 108 | GLN |
| 1 | 218-A | 118 | GLU |
| 1 | 218-A | 135 | SER |
| 1 | 218-A | 148 | SER |
| 1 | 218-A | 152 | CYS |
| 1 | 218-A | 154 | GLU |
| 1 | 218-A | 156 | LEU |
| 1 | 219-A | 4 | LEU |
| 1 | 219-A | 18 | ASN |
| 1 | 219-A | 23 | ASN |
| 1 | 219-A | 33 | ARG |
| 1 | 219-A | 52 | ARG |
| 1 | 219-A | 59 | ASN |
| 1 | 219-A | 79 | ASP |
| 1 | 219-A | 118 | GLU |
| 1 | 219-A | 119 | VAL |
| 1 | 219-A | 120 | GLU |
| 1 | 219-A | 148 | SER |
| 1 | 219-A | 154 | GLU |
| 1 | 219-A | 156 | LEU |
| 1 | 220-A | 1 | MET |
| 1 | 220-A | 4 | LEU |
| 1 | 220-A | 33 | ARG |
| 1 | 220-A | 52 | ARG |
| 1 | 220-A | 59 | ASN |
| 1 | 220-A | 79 | ASP |
| 1 | 220-A | 108 | GLN |
| 1 | 220-A | 119 | VAL |
| 1 | 220-A | 120 | GLU |
| 1 | 220-A | 128 | TYR |
| 1 | 220-A | 148 | SER |
| 1 | 220-A | 154 | GLU |
| 1 | 220-A | 157 | GLU |
| 1 | 221-A | 18 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 221-A | 20 | MET |
| 1 | 221-A | 21 | PRO |
| 1 | 221-A | 33 | ARG |
| 1 | 221-A | 52 | ARG |
| 1 | 221-A | 59 | ASN |
| 1 | 221-A | 66 | PRO |
| 1 | 221-A | 76 | LYS |
| 1 | 221-A | 108 | GLN |
| 1 | 221-A | 111 | TYR |
| 1 | 221-A | 118 | GLU |
| 1 | 221-A | 128 | TYR |
| 1 | 221-A | 148 | SER |
| 1 | 221-A | 156 | LEU |
| 1 | 221-A | 157 | GLU |
| 1 | 222-A | 1 | MET |
| 1 | 222-A | 16 | MET |
| 1 | 222-A | 23 | ASN |
| 1 | 222-A | 59 | ASN |
| 1 | 222-A | 76 | LYS |
| 1 | 222-A | 108 | GLN |
| 1 | 222-A | 118 | GLU |
| 1 | 222-A | 139 | GLU |
| 1 | 222-A | 152 | CYS |
| 1 | 222-A | 157 | GLU |
| 1 | 223-A | 1 | MET |
| 1 | 223-A | 16 | MET |
| 1 | 223-A | 20 | MET |
| 1 | 223-A | 59 | ASN |
| 1 | 223-A | 106 | LYS |
| 1 | 223-A | 119 | VAL |
| 1 | 223-A | 139 | GLU |
| 1 | 223-A | 148 | SER |
| 1 | 223-A | 152 | CYS |
| 1 | 224-A | 1 | MET |
| 1 | 224-A | 20 | MET |
| 1 | 224-A | 33 | ARG |
| 1 | 224-A | 59 | ASN |
| 1 | 224-A | 65 | GLN |
| 1 | 224-A | 76 | LYS |
| 1 | 224-A | 88 | VAL |
| 1 | 224-A | 98 | ARG |
| 1 | 224-A | 118 | GLU |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 224-A | 126 | PRO |
| 1 | 224-A | 152 | CYS |
| 1 | 225-A | 4 | LEU |
| 1 | 225-A | 33 | ARG |
| 1 | 225-A | 59 | ASN |
| 1 | 225-A | 65 | GLN |
| 1 | 225-A | 76 | LYS |
| 1 | 225-A | 98 | ARG |
| 1 | 225-A | 118 | GLU |
| 1 | 225-A | 128 | TYR |
| 1 | 225-A | 152 | CYS |
| 1 | 225-A | 154 | GLU |
| 1 | 225-A | 159 | ARG |
| 1 | 226-A | 1 | MET |
| 1 | 226-A | 10 | VAL |
| 1 | 226-A | 33 | ARG |
| 1 | 226-A | 59 | ASN |
| 1 | 226-A | 76 | LYS |
| 1 | 226-A | 98 | ARG |
| 1 | 226-A | 120 | GLU |
| 1 | 226-A | 128 | TYR |
| 1 | 226-A | 148 | SER |
| 1 | 227-A | 1 | MET |
| 1 | 227-A | 4 | LEU |
| 1 | 227-A | 20 | MET |
| 1 | 227-A | 33 | ARG |
| 1 | 227-A | 49 | SER |
| 1 | 227-A | 59 | ASN |
| 1 | 227-A | 98 | ARG |
| 1 | 227-A | 108 | GLN |
| 1 | 227-A | 120 | GLU |
| 1 | 227-A | 127 | ASP |
| 1 | 228-A | 4 | LEU |
| 1 | 228-A | 20 | MET |
| 1 | 228-A | 23 | ASN |
| 1 | 228-A | 52 | ARG |
| 1 | 228-A | 59 | ASN |
| 1 | 228-A | 101 | GLU |
| 1 | 228-A | 152 | CYS |
| 1 | 229-A | 4 | LEU |
| 1 | 229-A | 17 | GLU |
| 1 | 229-A | 23 | ASN |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 229-A | 49 | SER |
| 1 | 229-A | 52 | ARG |
| 1 | 229-A | 59 | ASN |
| 1 | 229-A | 139 | GLU |
| 1 | 229-A | 148 | SER |
| 1 | 229-A | 152 | CYS |
| 1 | 230-A | 1 | MET |
| 1 | 230-A | 20 | MET |
| 1 | 230-A | 23 | ASN |
| 1 | 230-A | 52 | ARG |
| 1 | 230-A | 59 | ASN |
| 1 | 230-A | 65 | GLN |
| 1 | 230-A | 76 | LYS |
| 1 | 230-A | 119 | VAL |
| 1 | 230-A | 152 | CYS |
| 1 | 230-A | 157 | GLU |
| 1 | 231-A | 20 | MET |
| 1 | 231-A | 28 | LEU |
| 1 | 231-A | 33 | ARG |
| 1 | 231-A | 59 | ASN |
| 1 | 231-A | 65 | GLN |
| 1 | 231-A | 76 | LYS |
| 1 | 231-A | 79 | ASP |
| 1 | 231-A | 120 | GLU |
| 1 | 231-A | 138 | SER |
| 1 | 231-A | 152 | CYS |
| 1 | 231-A | 157 | GLU |
| 1 | 232-A | 4 | LEU |
| 1 | 232-A | 23 | ASN |
| 1 | 232-A | 33 | ARG |
| 1 | 232-A | 52 | ARG |
| 1 | 232-A | 59 | ASN |
| 1 | 232-A | 65 | GLN |
| 1 | 232-A | 79 | ASP |
| 1 | 232-A | 87 | ASP |
| 1 | 232-A | 118 | GLU |
| 1 | 232-A | 120 | GLU |
| 1 | 232-A | 128 | TYR |
| 1 | 232-A | 139 | GLU |
| 1 | 232-A | 152 | CYS |
| 1 | 233-A | 23 | ASN |
| 1 | 233-A | 49 | SER |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 233-A | 52 | ARG |
| 1 | 233-A | 59 | ASN |
| 1 | 233-A | 108 | GLN |
| 1 | 233-A | 128 | TYR |
| 1 | 233-A | 132 | ASP |
| 1 | 233-A | 157 | GLU |
| 1 | 234-A | 4 | LEU |
| 1 | 234-A | 23 | ASN |
| 1 | 234-A | 28 | LEU |
| 1 | 234-A | 44 | ARG |
| 1 | 234-A | 52 | ARG |
| 1 | 234-A | 59 | ASN |
| 1 | 234-A | 120 | GLU |
| 1 | 234-A | 139 | GLU |
| 1 | 235-A | 4 | LEU |
| 1 | 235-A | 33 | ARG |
| 1 | 235-A | 52 | ARG |
| 1 | 235-A | 59 | ASN |
| 1 | 235-A | 118 | GLU |
| 1 | 236-A | 1 | MET |
| 1 | 236-A | 18 | ASN |
| 1 | 236-A | 20 | MET |
| 1 | 236-A | 52 | ARG |
| 1 | 236-A | 59 | ASN |
| 1 | 236-A | 101 | GLU |
| 1 | 236-A | 109 | LYS |
| 1 | 236-A | 157 | GLU |
| 1 | 236-A | 159 | ARG |
| 1 | 237-A | 16 | MET |
| 1 | 237-A | 18 | ASN |
| 1 | 237-A | 52 | ARG |
| 1 | 237-A | 59 | ASN |
| 1 | 237-A | 65 | GLN |
| 1 | 237-A | 108 | GLN |
| 1 | 237-A | 118 | GLU |
| 1 | 237-A | 120 | GLU |
| 1 | 238-A | 33 | ARG |
| 1 | 238-A | 52 | ARG |
| 1 | 238-A | 59 | ASN |
| 1 | 238-A | 118 | GLU |
| 1 | 238-A | 120 | GLU |
| 1 | 238-A | 157 | GLU |

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| Mol | Chain | Res | Type |
|------------|--------------|------------|-------------|
| 1 | 239-A | 52 | ARG |
| 1 | 239-A | 59 | ASN |
| 1 | 239-A | 106 | LYS |
| 1 | 239-A | 108 | GLN |
| 1 | 239-A | 136 | VAL |
| 1 | 239-A | 157 | GLU |
| 1 | 240-A | 1 | MET |
| 1 | 240-A | 4 | LEU |
| 1 | 240-A | 16 | MET |
| 1 | 240-A | 23 | ASN |
| 1 | 240-A | 52 | ARG |
| 1 | 240-A | 59 | ASN |
| 1 | 240-A | 106 | LYS |
| 1 | 240-A | 108 | GLN |
| 1 | 240-A | 119 | VAL |
| 1 | 240-A | 138 | SER |
| 1 | 241-A | 1 | MET |
| 1 | 241-A | 4 | LEU |
| 1 | 241-A | 20 | MET |
| 1 | 241-A | 59 | ASN |
| 1 | 241-A | 106 | LYS |
| 1 | 241-A | 108 | GLN |
| 1 | 241-A | 118 | GLU |
| 1 | 242-A | 16 | MET |
| 1 | 242-A | 17 | GLU |
| 1 | 242-A | 33 | ARG |
| 1 | 242-A | 49 | SER |
| 1 | 242-A | 52 | ARG |
| 1 | 242-A | 59 | ASN |
| 1 | 242-A | 79 | ASP |
| 1 | 242-A | 87 | ASP |
| 1 | 242-A | 98 | ARG |
| 1 | 242-A | 108 | GLN |
| 1 | 242-A | 119 | VAL |
| 1 | 242-A | 159 | ARG |
| 1 | 243-A | 4 | LEU |
| 1 | 243-A | 16 | MET |
| 1 | 243-A | 17 | GLU |
| 1 | 243-A | 23 | ASN |
| 1 | 243-A | 52 | ARG |
| 1 | 243-A | 59 | ASN |
| 1 | 243-A | 98 | ARG |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 243-A | 106 | LYS |
| 1 | 243-A | 108 | GLN |
| 1 | 243-A | 119 | VAL |
| 1 | 243-A | 138 | SER |
| 1 | 243-A | 159 | ARG |
| 1 | 244-A | 4 | LEU |
| 1 | 244-A | 17 | GLU |
| 1 | 244-A | 59 | ASN |
| 1 | 244-A | 106 | LYS |
| 1 | 244-A | 108 | GLN |
| 1 | 244-A | 159 | ARG |
| 1 | 245-A | 1 | MET |
| 1 | 245-A | 4 | LEU |
| 1 | 245-A | 20 | MET |
| 1 | 245-A | 23 | ASN |
| 1 | 245-A | 59 | ASN |
| 1 | 245-A | 109 | LYS |
| 1 | 245-A | 119 | VAL |
| 1 | 245-A | 120 | GLU |
| 1 | 245-A | 159 | ARG |
| 1 | 246-A | 1 | MET |
| 1 | 246-A | 4 | LEU |
| 1 | 246-A | 20 | MET |
| 1 | 246-A | 23 | ASN |
| 1 | 246-A | 59 | ASN |
| 1 | 246-A | 65 | GLN |
| 1 | 246-A | 106 | LYS |
| 1 | 246-A | 156 | LEU |
| 1 | 246-A | 158 | ARG |
| 1 | 246-A | 159 | ARG |
| 1 | 247-A | 1 | MET |
| 1 | 247-A | 23 | ASN |
| 1 | 247-A | 59 | ASN |
| 1 | 247-A | 65 | GLN |
| 1 | 247-A | 101 | GLU |
| 1 | 247-A | 135 | SER |
| 1 | 247-A | 156 | LEU |
| 1 | 248-A | 1 | MET |
| 1 | 248-A | 4 | LEU |
| 1 | 248-A | 23 | ASN |
| 1 | 248-A | 59 | ASN |
| 1 | 248-A | 60 | ILE |

Continued on next page...

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1 | 248-A | 148 | SER |
| 1 | 248-A | 156 | LEU |
| 1 | 249-A | 21 | PRO |
| 1 | 249-A | 23 | ASN |
| 1 | 249-A | 33 | ARG |
| 1 | 249-A | 59 | ASN |
| 1 | 249-A | 60 | ILE |
| 1 | 249-A | 101 | GLU |
| 1 | 249-A | 118 | GLU |
| 1 | 249-A | 119 | VAL |
| 1 | 249-A | 120 | GLU |
| 1 | 249-A | 134 | GLU |
| 1 | 249-A | 148 | SER |
| 1 | 249-A | 154 | GLU |
| 1 | 250-A | 1 | MET |
| 1 | 250-A | 18 | ASN |
| 1 | 250-A | 23 | ASN |
| 1 | 250-A | 33 | ARG |
| 1 | 250-A | 59 | ASN |
| 1 | 250-A | 65 | GLN |
| 1 | 250-A | 118 | GLU |
| 1 | 250-A | 127 | ASP |
| 1 | 250-A | 128 | TYR |
| 1 | 250-A | 154 | GLU |
| 1 | 250-A | 159 | ARG |

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

500 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
| | | | | | Counts | RMSZ | # $ Z > 2$ | Counts | RMSZ | # $ Z > 2$ |
| 2 | FOL | 125-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 34-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 76-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 202-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 85-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 174-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 56-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 54-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 187-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 68-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 10-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 149-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 161-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 107-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 81-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 129-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 6-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 21-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 238-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 98-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 208-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 165-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 31-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 119-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 105-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 39-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | NAP | 33-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 180-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 54-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 14-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 12-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 145-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 13-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 99-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 83-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 89-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 117-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 201-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 23-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 5-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 48-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 203-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 81-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 30-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 156-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 162-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 107-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 42-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 239-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 190-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 106-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 205-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 158-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 112-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 215-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 220-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 92-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 55-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 123-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 113-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 118-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | NAP | 82-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 38-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 176-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 144-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 49-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 44-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 70-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 166-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 186-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 138-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 104-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 149-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 164-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 156-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 188-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 121-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 48-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 133-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 6-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 7-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 225-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 30-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 97-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 3-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 80-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 223-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 17-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 96-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 78-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 246-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 101-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 176-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 72-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 235-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 154-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | NAP | 10-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 175-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 127-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 27-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 137-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 137-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 115-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 103-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 147-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 75-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 243-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 56-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 79-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 175-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 21-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 87-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 234-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 169-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 241-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 245-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 9-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 249-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 208-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 19-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 233-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 182-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 43-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 207-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 20-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 248-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 247-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 185-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 136-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 152-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 60-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | NAP | 51-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 53-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 226-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 195-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 204-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 110-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 211-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 126-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 244-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 134-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 236-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 198-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 244-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 183-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 153-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 135-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 68-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 240-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 202-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 140-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 17-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 119-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 240-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 66-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 84-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 100-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 27-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 170-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 1-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 228-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 14-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 234-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 130-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 161-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 122-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | NAP | 102-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 215-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 210-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 22-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 249-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 216-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 139-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 96-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 210-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 224-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 171-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 184-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 125-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 159-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 44-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 69-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 213-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 169-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 62-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 113-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 49-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 225-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 55-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 61-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 242-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 211-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 181-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 116-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 71-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 90-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 65-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 111-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 52-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 160-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 166-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 191-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 152-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 220-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 50-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 8-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 164-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 217-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 117-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 51-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 245-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 185-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 95-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 232-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 4-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 114-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 29-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 32-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 58-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 63-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 196-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 138-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 16-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 57-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 200-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 201-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 250-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 98-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 36-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 13-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 16-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 219-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 200-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 167-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 37-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 124-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | NAP | 120-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 63-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 80-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 34-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 106-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 140-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 218-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 26-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 243-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 157-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 94-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 108-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 91-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 209-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 57-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 111-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 60-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 90-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 143-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 246-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 155-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 122-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 151-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 86-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 50-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 45-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 232-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 128-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 74-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 11-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 177-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 207-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 241-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 189-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 158-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | NAP | 198-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 116-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 2-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 155-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 88-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 179-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 5-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 170-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 18-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 97-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 229-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 222-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 47-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 76-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 35-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 123-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 41-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 108-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 71-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 8-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 121-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 104-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 167-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 47-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 67-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 141-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 15-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 25-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 87-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 32-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 206-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 73-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 194-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 77-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 205-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | NAP | 236-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 151-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 93-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 85-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 233-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 4-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 24-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 237-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 226-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 75-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 28-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 128-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 238-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 26-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 129-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 223-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 41-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 230-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 162-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 178-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 46-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 38-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 163-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 227-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 179-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 192-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 219-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 172-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 172-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 58-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 168-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 183-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 114-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 204-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 120-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 23-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 72-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 135-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 189-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 127-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 143-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 1-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 237-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 62-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 46-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 82-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 15-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 103-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 31-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 136-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 184-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 100-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 146-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 145-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 173-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 197-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 105-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 36-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 148-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 59-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 188-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 24-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 118-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 231-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 224-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 83-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 195-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 39-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 131-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 209-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 242-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 132-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 197-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 186-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 182-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 70-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 79-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 177-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 222-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 227-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 148-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 157-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 190-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 109-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 9-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 40-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 181-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 2-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 77-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 86-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 150-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 216-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 146-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 228-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 187-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 144-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 43-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 193-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 221-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 147-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 59-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 248-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 94-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 174-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 64-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 64-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 115-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 65-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 124-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 142-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 247-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 180-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 78-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 163-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 214-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 178-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 206-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 102-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 231-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 235-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 141-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 132-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 168-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 99-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 173-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 130-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 142-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 217-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 212-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 171-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 35-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 22-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 29-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 18-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 89-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 165-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 139-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 133-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 95-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 159-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | FOL | 239-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 74-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 199-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 93-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 229-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 221-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 67-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 154-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 101-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 112-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 84-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 91-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 109-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 66-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 20-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 150-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 7-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 69-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 88-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 193-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 73-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 28-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 40-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 203-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 230-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 250-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 199-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 52-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 45-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 160-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 53-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 33-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 191-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 131-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 126-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | NAP | 11-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 110-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 37-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 153-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 212-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 25-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 194-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 213-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 12-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 134-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 19-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 192-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 3-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 92-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 214-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 3 | NAP | 218-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |
| 2 | FOL | 196-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 2 | FOL | 61-A | 201 | - | 28,34,34 | 1.00 | 2 (7%) | 36,47,47 | 2.27 | 11 (30%) |
| 3 | NAP | 42-A | 202 | - | 45,52,52 | 1.95 | 6 (13%) | 56,80,80 | 2.99 | 13 (23%) |

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 | 125-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 34-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 76-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 202-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 85-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 174-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 56-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 54-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 187-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 68-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|------------|---------|
| 2 | FOL | 10-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 149-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 161-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 107-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 81-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 129-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 164-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 21-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 238-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 98-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 208-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 165-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 31-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 119-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 105-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 39-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 33-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 180-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 54-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 14-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 12-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 145-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 13-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 99-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 83-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 89-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 117-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 201-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 23-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 5-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 48-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 203-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 81-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 30-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|------------|---------|
| 2 | FOL | 156-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 162-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 107-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 42-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 239-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 190-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 106-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 205-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 158-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 112-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 215-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 220-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 92-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 55-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 123-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 113-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 118-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 82-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 38-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 176-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 144-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 49-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 44-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 70-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 166-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 186-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 138-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 104-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 149-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 6-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 156-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 188-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 121-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 48-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|------------|---------|
| 2 | FOL | 133-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 6-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 7-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 225-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 30-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 97-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 3-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 80-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 223-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 17-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 96-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 78-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 246-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 101-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 176-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 72-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 235-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 154-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 10-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 175-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 127-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 27-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 137-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 137-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 115-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 103-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 147-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 75-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 243-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 56-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 79-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 175-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 21-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 87-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 3 | NAP | 234-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 169-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 241-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 245-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 9-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 249-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 208-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 19-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 233-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 182-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 43-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 207-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 20-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 248-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 247-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 185-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 136-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 152-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 60-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 51-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 53-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 226-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 195-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 204-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 110-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 211-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 126-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 244-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 134-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 236-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 198-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 244-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 183-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 153-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 2 | FOL | 135-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 68-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 240-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 202-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 140-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 17-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 119-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 240-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 66-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 84-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 100-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 27-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 170-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 1-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 228-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 14-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 234-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 130-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 161-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 122-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 102-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 215-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 210-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 22-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 249-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 216-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 139-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 96-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 210-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 224-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 171-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 184-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 125-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 159-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|------------|---------|
| 3 | NAP | 44-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 69-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 213-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 169-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 62-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 113-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 49-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 225-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 55-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 61-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 242-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 211-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 181-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 116-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 71-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 90-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 65-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 111-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 52-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 160-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 166-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 191-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 152-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 220-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 50-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 8-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 164-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 217-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 117-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 51-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 245-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 185-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 95-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 232-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|------------|---------|
| 3 | NAP | 4-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 114-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 29-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 32-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 58-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 63-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 196-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 138-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 16-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 57-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 200-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 201-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 250-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 98-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 36-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 13-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 16-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 219-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 200-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 167-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 37-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 124-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 120-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 63-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 80-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 34-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 106-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 140-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 218-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 26-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 243-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 157-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 94-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 108-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|------------|---------|
| 3 | NAP | 91-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 209-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 57-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 111-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 60-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 90-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 143-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 246-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 155-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 122-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 151-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 86-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 50-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 45-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 232-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 128-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 74-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 11-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 177-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 207-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 241-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 189-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 158-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 198-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 116-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 2-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 155-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 88-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 179-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 5-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 170-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 18-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 97-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 229-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|------------|---------|
| 2 | FOL | 222-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 47-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 76-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 35-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 123-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 41-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 108-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 71-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 8-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 121-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 104-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 167-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 47-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 67-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 141-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 15-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 25-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 87-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 62-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 206-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 73-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 194-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 77-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 205-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 236-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 151-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 93-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 85-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 233-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 4-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 24-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 237-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 226-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 75-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|------------|---------|
| 2 | FOL | 28-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 128-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 238-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 26-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 129-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 223-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 41-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 230-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 162-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 178-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 46-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 38-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 163-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 227-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 179-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 192-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 219-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 172-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 172-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 58-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 168-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 183-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 114-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 204-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 120-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 23-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 72-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 135-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 189-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 127-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 143-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 1-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 237-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 32-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|------------|---------|
| 3 | NAP | 46-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 82-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 15-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 103-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 31-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 136-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 184-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 100-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 146-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 145-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 173-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 197-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 105-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 36-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 148-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 59-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 188-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 24-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 118-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 231-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 224-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 83-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 195-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 39-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 131-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 209-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 242-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 132-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 197-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 186-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 182-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 70-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 79-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 177-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|------------|---------|
| 3 | NAP | 222-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 227-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 148-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 157-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 190-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 109-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 9-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 40-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 181-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 2-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 77-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 86-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 150-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 216-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 146-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 228-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 187-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 144-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 43-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 193-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 221-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 147-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 59-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 248-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 94-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 174-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 64-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 64-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 115-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 65-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 124-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 142-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 247-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 180-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|------------|---------|
| 3 | NAP | 78-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 163-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 214-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 178-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 206-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 102-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 231-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 235-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 141-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 132-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 168-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 99-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 173-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 130-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 142-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 217-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 212-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 171-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 35-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 22-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 29-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 18-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 89-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 165-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 139-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 133-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 95-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 159-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 239-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 74-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 199-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 93-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 229-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 221-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|-----------|------------|---------|
| 2 | FOL | 67-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 154-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 101-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 112-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 84-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 91-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 109-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 66-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 20-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 150-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 7-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 69-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 88-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 193-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 73-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 28-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 40-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 203-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 230-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 250-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 199-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 52-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 45-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 160-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 53-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 33-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 191-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 131-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 126-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 11-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 110-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 37-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 153-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 212-A | 202 | - | 1/1/12/12 | 4/31/67/67 | 0/5/5/5 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 3 | NAP | 25-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 194-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 213-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 12-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 134-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 19-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 192-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 3-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 92-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 214-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 3 | NAP | 218-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |
| 2 | FOL | 196-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 2 | FOL | 61-A | 201 | - | - | 4/16/22/22 | 0/3/3/3 |
| 3 | NAP | 42-A | 202 | - | - | 4/31/67/67 | 0/5/5/5 |

All (2000) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 34-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 76-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 202-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 174-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 54-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 161-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 129-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 238-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 208-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 119-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 39-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 33-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 12-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 89-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 23-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 5-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 81-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 162-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 107-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 239-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 190-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 215-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 92-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 55-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 82-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 38-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 144-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 186-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 138-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 104-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 149-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 164-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 156-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 48-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 6-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 225-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 30-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 3-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 223-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 96-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 176-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 72-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 154-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 10-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 175-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 127-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 27-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 137-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 243-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 56-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 21-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 87-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 234-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 169-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 241-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 249-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 233-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 182-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 43-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 207-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 20-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 247-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 136-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 51-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 195-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 204-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 211-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 126-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 244-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 68-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 240-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 17-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 66-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 170-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 228-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 14-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 122-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 102-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 22-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 210-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 224-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 171-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 184-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 125-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 44-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 158-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 213-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 113-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 49-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 61-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 242-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 90-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 65-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 111-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 52-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 166-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 152-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 220-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 217-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 245-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 185-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 95-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 4-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 114-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 29-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 32-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 58-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 196-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 201-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 98-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 13-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 16-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 219-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 200-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 120-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 63-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 80-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 106-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 140-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 26-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 157-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 94-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 108-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 91-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 57-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 60-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 143-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 246-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 155-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 86-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 50-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 232-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 177-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 189-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 145-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 198-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 116-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 179-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 117-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 97-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 123-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 71-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 121-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 8-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 167-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 47-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 67-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 15-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 206-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 73-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 194-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 205-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 236-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 151-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 85-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 226-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 75-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 128-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 41-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 230-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 163-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 192-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 172-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 168-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 183-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 135-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 1-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 237-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 62-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 46-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 103-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 31-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 100-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 146-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 173-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 105-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 36-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 59-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 188-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 24-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 118-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 83-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 209-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 132-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 197-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 70-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 79-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 222-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 227-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 148-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 109-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 9-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 40-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 181-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 2-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 77-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 214-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 216-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 187-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 221-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 147-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 248-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 64-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 115-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 124-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 180-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 78-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 178-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 231-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 235-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 141-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 99-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 130-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 142-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 35-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 18-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 165-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 139-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 133-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 159-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 74-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 199-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 93-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 229-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 101-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 112-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 84-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 150-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 7-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 69-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 88-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 3 | 193-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 28-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 203-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 250-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 45-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 160-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 53-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 191-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 11-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 110-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 37-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 153-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 212-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 25-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 134-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 19-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 131-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 218-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 42-A | 202 | NAP | O3B-C3B | -9.03 | 1.21 | 1.43 |
| 3 | 34-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 76-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 202-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 174-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 54-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 161-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 129-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 238-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 208-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 119-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 39-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 33-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 12-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 89-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 23-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 5-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 81-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 162-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 107-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 239-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 190-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 215-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 92-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 55-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 82-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 38-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 144-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 186-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 138-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 104-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 149-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 164-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 156-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 48-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 6-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 225-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 30-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 3-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 223-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 96-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 176-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 72-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 154-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 10-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 175-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 127-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 27-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 137-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 243-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 56-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 21-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 87-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 234-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 169-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 241-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 249-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 233-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 182-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 43-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 207-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 20-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 247-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 136-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 51-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 195-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 204-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 211-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 126-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 244-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 68-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 240-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 17-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 66-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 170-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 228-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 14-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 122-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 102-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 22-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 210-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 224-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 171-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 184-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 125-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 44-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 158-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 213-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 113-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 49-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 61-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 242-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 90-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 65-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 111-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 52-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 166-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 152-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 220-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 217-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 245-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 185-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 95-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 4-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 114-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 29-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 32-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 58-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 196-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 201-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 98-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 13-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 16-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 219-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 200-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 120-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 63-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 80-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 106-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 140-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 26-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 157-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 94-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 108-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 91-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 57-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 60-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 143-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 246-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 155-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 86-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 50-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 232-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 177-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 189-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 145-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 198-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 116-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 179-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 117-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 97-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 123-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 71-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 121-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 8-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 167-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 47-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 67-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 15-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 206-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 73-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 194-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 205-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 236-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 151-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 85-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 226-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 75-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 128-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 41-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 230-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 163-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 192-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 172-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 168-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 183-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 135-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 1-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 237-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 62-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 46-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 103-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 31-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 100-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 146-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 173-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 105-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 36-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 59-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 188-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 24-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 118-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 83-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 209-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 132-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 197-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 70-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 79-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 222-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 227-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 148-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 109-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 9-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 40-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 181-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 2-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 77-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 214-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 216-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 187-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 221-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 147-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 248-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 64-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 115-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 124-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 180-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 78-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 178-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 231-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 235-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 141-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 99-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 130-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 142-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 35-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 18-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 165-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 139-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 133-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 159-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 74-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 199-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 93-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 229-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 101-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 112-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 84-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 150-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 7-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 69-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 88-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 193-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 28-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 203-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 250-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 45-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 160-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 53-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 191-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 11-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 110-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 37-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 153-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 212-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 25-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 134-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 19-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 131-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 218-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 42-A | 202 | NAP | C2N-N1N | 4.30 | 1.40 | 1.35 |
| 3 | 34-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 76-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 202-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 174-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 54-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 161-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 129-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 238-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 208-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 119-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 39-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 33-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 12-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 89-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 23-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 5-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 81-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 162-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 107-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 239-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 190-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 215-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 92-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 55-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 82-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 38-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 144-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 186-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 138-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 104-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 149-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 164-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 156-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 48-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 6-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 225-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 30-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 3-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 223-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 96-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 176-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 72-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 154-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 10-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 175-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 127-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 27-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 137-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 243-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 56-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 21-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 87-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 234-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 169-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 241-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 249-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 233-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 182-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 43-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 207-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 20-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 247-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 136-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 51-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 195-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 204-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 211-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 126-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 244-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 68-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 240-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 17-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 66-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 170-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 228-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 14-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 122-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 102-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 22-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 210-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 224-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 171-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 184-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 125-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 44-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 158-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 213-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 113-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 49-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 61-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 242-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 90-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 65-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 111-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 52-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 166-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 152-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 220-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 217-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 245-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 185-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 95-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 4-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 114-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 29-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 32-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 58-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 196-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 201-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 98-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 13-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 16-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 219-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 200-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 120-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 63-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 80-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 106-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 140-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 26-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 157-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 94-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 108-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 91-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 57-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 60-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 143-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 246-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 155-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 86-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 50-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 232-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 177-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 189-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 145-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 198-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 116-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 179-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 117-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 97-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 123-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 71-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 121-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 8-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 167-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 47-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 67-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 15-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 206-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 73-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 194-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 205-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 236-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 151-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 85-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 226-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 75-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 128-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 41-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 230-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 163-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 192-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 172-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 168-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 183-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 135-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 1-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 237-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 62-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 46-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 103-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 31-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 100-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 146-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 173-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 105-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 36-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 59-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 188-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 24-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 118-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 83-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 209-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 132-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 197-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 70-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 79-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 222-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 227-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 148-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 109-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 9-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 40-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 181-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 2-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 77-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 214-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 216-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 187-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 221-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 147-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 248-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 64-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 115-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 124-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 180-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 78-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 178-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 231-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 235-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 141-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 99-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 130-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 142-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 35-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 18-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 165-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 139-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 133-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 159-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 74-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 199-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 93-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 229-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 101-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 112-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 84-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 150-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 7-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 69-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 88-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 193-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 28-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 203-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 250-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 45-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 160-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 53-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 191-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 11-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 110-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 37-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 153-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 212-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 25-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 134-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 19-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 131-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 218-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 42-A | 202 | NAP | O4B-C1B | 3.62 | 1.46 | 1.41 |
| 3 | 34-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 76-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 202-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 174-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 54-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 161-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 129-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 238-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 208-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 119-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 39-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 33-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 12-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 89-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 23-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 5-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 81-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 162-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 107-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 239-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 190-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 215-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 92-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 55-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 82-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 38-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 144-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 186-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 138-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 104-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 149-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 164-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 156-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 48-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 6-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 225-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 30-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 3-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 223-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 96-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 176-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 72-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 154-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 10-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 175-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 127-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 27-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 137-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 243-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 56-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 21-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 87-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 234-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 169-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 241-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 249-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 233-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 182-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 43-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 207-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 20-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 247-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 136-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 51-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 195-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 204-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 211-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 126-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 244-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 68-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 240-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 17-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 66-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 170-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 228-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 14-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 122-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 102-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 22-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 210-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 224-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 171-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 184-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 125-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 44-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 158-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 213-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 113-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 49-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 61-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 242-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 90-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 65-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 111-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 52-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 166-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 152-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 220-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 217-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 245-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 185-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 95-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 4-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 114-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 29-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 32-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 58-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 196-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 201-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 98-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 13-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 16-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 219-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 200-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 120-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 63-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 80-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 106-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 140-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 26-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 157-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 94-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 108-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 91-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 57-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 60-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 143-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 246-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 155-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 86-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 50-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 232-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 177-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 189-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 145-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 198-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 116-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 179-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 117-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 97-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 123-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 71-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 121-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 8-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 167-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 47-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 67-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 15-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 206-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 73-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 194-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 205-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 236-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 151-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 85-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 226-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 75-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 128-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 41-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 230-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 163-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 192-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 172-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 168-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 183-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 135-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 1-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 237-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 62-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 46-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 103-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 31-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 100-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 146-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 173-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 105-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 36-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 59-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 188-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 24-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 118-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 83-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 209-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 132-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 197-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 70-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 79-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 222-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 227-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 148-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 109-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 9-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 40-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 181-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 2-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 77-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 214-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 216-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 187-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 221-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 147-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 248-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 64-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 115-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 124-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 180-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 78-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 178-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 231-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 235-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 141-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 99-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 130-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 142-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 35-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 18-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 165-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 139-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 133-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 159-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 74-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 199-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 93-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 229-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 101-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 112-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 84-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 150-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 7-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 69-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 88-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 193-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 28-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 203-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 250-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 45-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 160-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 53-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 191-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 11-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 110-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 37-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 153-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 212-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 25-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 134-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 19-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 131-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 218-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 42-A | 202 | NAP | C7N-N7N | 3.27 | 1.39 | 1.33 |
| 3 | 34-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 76-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 202-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 174-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 54-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 161-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 129-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 238-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 208-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 119-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 39-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 33-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 12-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 89-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 23-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 5-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 81-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 162-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 107-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 239-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 190-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 215-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 92-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 55-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 82-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 38-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 144-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 186-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 138-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 104-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 149-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 164-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 156-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 48-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 6-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 225-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 30-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 3-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 223-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 96-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 176-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 72-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 154-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 10-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 175-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 127-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 27-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 137-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 243-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 56-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 21-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 87-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 234-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 169-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 241-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 249-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 233-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 182-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 43-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 207-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 20-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 247-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 136-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 51-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 195-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 204-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 211-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 126-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 244-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 68-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 240-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 17-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 66-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 170-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 228-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 14-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 122-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 102-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 22-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 210-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 224-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 171-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 184-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 125-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 44-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 158-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 213-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 113-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 49-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 61-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 242-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 90-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 65-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 111-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 52-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 166-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 152-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 220-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 217-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 245-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 185-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 95-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 4-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 114-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 29-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 32-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 58-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 196-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 201-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 98-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 13-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 16-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 219-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 200-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 120-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 63-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 80-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 106-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 140-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 26-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 157-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 94-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 108-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 91-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 57-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 60-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 143-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 246-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 155-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 86-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 50-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 232-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 177-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 189-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 145-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 198-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 116-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 179-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 117-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 97-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 123-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 71-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 121-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 8-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 167-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 47-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 67-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 15-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 206-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 73-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 194-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 205-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 236-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 151-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 85-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 226-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 75-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 128-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 41-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 230-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 163-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 192-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 172-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 168-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 183-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 135-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 1-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 237-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 62-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 46-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 103-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 31-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 100-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 146-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 173-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 105-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 36-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 59-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 188-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 24-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 118-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 83-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 209-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 132-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 197-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 70-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 79-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 222-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 227-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 148-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 109-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 9-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 40-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 181-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 2-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 77-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 214-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 216-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 187-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 221-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 147-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 248-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 64-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 115-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 124-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 180-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 78-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 178-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 231-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 235-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 141-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 99-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 130-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 142-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 35-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 18-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 165-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 139-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 133-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 159-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 74-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 199-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 93-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 229-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 101-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 112-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 84-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 150-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 7-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 69-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 88-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 193-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 28-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 203-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 250-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 45-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 160-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 53-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 191-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 11-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 110-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 37-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 153-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 212-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 25-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 134-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 19-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 131-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 218-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 42-A | 202 | NAP | C6N-N1N | 2.87 | 1.42 | 1.35 |
| 3 | 34-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 76-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 202-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 174-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 54-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 161-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 129-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 238-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 208-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 119-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 39-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 33-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 12-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 89-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 23-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 5-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 81-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 162-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 107-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 239-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 190-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 215-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 92-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 55-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 82-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 38-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 144-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 186-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 138-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 104-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 149-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 164-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 156-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 48-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 6-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 225-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 30-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 3-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 223-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 96-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 176-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 72-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 154-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 10-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 175-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 127-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 27-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 137-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 243-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 56-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 21-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 87-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 234-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 169-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 241-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 249-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 233-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 182-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 43-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 207-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 20-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 247-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 136-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 51-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 195-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 204-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 211-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 126-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 244-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 68-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 240-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 17-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 66-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 170-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 228-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 14-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 122-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 102-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 22-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 210-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 224-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 171-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 184-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 125-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 44-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 158-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 213-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 113-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 49-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 61-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 242-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 90-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 65-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 111-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 52-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 166-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 152-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 220-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 217-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 245-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 185-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 95-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 4-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 114-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 29-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 32-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 58-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 196-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 201-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 98-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 13-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 16-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 219-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 200-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 120-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 63-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 80-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 106-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 140-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 26-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 157-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 94-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 108-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 91-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 57-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 60-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 143-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 246-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 155-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 86-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 50-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 232-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 177-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 189-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 145-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 198-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 116-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 179-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 117-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 97-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 123-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 71-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 121-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 8-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 167-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 47-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 67-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 15-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 206-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 73-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 194-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 205-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 236-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 151-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 85-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 226-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 75-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 128-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 41-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 230-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 163-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 192-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 172-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 168-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 183-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 135-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 1-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 237-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 62-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 46-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 103-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 31-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 100-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 146-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 173-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 105-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 36-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 59-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 188-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 24-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 118-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 83-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 209-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 132-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 197-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 70-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 79-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 222-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 227-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 148-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 109-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 9-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 40-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 181-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 2-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 77-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 214-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 216-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 187-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 221-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 147-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 248-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 64-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 115-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 124-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 180-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 78-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 178-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 231-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 235-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 141-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 99-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 130-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 142-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 35-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 18-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 165-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 139-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 133-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 159-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 74-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 199-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 93-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 229-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 101-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 112-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 84-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 150-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 7-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 69-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 88-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 193-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 28-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 203-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 250-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 45-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 160-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 53-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 191-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 11-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 110-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 3 | 37-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 153-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 212-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 25-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 134-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 19-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 131-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 218-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 3 | 42-A | 202 | NAP | P2B-O2B | 2.73 | 1.64 | 1.59 |
| 2 | 125-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 85-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 56-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 187-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 68-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 10-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 149-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 107-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 81-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 6-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 21-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 98-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 165-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 | 105-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 180-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 54-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 14-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 145-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 13-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 99-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 83-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 117-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 201-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 48-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 203-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 30-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 156-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 42-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 106-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 205-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 158-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 112-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 220-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 123-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 113-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 118-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 176-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 49-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 44-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 70-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 166-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 188-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 121-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 133-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 7-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 97-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 80-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 17-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 78-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 246-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 101-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 235-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 137-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 115-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 103-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 147-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 75-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 79-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 175-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 245-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 9-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 208-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 19-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 248-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 185-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 152-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 60-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 53-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 226-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 110-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 244-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 134-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 236-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 198-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 183-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 153-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 135-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 202-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 140-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 119-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 240-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 84-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 100-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 27-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 1-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 234-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 130-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 161-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 215-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 210-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 249-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 216-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 139-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 96-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 159-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 69-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 169-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 62-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 225-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 55-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 211-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 181-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 116-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 71-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 160-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 191-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 50-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 8-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 164-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 18-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 51-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 232-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 63-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 138-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 16-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 57-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 200-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 250-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 36-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 167-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 37-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 124-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 34-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 218-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 243-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 209-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 111-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 90-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 122-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 151-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 45-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 128-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 74-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 11-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 207-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 241-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 2-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 155-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 88-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 5-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 170-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 229-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 222-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 47-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 76-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 35-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 41-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 108-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 104-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 141-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 25-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 87-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 32-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 77-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 93-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 233-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 4-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 24-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 237-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 28-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 238-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 26-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 129-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 223-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 162-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 178-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 46-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 38-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 227-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 179-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 219-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 172-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 58-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 114-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 204-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 120-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 23-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 72-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 189-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 127-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 143-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 82-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 15-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 136-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 184-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 197-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 148-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 231-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 224-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 195-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 39-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 131-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 242-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 186-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 182-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 177-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 157-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 190-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 86-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 150-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 146-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 228-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 144-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 43-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 193-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 59-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 94-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 174-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 64-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 65-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 142-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 247-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 163-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 214-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 206-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 102-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 132-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 168-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 173-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 217-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 212-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 171-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 22-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 29-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 89-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 95-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 239-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 221-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 67-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 154-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 91-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 109-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 66-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 20-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 73-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 40-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 230-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 199-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 52-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 33-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 126-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 194-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 213-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 12-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 192-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 3-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 92-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 196-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 61-A | 201 | FOL | C4A-C8A | 2.66 | 1.45 | 1.40 |
| 2 | 125-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 85-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 56-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 187-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 68-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 10-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 149-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 107-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 81-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 6-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 21-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 98-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 165-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 31-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 105-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 180-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 54-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 14-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 145-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 13-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 99-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 83-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 117-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 201-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 48-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 203-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 30-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 156-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 42-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 106-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 205-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 158-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 112-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 220-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 123-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) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | 113-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 118-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 176-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 49-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 44-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 70-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 166-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 188-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 121-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 133-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 7-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 97-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 80-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 17-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 78-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 246-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 101-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 235-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 137-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 115-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 103-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 147-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 75-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 79-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 175-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 245-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 9-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 208-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 19-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 248-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 185-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 152-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 60-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 53-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 226-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 110-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 244-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 134-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 236-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 198-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 183-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 153-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) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | 135-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 202-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 140-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 119-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 240-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 84-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 100-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 27-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 1-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 234-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 130-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 161-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 215-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 210-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 249-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 216-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 139-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 96-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 159-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 69-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 169-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 62-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 225-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 55-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 211-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 181-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 116-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 71-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 160-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 191-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 50-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 8-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 164-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 18-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 51-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 232-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 63-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 138-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 16-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 57-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 200-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 250-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) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | 36-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 167-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 37-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 124-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 34-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 218-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 243-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 209-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 111-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 90-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 122-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 151-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 45-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 128-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 74-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 11-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 207-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 241-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 2-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 155-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 88-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 5-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 170-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 229-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 222-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 47-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 76-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 35-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 41-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 108-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 104-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 141-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 25-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 87-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 32-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 77-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 93-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 233-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 4-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 24-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 237-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 28-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) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | 238-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 26-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 129-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 223-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 162-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 178-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 46-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 38-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 227-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 179-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 219-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 172-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 58-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 114-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 204-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 120-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 23-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 72-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 189-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 127-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 143-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 82-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 15-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 136-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 184-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 197-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 148-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 231-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 224-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 195-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 39-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 131-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 242-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 186-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 182-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 177-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 157-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 190-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 86-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 150-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 146-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 228-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) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | 144-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 43-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 193-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 59-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 94-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 174-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 64-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 65-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 142-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 247-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 163-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 214-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 206-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 102-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 132-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 168-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 173-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 217-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 212-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 171-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 22-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 29-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 89-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 95-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 239-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 221-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 67-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 154-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 91-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 109-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 66-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 20-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 73-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 40-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 230-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 199-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 52-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 33-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 126-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 194-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 213-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 12-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) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | 192-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 3-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 92-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 196-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |
| 2 | 61-A | 201 | FOL | CB-CA | 2.22 | 1.56 | 1.53 |

All (6000) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 3 | 34-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 76-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 202-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 174-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 54-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 161-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 129-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 238-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 208-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 119-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 39-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 33-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 12-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 89-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 23-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 5-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 81-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 162-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 107-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 239-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 190-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 215-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 92-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 55-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 82-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 38-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 144-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 186-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 138-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 104-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 149-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 164-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 156-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 3 | 48-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 6-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 225-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 30-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 3-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 223-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 96-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 176-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 72-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 154-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 10-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 175-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 127-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 27-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 137-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 243-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 56-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 21-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 87-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 234-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 169-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 241-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 249-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 233-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 182-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 43-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 207-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 20-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 247-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 136-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 51-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 195-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 204-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 211-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 126-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 244-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 68-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 240-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 17-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 66-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 170-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 228-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 3 | 14-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 122-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 102-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 22-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 210-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 224-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 171-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 184-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 125-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 44-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 158-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 213-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 113-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 49-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 61-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 242-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 90-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 65-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 111-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 52-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 166-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 152-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 220-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 217-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 245-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 185-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 95-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 4-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 114-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 29-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 32-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 58-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 196-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 201-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 98-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 13-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 16-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 219-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 200-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 120-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 63-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 80-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 3 | 106-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 140-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 26-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 157-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 94-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 108-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 91-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 57-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 60-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 143-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 246-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 155-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 86-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 50-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 232-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 177-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 189-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 145-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 198-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 116-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 179-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 117-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 97-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 123-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 71-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 121-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 8-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 167-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 47-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 67-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 15-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 206-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 73-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 194-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 205-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 236-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 151-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 85-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 226-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 75-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 128-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 41-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 3 | 230-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 163-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 192-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 172-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 168-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 183-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 135-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 1-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 237-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 62-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 46-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 103-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 31-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 100-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 146-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 173-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 105-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 36-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 59-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 188-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 24-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 118-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 83-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 209-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 132-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 197-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 70-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 79-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 222-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 227-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 148-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 109-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 9-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 40-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 181-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 2-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 77-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 214-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 216-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 187-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 221-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 147-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 3 | 248-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 64-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 115-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 124-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 180-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 78-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 178-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 231-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 235-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 141-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 99-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 130-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 142-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 35-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 18-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 165-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 139-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 133-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 159-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 74-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 199-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 93-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 229-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 101-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 112-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 84-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 150-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 7-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 69-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 88-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 193-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 28-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 203-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 250-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 45-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 160-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 53-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 191-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 11-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 110-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 37-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 153-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|--------|-------------|----------|
| 3 | 212-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 25-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 134-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 19-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 131-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 218-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 42-A | 202 | NAP | O2N-PN-O5D | -11.01 | 56.61 | 107.75 |
| 3 | 34-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 76-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 202-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 174-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 54-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 161-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 129-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 238-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 208-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 119-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 39-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 33-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 12-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 89-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 23-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 5-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 81-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 162-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 107-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 239-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 190-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 215-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 92-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 55-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 82-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 38-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 144-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 186-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 138-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 104-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 149-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 164-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 156-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 48-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 6-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 225-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 30-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 3-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 223-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 96-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 176-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 72-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 154-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 10-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 175-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 127-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 27-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 137-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 243-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 56-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 21-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 87-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 234-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 169-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 241-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 249-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 233-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 182-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 43-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 207-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 20-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 247-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 136-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 51-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 195-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 204-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 211-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 126-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 244-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 68-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 240-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 17-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 66-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 170-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 228-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 14-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 122-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 102-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 22-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 210-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 224-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 171-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 184-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 125-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 44-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 158-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 213-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 113-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 49-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 61-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 242-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 90-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 65-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 111-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 52-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 166-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 152-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 220-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 217-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 245-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 185-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 95-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 4-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 114-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 29-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 32-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 58-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 196-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 201-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 98-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 13-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 16-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 219-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 200-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 120-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 63-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 80-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 106-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 140-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 26-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 157-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 94-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 108-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 91-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 57-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 60-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 143-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 246-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 155-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 86-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 50-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 232-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 177-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 189-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 145-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 198-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 116-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 179-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 117-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 97-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 123-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 71-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 121-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 8-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 167-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 47-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 67-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 15-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 206-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 73-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 194-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 205-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 236-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 151-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 85-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 226-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 75-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 128-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 41-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 230-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 163-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 192-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 172-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 168-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 183-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 135-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 1-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 237-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 62-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 46-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 103-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 31-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 100-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 146-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 173-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 105-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 36-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 59-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 188-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 24-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 118-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 83-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 209-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 132-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 197-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 70-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 79-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 222-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 227-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 148-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 109-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 9-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 40-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 181-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 2-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 77-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 214-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 216-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 187-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 221-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 147-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 248-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 64-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 115-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 124-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 180-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 78-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 178-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 231-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 235-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 141-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 99-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 130-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 142-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 35-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 18-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 165-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 139-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 133-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 159-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 74-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 199-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 93-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 229-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 101-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 112-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 84-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 150-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 7-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 69-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 88-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 193-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 28-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 203-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 250-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 45-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 160-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 53-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 191-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 11-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 110-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 37-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 153-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 212-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 25-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 134-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 19-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 131-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 218-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 42-A | 202 | NAP | O2N-PN-O1N | 9.97 | 161.53 | 112.24 |
| 3 | 34-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 76-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 202-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 174-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 54-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 161-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 129-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 238-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 208-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 119-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 39-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 33-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 12-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 89-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 23-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 5-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 81-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 162-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 107-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 239-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 190-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 215-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 92-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 55-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 82-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 38-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 144-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 186-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 138-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 104-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 149-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 164-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 156-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 48-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 6-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 225-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 30-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 3-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 223-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 96-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 176-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 72-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 154-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 10-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 175-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 127-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 27-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 137-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 243-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 56-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 21-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 87-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 234-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 169-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 241-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 249-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 233-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 182-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 43-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 207-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 20-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 247-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 136-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 51-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 195-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 204-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 211-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 126-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 244-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 68-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 240-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 17-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 66-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 170-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 228-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 14-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 122-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 102-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 22-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 210-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 224-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 171-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 184-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 125-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 44-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 158-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 213-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 113-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 49-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 61-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 242-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 90-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 65-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 111-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 52-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 166-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 152-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 220-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 217-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 245-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 185-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 95-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 4-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 114-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 29-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 32-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 58-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 196-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 201-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 98-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 13-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 16-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 219-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 200-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 120-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 63-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 80-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 106-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 140-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 26-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 157-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 94-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 108-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 91-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 57-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 60-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 143-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 246-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 155-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 86-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 50-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 232-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 177-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 189-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 145-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 198-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 116-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 179-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 117-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 97-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 123-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 71-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 121-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 8-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 167-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 47-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 67-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 15-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 206-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 73-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 194-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 205-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 236-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 151-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 85-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 226-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 75-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 128-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 41-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 230-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 163-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 192-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 172-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 168-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 183-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 135-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 1-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 237-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 62-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 46-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 103-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 31-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 100-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 146-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 173-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 105-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 36-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 59-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 188-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 24-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 118-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 83-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 209-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 132-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 197-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 70-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 79-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 222-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 227-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 148-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 109-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 9-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 40-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 181-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 2-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 77-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 214-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 216-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 187-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 221-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 147-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 248-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 64-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 115-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 124-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 180-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 78-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 178-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 231-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 235-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 141-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 99-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 130-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 142-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 35-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 18-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 165-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 139-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 133-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 159-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 74-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 199-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 93-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 229-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 101-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 112-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 84-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 150-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 7-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 69-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 88-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 193-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 28-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 203-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 250-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 45-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 160-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 53-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 191-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 11-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 110-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 37-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 153-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 212-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 25-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 134-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 19-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 131-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 218-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 42-A | 202 | NAP | C3B-C2B-C1B | -8.62 | 86.68 | 102.89 |
| 3 | 34-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 76-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 202-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 174-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 54-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 161-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 129-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 238-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 208-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 119-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 39-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 33-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 12-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 89-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 23-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 5-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 81-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 162-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 107-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 239-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 190-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 215-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 92-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 55-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 82-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 38-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 144-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 186-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 138-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 104-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 149-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 164-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 156-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 48-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 6-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 225-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 30-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 3-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 223-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 96-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 176-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 72-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 154-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 10-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 175-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 127-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 27-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 137-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 243-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 56-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 21-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 87-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 234-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 169-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 241-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 249-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 233-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 182-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 43-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 207-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 20-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 247-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 136-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 51-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 195-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 204-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 211-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 126-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 244-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 68-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 240-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 17-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 66-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 170-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 228-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 14-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 122-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 102-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 22-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 210-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 224-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 171-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 184-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 125-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 44-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 158-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 213-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 113-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 49-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 61-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 242-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 90-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 65-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 111-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 52-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 166-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 152-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 220-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 217-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 245-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 185-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 95-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 4-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 114-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 29-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 32-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 58-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 196-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 201-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 98-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 13-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 16-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 219-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 200-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 120-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 63-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 80-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 106-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 140-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 26-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 157-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 94-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 108-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 91-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 57-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 60-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 143-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 246-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 155-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 86-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 50-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 232-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 177-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 189-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 145-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 198-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 116-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 179-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 117-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 97-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 123-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 71-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 121-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 8-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 167-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 47-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 67-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 15-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 206-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 73-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 194-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 205-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 236-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 151-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 85-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 226-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 75-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 128-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 41-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 230-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 163-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 192-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 172-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 168-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 183-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 135-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 1-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 237-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 62-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 46-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 103-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 31-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 100-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 146-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 173-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 105-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 36-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 59-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 188-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 24-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 118-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 83-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 209-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 132-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 197-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 70-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 79-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 222-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 227-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 148-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 109-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 9-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 40-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 181-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 2-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 77-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 214-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 216-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 187-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 221-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 147-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 248-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 64-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 115-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 124-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 180-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 78-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 178-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 231-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 235-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 141-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 99-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 130-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 142-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 35-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 18-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 165-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 139-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 133-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 159-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 74-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 199-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 93-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 229-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 101-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 112-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 84-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 150-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 7-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 69-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 88-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 193-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 28-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 203-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 250-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 45-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 160-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 53-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 191-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 11-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 110-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 37-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 153-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 212-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 25-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 134-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 19-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 131-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 218-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 42-A | 202 | NAP | O3B-C3B-C2B | 7.11 | 131.35 | 111.17 |
| 3 | 34-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 76-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 202-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 174-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 54-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 161-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 129-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 238-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 208-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 119-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 39-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 33-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 12-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 89-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 23-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 5-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 81-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 162-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 107-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 239-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 190-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 215-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 92-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 55-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 82-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 38-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 144-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 186-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 138-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 104-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 149-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 164-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 156-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 48-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 6-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 225-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 30-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 3-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 223-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 96-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 176-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 72-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 154-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 10-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 175-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 127-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 27-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 137-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 243-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 56-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 21-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 87-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 234-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 169-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 241-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 249-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 233-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 182-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 43-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 207-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 20-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 247-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 136-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 51-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 195-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 204-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 211-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 126-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 244-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 68-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 240-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 17-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 66-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 170-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 228-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 14-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 122-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 102-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 22-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 210-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 224-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 171-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 184-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 125-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 44-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 158-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 213-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 113-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 49-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 61-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 242-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 90-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 65-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 111-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 52-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 166-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 152-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 220-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 217-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 245-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 185-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 95-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 4-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 114-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 29-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 32-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 58-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 196-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 201-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 98-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 13-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 16-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 219-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 200-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 120-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 63-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 80-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 106-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 140-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 26-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 157-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 94-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 108-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 91-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 57-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 60-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 143-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 246-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 155-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 86-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 50-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 232-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 177-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 189-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 145-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 198-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 116-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 179-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 117-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 97-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 123-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 71-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 121-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 8-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 167-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 47-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 67-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 15-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 206-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 73-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 194-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 205-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 236-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 151-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 85-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 226-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 75-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 128-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 41-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 230-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 163-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 192-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 172-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 168-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 183-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 135-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 1-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 237-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 62-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 46-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 103-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 31-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 100-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 146-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 173-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 105-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 36-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 59-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 188-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 24-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 118-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 83-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 209-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 132-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 197-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 70-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 79-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 222-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 227-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 148-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 109-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 9-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 40-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 181-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 2-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 77-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 214-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 216-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 187-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 221-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 147-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 248-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 64-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 115-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 124-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 180-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 78-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 178-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 231-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 235-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 141-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 99-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 130-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 142-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 35-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 18-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 165-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 139-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 133-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 159-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 74-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 199-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 93-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 229-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 101-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 112-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 84-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 150-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 7-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 69-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 88-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 193-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 28-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 203-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 250-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 45-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 160-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 53-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 191-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 11-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 110-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 37-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 153-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 212-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 25-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 134-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 19-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 131-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 218-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 3 | 42-A | 202 | NAP | O4B-C4B-C3B | -6.41 | 92.43 | 105.11 |
| 2 | 125-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 85-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 56-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 187-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 68-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 10-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 149-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 107-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 81-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 6-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 21-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 98-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 165-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 31-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 105-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 180-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 54-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 14-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 145-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 13-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 99-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 83-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 117-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 201-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 48-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 203-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 30-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 156-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 42-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 106-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 205-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 158-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 112-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 220-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 123-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 113-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 118-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 176-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 49-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 44-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 70-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 166-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 188-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 121-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 133-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 7-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 97-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 80-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 17-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 78-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 246-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 101-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 235-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 137-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 115-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 103-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 147-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 75-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 79-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 175-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 245-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 9-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 208-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 19-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 248-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 185-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 152-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 60-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 53-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 226-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 110-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 244-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 134-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 236-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 198-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 183-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 153-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 135-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 202-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 140-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 119-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 240-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 84-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 100-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 27-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 1-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 234-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 130-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 161-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 215-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 210-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 249-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 216-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 139-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 96-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 159-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 69-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 169-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 62-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 225-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 55-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 211-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 181-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 116-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 71-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 160-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 191-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 50-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 8-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 164-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 18-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 51-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 232-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 63-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 138-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 16-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 57-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 200-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 250-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 36-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 167-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 37-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 124-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 34-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 218-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 243-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 209-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 111-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 90-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 122-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 151-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 45-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 128-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 74-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 11-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 207-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 241-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 2-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 155-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 88-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 5-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 170-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 229-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 222-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 47-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 76-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 35-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 41-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 108-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 104-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 141-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 25-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 87-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 32-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 77-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 93-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 233-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 4-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 24-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 237-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 28-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 238-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 26-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 129-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 223-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 162-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 178-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 46-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 38-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 227-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 179-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 219-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 172-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 58-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 114-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 204-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 120-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 23-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 72-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 189-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 127-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 143-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 82-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 15-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 136-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 184-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 197-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 148-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 231-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 224-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 195-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 39-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 131-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 242-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 186-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 182-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 177-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 157-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 190-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 86-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 150-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 146-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 228-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 144-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 43-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 193-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 59-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 94-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 174-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 64-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 65-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | 142-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 247-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 163-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 214-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 206-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 102-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 132-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 168-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 173-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 217-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 212-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 171-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 22-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 29-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 89-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 95-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 239-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 221-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 67-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 154-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 91-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 109-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 66-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 20-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 73-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 40-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 230-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 199-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 52-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 33-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 126-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 194-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 213-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 12-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 192-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 3-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 92-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 196-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 61-A | 201 | FOL | N8-C8A-N1 | 5.83 | 122.48 | 115.82 |
| 2 | 125-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 85-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 56-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | 187-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 68-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 10-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 149-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 107-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 81-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 6-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 21-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 98-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 165-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 31-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 105-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 180-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 54-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 14-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 145-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 13-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 99-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 83-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 117-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 201-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 48-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 203-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 30-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 156-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 42-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 106-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 205-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 158-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 112-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 220-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 123-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 113-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 118-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 176-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 49-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 44-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 70-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 166-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 188-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 121-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 133-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | 7-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 97-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 80-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 17-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 78-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 246-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 101-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 235-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 137-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 115-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 103-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 147-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 75-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 79-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 175-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 245-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 9-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 208-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 19-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 248-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 185-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 152-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 60-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 53-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 226-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 110-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 244-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 134-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 236-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 198-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 183-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 153-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 135-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 202-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 140-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 119-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 240-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 84-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 100-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 27-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 1-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 234-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | 130-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 161-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 215-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 210-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 249-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 216-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 139-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 96-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 159-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 69-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 169-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 62-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 225-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 55-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 211-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 181-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 116-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 71-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 160-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 191-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 50-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 8-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 164-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 18-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 51-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 232-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 63-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 138-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 16-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 57-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 200-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 250-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 36-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 167-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 37-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 124-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 34-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 218-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 243-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 209-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 111-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 90-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | 122-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 151-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 45-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 128-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 74-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 11-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 207-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 241-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 2-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 155-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 88-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 5-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 170-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 229-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 222-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 47-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 76-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 35-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 41-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 108-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 104-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 141-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 25-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 87-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 32-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 77-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 93-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 233-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 4-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 24-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 237-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 28-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 238-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 26-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 129-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 223-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 162-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 178-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 46-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 38-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 227-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 179-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | 219-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 172-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 58-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 114-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 204-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 120-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 23-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 72-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 189-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 127-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 143-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 82-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 15-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 136-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 184-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 197-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 148-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 231-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 224-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 195-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 39-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 131-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 242-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 186-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 182-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 177-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 157-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 190-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 86-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 150-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 146-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 228-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 144-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 43-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 193-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 59-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 94-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 174-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 64-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 65-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 142-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 247-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 2 | 163-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 214-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 206-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 102-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 132-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 168-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 173-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 217-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 212-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 171-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 22-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 29-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 89-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 95-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 239-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 221-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 67-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 154-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 91-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 109-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 66-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 20-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 73-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 40-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 230-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 199-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 52-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 33-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 126-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 194-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 213-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 12-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 192-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 3-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 92-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 196-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 61-A | 201 | FOL | C4A-C4-N3 | -5.23 | 116.28 | 123.43 |
| 2 | 125-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 85-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 56-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 187-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 68-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2 | 10-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 149-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 107-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 81-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 6-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 21-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 98-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 165-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 31-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 105-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 180-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 54-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 14-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 145-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 13-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 99-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 83-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 117-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 201-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 48-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 203-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 30-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 156-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 42-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 106-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 205-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 158-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 112-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 220-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 123-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 113-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 118-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 176-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 49-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 44-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 70-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 166-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 188-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 121-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 133-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 7-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 97-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2 | 80-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 17-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 78-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 246-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 101-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 235-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 137-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 115-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 103-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 147-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 75-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 79-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 175-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 245-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 9-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 208-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 19-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 248-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 185-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 152-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 60-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 53-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 226-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 110-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 244-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 134-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 236-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 198-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 183-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 153-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 135-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 202-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 140-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 119-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 240-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 84-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 100-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 27-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 1-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 234-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 130-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 161-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2 | 215-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 210-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 249-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 216-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 139-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 96-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 159-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 69-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 169-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 62-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 225-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 55-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 211-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 181-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 116-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 71-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 160-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 191-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 50-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 8-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 164-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 18-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 51-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 232-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 63-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 138-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 16-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 57-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 200-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 250-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 36-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 167-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 37-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 124-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 34-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 218-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 243-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 209-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 111-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 90-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 122-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 151-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2 | 45-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 128-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 74-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 11-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 207-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 241-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 2-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 155-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 88-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 5-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 170-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 229-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 222-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 47-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 76-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 35-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 41-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 108-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 104-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 141-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 25-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 87-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 32-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 77-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 93-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 233-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 4-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 24-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 237-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 28-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 238-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 26-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 129-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 223-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 162-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 178-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 46-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 38-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 227-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 179-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 219-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 172-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2 | 58-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 114-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 204-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 120-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 23-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 72-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 189-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 127-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 143-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 82-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 15-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 136-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 184-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 197-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 148-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 231-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 224-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 195-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 39-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 131-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 242-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 186-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 182-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 177-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 157-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 190-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 86-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 150-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 146-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 228-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 144-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 43-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 193-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 59-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 94-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 174-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 64-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 65-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 142-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 247-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 163-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 214-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2 | 206-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 102-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 132-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 168-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 173-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 217-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 212-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 171-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 22-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 29-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 89-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 95-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 239-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 221-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 67-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 154-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 91-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 109-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 66-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 20-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 73-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 40-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 230-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 199-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 52-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 33-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 126-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 194-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 213-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 12-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 192-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 3-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 92-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 196-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 2 | 61-A | 201 | FOL | C4-N3-C2 | 4.91 | 123.74 | 115.93 |
| 3 | 34-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 76-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 202-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 174-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 54-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 161-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 129-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 238-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 208-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 119-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 39-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 33-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 12-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 89-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 23-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 5-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 81-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 162-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 107-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 239-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 190-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 215-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 92-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 55-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 82-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 38-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 144-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 186-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 138-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 104-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 149-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 164-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 156-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 48-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 6-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 225-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 30-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 3-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 223-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 96-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 176-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 72-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 154-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 10-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 175-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 127-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 27-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 137-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 243-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 56-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 21-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 87-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 234-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 169-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 241-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 249-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 233-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 182-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 43-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 207-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 20-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 247-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 136-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 51-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 195-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 204-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 211-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 126-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 244-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 68-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 240-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 17-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 66-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 170-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 228-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 14-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 122-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 102-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 22-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 210-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 224-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 171-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 184-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 125-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 44-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 158-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 213-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 113-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 49-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 61-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 242-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 90-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 65-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 111-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 52-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 166-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 152-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 220-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 217-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 245-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 185-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 95-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 4-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 114-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 29-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 32-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 58-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 196-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 201-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 98-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 13-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 16-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 219-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 200-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 120-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 63-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 80-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 106-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 140-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 26-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 157-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 94-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 108-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 91-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 57-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 60-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 143-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 246-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 155-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 86-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 50-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 232-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 177-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 189-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 145-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 198-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 116-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 179-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 117-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 97-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 123-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 71-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 121-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 8-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 167-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 47-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 67-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 15-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 206-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 73-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 194-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 205-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 236-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 151-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 85-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 226-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 75-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 128-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 41-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 230-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 163-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 192-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 172-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 168-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 183-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 135-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 1-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 237-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 62-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 46-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 103-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 31-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 100-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 146-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 173-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 105-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 36-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 59-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 188-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 24-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 118-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 83-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 209-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 132-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 197-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 70-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 79-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 222-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 227-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 148-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 109-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 9-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 40-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 181-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 2-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 77-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 214-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 216-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 187-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 221-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 147-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 248-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 64-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 115-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 124-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 180-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 78-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 178-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 231-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 235-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 141-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 99-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 130-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 142-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 35-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 18-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 165-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 139-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 133-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 159-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 74-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 199-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 93-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 229-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 101-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 112-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 84-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 150-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 7-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 69-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 88-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 193-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 28-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 203-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 250-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 45-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 160-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 53-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 191-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 11-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 110-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 37-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 153-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 212-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 25-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 134-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 19-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 131-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 218-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 42-A | 202 | NAP | O2B-C2B-C3B | 4.39 | 127.59 | 111.68 |
| 3 | 34-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 76-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 202-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 174-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 54-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 161-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 129-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 238-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 208-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 119-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 39-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 33-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 12-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 89-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 23-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 5-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 81-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 162-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 107-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 239-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 190-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 215-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 92-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 55-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 82-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 38-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 144-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 186-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 138-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 104-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 149-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 164-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 156-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 48-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 6-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 225-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 30-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 3-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 223-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 96-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 176-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 72-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 154-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 10-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 175-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 127-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 27-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 137-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 243-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 56-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 21-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 87-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 234-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 169-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 241-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 249-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 233-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 182-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 43-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 207-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 20-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 247-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 136-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 51-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 195-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 204-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 211-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 126-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 244-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 68-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 240-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 17-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 66-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 170-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 228-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 14-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 122-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 102-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 22-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 210-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 224-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 171-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 184-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 125-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 44-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 158-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 213-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 113-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 49-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 61-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 242-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 90-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 65-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 111-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 52-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 166-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 152-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 220-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 217-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 245-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 185-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 95-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 4-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 114-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 29-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 32-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 58-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 196-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 201-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 98-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 13-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 16-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 219-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 200-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 120-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 63-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 80-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 106-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 140-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 26-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 157-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 94-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 108-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 91-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 57-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 60-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 143-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 246-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 155-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 86-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 50-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 232-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 177-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 189-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 145-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 198-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 116-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 179-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 117-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 97-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 123-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 71-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 121-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 8-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 167-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 47-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 67-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 15-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 206-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 73-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 194-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 205-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 236-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 151-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 85-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 226-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 75-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 128-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 41-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 230-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 163-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 192-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 172-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 168-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 183-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 135-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 1-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 237-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 62-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 46-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 103-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 31-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 100-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 146-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 173-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 105-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 36-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 59-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 188-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 24-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 118-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 83-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 209-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 132-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 197-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 70-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 79-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 222-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 227-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 148-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 109-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 9-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 40-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 181-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 2-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 77-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 214-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 216-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 187-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 221-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 147-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 248-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 64-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 115-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 124-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 180-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 78-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 178-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 231-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 235-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 141-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 99-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 130-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 142-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 35-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 18-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 165-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 139-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 133-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 159-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 74-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 199-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 93-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 229-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 101-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 112-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 84-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 150-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 7-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 69-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 88-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 193-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 28-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 203-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 250-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 45-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 160-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 53-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 191-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 11-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 110-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 37-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 153-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 212-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 25-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 134-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 19-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 131-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 218-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 3 | 42-A | 202 | NAP | O3B-C3B-C4B | 3.80 | 122.03 | 111.05 |
| 2 | 125-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 85-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 56-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 187-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 68-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 10-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 149-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 107-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 81-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 6-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 21-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 98-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 165-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 31-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 105-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 180-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 54-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 14-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 145-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 13-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 99-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 83-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 117-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 201-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 48-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 203-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 30-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 156-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 42-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 106-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 205-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 158-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 112-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 220-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 123-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 113-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 118-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 176-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 49-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 44-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 70-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 166-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 188-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 121-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 133-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 7-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 97-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 80-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 17-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 78-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 246-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 101-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 235-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 137-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 115-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 103-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 147-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 75-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 79-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 175-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 245-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 9-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 208-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 19-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 248-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 185-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 152-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 60-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 53-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 226-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 110-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 244-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 134-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 236-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 198-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 183-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 153-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 135-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 202-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 140-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 119-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 240-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 84-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 100-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 27-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 1-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 234-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 130-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 161-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 215-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 210-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 249-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 216-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 139-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 96-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 159-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 69-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 169-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 62-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 225-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 55-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 211-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 181-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 116-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 71-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 160-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 191-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 50-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 8-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 164-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 18-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 51-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 232-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 63-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 138-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 16-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 57-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 200-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 250-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 36-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 167-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 37-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 124-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 34-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 218-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 243-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 209-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 111-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 90-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 122-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 151-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 45-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 128-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 74-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 11-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 207-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 241-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 2-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 155-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 88-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 5-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 170-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 229-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 222-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 47-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 76-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 35-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 41-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 108-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 104-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 141-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 25-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 87-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 32-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 77-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 93-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 233-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 4-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 24-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 237-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 28-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 238-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 26-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 129-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 223-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 162-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 178-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 46-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 38-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 227-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 179-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 219-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 172-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 58-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 114-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 204-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 120-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 23-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 72-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 189-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 127-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 143-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 82-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 15-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 136-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 184-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 197-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 148-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 231-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 224-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 195-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 39-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 131-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 242-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 186-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 182-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 177-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 157-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 190-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 86-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 150-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 146-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 228-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 144-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 43-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 193-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 59-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 94-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 174-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 64-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 65-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 142-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 247-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 163-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 214-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 206-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 102-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 132-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 168-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 173-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 217-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | 212-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 171-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 22-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 29-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 89-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 95-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 239-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 221-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 67-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 154-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 91-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 109-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 66-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 20-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 73-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 40-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 230-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 199-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 52-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 33-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 126-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 194-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 213-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 12-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 192-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 3-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 92-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 196-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 61-A | 201 | FOL | N1-C2-N3 | -3.62 | 122.40 | 127.22 |
| 2 | 125-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 85-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 56-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 187-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 68-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 10-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 149-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 107-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 81-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 6-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 21-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 98-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 165-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | 31-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 105-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 180-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 54-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 14-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 145-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 13-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 99-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 83-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 117-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 201-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 48-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 203-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 30-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 156-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 42-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 106-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 205-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 158-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 112-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 220-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 123-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 113-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 118-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 176-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 49-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 44-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 70-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 166-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 188-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 121-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 133-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 7-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 97-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 80-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 17-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 78-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 246-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 101-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 235-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 137-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 115-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | 103-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 147-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 75-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 79-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 175-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 245-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 9-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 208-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 19-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 248-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 185-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 152-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 60-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 53-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 226-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 110-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 244-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 134-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 236-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 198-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 183-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 153-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 135-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 202-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 140-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 119-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 240-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 84-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 100-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 27-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 1-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 234-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 130-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 161-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 215-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 210-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 249-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 216-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 139-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 96-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 159-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 69-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | 169-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 62-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 225-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 55-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 211-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 181-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 116-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 71-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 160-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 191-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 50-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 8-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 164-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 18-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 51-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 232-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 63-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 138-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 16-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 57-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 200-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 250-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 36-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 167-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 37-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 124-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 34-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 218-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 243-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 209-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 111-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 90-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 122-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 151-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 45-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 128-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 74-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 11-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 207-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 241-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 2-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 155-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | 88-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 5-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 170-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 229-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 222-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 47-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 76-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 35-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 41-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 108-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 104-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 141-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 25-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 87-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 32-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 77-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 93-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 233-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 4-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 24-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 237-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 28-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 238-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 26-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 129-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 223-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 162-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 178-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 46-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 38-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 227-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 179-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 219-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 172-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 58-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 114-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 204-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 120-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 23-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 72-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 189-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 127-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | 143-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 82-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 15-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 136-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 184-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 197-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 148-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 231-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 224-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 195-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 39-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 131-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 242-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 186-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 182-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 177-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 157-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 190-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 86-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 150-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 146-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 228-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 144-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 43-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 193-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 59-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 94-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 174-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 64-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 65-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 142-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 247-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 163-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 214-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 206-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 102-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 132-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 168-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 173-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 217-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 212-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 171-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 22-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 29-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 89-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 95-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 239-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 221-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 67-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 154-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 91-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 109-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 66-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 20-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 73-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 40-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 230-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 199-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 52-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 33-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 126-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 194-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 213-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 12-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 192-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 3-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 92-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 196-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 2 | 61-A | 201 | FOL | C4-C4A-C8A | -3.54 | 117.61 | 119.95 |
| 3 | 34-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 76-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 202-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 174-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 54-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 161-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 129-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 238-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 208-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 119-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 39-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 33-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 12-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 89-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 23-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 5-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 81-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 162-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 107-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 239-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 190-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 215-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 92-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 55-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 82-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 38-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 144-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 186-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 138-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 104-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 149-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 164-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 156-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 48-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 6-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 225-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 30-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 3-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 223-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 96-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 176-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 72-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 154-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 10-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 175-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 127-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 27-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 137-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 243-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 56-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 21-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 87-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 234-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 169-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 241-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 249-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 233-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 182-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 43-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 207-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 20-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 247-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 136-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 51-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 195-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 204-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 211-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 126-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 244-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 68-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 240-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 17-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 66-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 170-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 228-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 14-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 122-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 102-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 22-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 210-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 224-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 171-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 184-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 125-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 44-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 158-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 213-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 113-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 49-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 61-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 242-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 90-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 65-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 111-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 52-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 166-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 152-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 220-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 217-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 245-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 185-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 95-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 4-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 114-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 29-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 32-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 58-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 196-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 201-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 98-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 13-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 16-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 219-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 200-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 120-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 63-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 80-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 106-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 140-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 26-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 157-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 94-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 108-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 91-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 57-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 60-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 143-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 246-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 155-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 86-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 50-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 232-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 177-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 189-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 145-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 198-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 116-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 179-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 117-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 97-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 123-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 71-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 121-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 8-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 167-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 47-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 67-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 15-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 206-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 73-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 194-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 205-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 236-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 151-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 85-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 226-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 75-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 128-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 41-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 230-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 163-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 192-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 172-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 168-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 183-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 135-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 1-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 237-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 62-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 46-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 103-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 31-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 100-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 146-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 173-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 105-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 36-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 59-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 188-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 24-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 118-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 83-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 209-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 132-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 197-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 70-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 79-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 222-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 227-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 148-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 109-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 9-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 40-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 181-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 2-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 77-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 214-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 216-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 187-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 221-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 147-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 248-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 64-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 115-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 124-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 180-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 78-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 178-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 231-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 235-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 141-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 99-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 130-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 142-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 35-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 18-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 165-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 139-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 133-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 159-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 74-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 199-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 93-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 229-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 101-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 112-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 84-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 150-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 7-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 69-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 88-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 193-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 28-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 203-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 250-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 45-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 160-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 53-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 191-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 11-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 110-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 37-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 153-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 212-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 25-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 134-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 19-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 131-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 218-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 3 | 42-A | 202 | NAP | C1B-N9A-C4A | -3.49 | 120.52 | 126.64 |
| 2 | 125-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 85-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 56-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 187-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 68-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 10-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 149-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 107-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 81-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 6-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 21-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 98-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 165-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 31-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 105-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 180-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 54-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | 14-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 145-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 13-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 99-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 83-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 117-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 201-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 48-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 203-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 30-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 156-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 42-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 106-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 205-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 158-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 112-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 220-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 123-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 113-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 118-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 176-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 49-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 44-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 70-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 166-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 188-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 121-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 133-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 7-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 97-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 80-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 17-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 78-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 246-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 101-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 235-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 137-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 115-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 103-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 147-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 75-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 79-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | 175-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 245-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 9-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 208-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 19-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 248-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 185-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 152-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 60-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 53-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 226-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 110-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 244-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 134-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 236-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 198-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 183-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 153-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 135-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 202-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 140-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 119-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 240-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 84-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 100-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 27-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 1-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 234-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 130-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 161-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 215-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 210-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 249-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 216-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 139-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 96-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 159-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 69-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 169-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 62-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 225-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 55-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | 211-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 181-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 116-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 71-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 160-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 191-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 50-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 8-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 164-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 18-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 51-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 232-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 63-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 138-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 16-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 57-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 200-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 250-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 36-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 167-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 37-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 124-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 34-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 218-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 243-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 209-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 111-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 90-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 122-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 151-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 45-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 128-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 74-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 11-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 207-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 241-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 2-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 155-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 88-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 5-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 170-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 229-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | 222-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 47-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 76-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 35-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 41-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 108-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 104-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 141-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 25-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 87-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 32-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 77-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 93-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 233-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 4-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 24-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 237-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 28-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 238-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 26-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 129-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 223-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 162-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 178-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 46-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 38-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 227-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 179-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 219-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 172-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 58-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 114-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 204-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 120-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 23-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 72-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 189-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 127-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 143-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 82-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 15-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 136-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 2 | 184-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 197-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 148-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 231-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 224-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 195-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 39-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 131-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 242-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 186-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 182-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 177-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 157-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 190-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 86-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 150-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 146-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 228-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 144-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 43-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 193-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 59-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 94-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 174-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 64-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 65-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 142-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 247-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 163-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 214-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 206-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 102-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 132-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 168-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 173-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 217-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 212-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 171-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 22-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 29-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 89-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 95-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 239-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 221-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 67-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 154-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 91-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 109-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 66-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 20-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 73-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 40-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 230-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 199-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 52-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 33-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 126-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 194-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 213-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 12-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 192-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 3-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 92-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 196-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 61-A | 201 | FOL | CA-N-C | 3.40 | 126.73 | 122.34 |
| 2 | 125-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 85-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 56-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 187-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 68-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 10-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 149-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 107-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 81-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 6-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 21-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 98-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 165-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 31-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 105-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 180-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 54-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 14-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 145-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 13-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 99-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 83-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 117-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 201-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 48-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 203-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 30-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 156-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 42-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 106-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 205-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 158-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 112-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 220-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 123-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 113-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 118-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 176-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 49-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 44-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 70-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 166-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 188-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 121-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 133-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 7-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 97-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 80-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 17-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 78-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 246-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 101-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 235-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 137-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 115-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 103-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 147-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 75-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 79-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 175-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 245-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 9-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 208-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 19-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 248-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 185-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 152-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 60-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 53-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 226-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 110-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 244-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 134-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 236-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 198-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 183-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 153-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 135-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 202-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 140-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 119-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 240-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 84-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 100-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 27-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 1-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 234-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 130-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 161-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 215-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 210-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 249-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 216-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 139-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 96-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 159-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 69-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 169-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 62-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 225-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 55-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 211-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 181-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 116-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 71-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 160-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 191-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 50-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 8-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 164-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 18-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 51-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 232-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 63-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 138-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 16-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 57-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 200-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 250-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 36-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 167-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 37-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 124-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 34-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 218-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 243-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 209-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 111-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 90-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 122-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 151-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 45-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 128-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 74-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 11-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 207-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 241-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 2-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 155-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 88-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 5-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 170-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 229-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 222-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 47-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 76-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 35-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 41-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 108-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 104-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 141-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 25-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 87-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 32-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 77-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 93-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 233-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 4-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 24-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 237-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 28-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 238-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 26-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 129-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 223-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 162-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 178-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 46-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 38-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 227-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 179-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 219-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 172-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 58-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 114-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 204-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 120-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 23-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 72-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 189-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 127-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 143-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 82-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 15-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 136-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 184-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 197-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2 | 148-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 231-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 224-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 195-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 39-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 131-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 242-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 186-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 182-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 177-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 157-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 190-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 86-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 150-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 146-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 228-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 144-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 43-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 193-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 59-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 94-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 174-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 64-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 65-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 142-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 247-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 163-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 214-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 206-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 102-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 132-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 168-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 173-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 217-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 212-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 171-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 22-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 29-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 89-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 95-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 239-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 221-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 67-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 154-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 91-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 109-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 66-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 20-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 73-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 40-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 230-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 199-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 52-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 33-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 126-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 194-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 213-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 12-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 192-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 3-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 92-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 196-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 61-A | 201 | FOL | CB-CG-CD | -3.19 | 106.74 | 113.59 |
| 2 | 125-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 85-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 56-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 187-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 68-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 10-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 149-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 107-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 81-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 6-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 21-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 98-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 165-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 31-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 105-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 180-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 54-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 14-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 145-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 13-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 99-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 83-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 117-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 201-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 48-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 203-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 30-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 156-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 42-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 106-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 205-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 158-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 112-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 220-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 123-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 113-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 118-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 176-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 49-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 44-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 70-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 166-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 188-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 121-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 133-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 7-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 97-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 80-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 17-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 78-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 246-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 101-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 235-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 137-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 115-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 103-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 147-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 75-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 79-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 175-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 245-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 9-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 208-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 19-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 248-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 185-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 152-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 60-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 53-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 226-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 110-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 244-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 134-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 236-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 198-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 183-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 153-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 135-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 202-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 140-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 119-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 240-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 84-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 100-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 27-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 1-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 234-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 130-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 161-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 215-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 210-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 249-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 216-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 139-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 96-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 159-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 69-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 169-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 62-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 225-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 55-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 211-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 181-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 116-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 71-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 160-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 191-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 50-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 8-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 164-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 18-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 51-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 232-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 63-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 138-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 16-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 57-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 200-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 250-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 36-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 167-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 37-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 124-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 34-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 218-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 243-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 209-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 111-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 90-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 122-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 151-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 45-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 128-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 74-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 11-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 207-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 241-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 2-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 155-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 88-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 5-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 170-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 229-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 222-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 47-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 76-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 35-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 41-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 108-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 104-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 141-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 25-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 87-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 32-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 77-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 93-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 233-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 4-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 24-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 237-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 28-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 238-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 26-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 129-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 223-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 162-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 178-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 46-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 38-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 227-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 179-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 219-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 172-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 58-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 114-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 204-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 120-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 23-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 72-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 189-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 127-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 143-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 82-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 15-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 136-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 184-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 197-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 148-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 231-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 224-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 195-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 39-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 131-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 242-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 186-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 182-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 177-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 157-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 190-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 86-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 150-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 146-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 228-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 144-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 43-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 193-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 59-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 94-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 174-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 64-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 65-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 142-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 247-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 163-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 214-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 206-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 102-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 132-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 168-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 173-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 217-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 212-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 171-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 22-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 29-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 89-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 95-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 239-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 221-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 67-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 154-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 91-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 109-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 66-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 20-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 73-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 40-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 230-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 199-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 52-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 33-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 126-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 194-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 213-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 12-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 192-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 3-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 92-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 196-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 61-A | 201 | FOL | C13-C14-N10 | -3.06 | 114.63 | 120.97 |
| 2 | 125-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 85-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 56-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 187-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 68-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 10-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 149-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 107-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 81-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 6-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 21-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 98-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 165-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 31-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 105-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 180-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 54-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 14-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 145-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 13-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 99-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 83-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 117-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 201-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 48-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 203-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 30-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 156-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 42-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 106-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 205-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 158-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 112-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 220-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 123-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 113-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 118-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 176-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 49-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 44-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 70-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 166-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 188-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 121-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 133-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 7-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 97-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 80-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 17-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 78-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 246-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 101-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 235-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 137-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 115-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 103-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 147-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 75-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 79-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 175-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 245-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 9-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 208-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 19-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 248-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 185-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 152-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 60-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 53-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 226-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 110-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 244-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 134-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 236-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 198-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 183-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 153-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 135-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 202-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 140-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 119-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 240-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 84-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 100-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 27-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 1-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 234-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 130-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 161-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 215-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 210-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 249-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 216-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 139-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 96-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 159-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 69-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 169-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 62-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 225-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 55-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 211-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 181-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 116-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 71-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 160-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 191-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 50-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 8-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 164-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 18-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 51-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 232-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 63-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 138-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 16-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 57-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 200-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 250-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 36-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 167-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 37-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 124-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 34-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 218-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 243-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 209-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 111-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 90-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 122-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 151-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 45-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 128-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 74-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 11-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 207-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 241-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 2-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 155-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 88-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 5-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 170-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 229-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 222-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 47-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 76-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 35-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 41-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 108-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 104-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 141-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 25-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 87-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 32-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 77-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 93-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 233-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 4-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 24-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 237-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 28-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 238-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 26-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 129-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 223-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 162-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 178-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 46-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 38-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 227-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 179-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 219-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 172-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 58-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 114-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 204-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 120-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 23-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 72-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 189-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 127-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 143-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 82-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 15-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 136-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 184-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 197-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 148-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 231-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 224-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 195-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 39-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 131-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 242-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 186-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 182-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 177-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 157-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 190-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 86-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 150-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 146-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 228-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 144-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 43-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 193-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 59-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 94-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 174-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 64-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 65-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 142-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 247-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 163-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 214-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 206-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 102-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 132-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 168-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 173-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 217-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 212-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 171-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 22-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 29-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 89-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 95-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 239-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 221-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 67-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 154-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 91-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 109-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 66-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 20-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 73-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 40-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 230-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 199-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 52-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 33-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 126-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 194-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 213-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 12-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 192-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 3-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 92-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 196-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 61-A | 201 | FOL | C2-N1-C8A | 3.00 | 118.79 | 115.36 |
| 2 | 125-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 85-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 56-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 187-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 68-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 10-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 149-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 107-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 81-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 6-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 21-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 98-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 165-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 31-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 105-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 180-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 54-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 14-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 145-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 13-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 99-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 83-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 117-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 201-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 48-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 203-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 30-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 156-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 42-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 106-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 205-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 158-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 112-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 220-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 123-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 113-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 118-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 176-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 49-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 44-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 70-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 166-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 188-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 121-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 133-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 7-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 97-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 80-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 17-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 78-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 246-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 101-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 235-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 137-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 115-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 103-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 147-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 75-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 79-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 175-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 245-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 9-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 208-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 19-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 248-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 185-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 152-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 60-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 53-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 226-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 110-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 244-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 134-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 236-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 198-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 183-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 153-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 135-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 202-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 140-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 119-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 240-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 84-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 100-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 27-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 1-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 234-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 130-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 161-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 215-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 210-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 249-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 216-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 139-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 96-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 159-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 69-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 169-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 62-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 225-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 55-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 211-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 181-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 116-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 71-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 160-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 191-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 50-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 8-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 164-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 18-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 51-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 232-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 63-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 138-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 16-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 57-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 200-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 250-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 36-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 167-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 37-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 124-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 34-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 218-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 243-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 209-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 111-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 90-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 122-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 151-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 45-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 128-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 74-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 11-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 207-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 241-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 2-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 155-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 88-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 5-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 170-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 229-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 222-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 47-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 76-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 35-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 41-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 108-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 104-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 141-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 25-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 87-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 32-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 77-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 93-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 233-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 4-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 24-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 237-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 28-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 238-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 26-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 129-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 223-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 162-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 178-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 46-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 38-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 227-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 179-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 219-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 172-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 58-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 114-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 204-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 120-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 23-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 72-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 189-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 127-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 143-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 82-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 15-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 136-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 184-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 197-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 148-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 231-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 224-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 195-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 39-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 131-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|------|-------------|----------|
| 2 | 242-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 186-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 182-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 177-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 157-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 190-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 86-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 150-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 146-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 228-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 144-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 43-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 193-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 59-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 94-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 174-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 64-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 65-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 142-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 247-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 163-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 214-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 206-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 102-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 132-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 168-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 173-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 217-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 212-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 171-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 22-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 29-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 89-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 95-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 239-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 221-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 67-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 154-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 91-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 109-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 66-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 20-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 2 | 73-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 40-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 230-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 199-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 52-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 33-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 126-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 194-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 213-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 12-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 192-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 3-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 92-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 196-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 2 | 61-A | 201 | FOL | CB-CA-N | 2.78 | 114.24 | 110.19 |
| 3 | 34-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 76-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 202-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 174-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 54-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 161-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 129-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 238-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 208-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 119-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 39-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 33-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 12-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 89-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 23-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 5-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 81-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 162-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 107-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 239-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 190-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 215-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 92-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 55-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 82-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 38-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 144-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 186-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 138-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 104-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 149-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 164-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 156-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 48-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 6-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 225-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 30-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 3-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 223-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 96-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 176-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 72-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 154-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 10-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 175-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 127-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 27-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 137-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 243-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 56-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 21-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 87-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 234-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 169-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 241-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 249-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 233-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 182-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 43-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 207-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 20-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 247-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 136-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 51-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 195-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 204-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 211-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 126-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 244-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 68-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 240-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 17-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 66-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 170-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 228-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 14-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 122-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 102-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 22-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 210-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 224-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 171-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 184-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 125-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 44-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 158-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 213-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 113-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 49-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 61-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 242-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 90-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 65-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 111-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 52-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 166-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 152-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 220-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 217-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 245-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 185-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 95-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 4-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 114-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 29-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 32-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 58-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 196-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 201-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 98-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 13-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 16-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 219-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 200-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 120-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 63-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 80-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 106-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 140-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 26-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 157-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 94-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 108-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 91-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 57-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 60-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 143-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 246-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 155-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 86-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 50-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 232-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 177-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 189-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 145-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 198-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 116-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 179-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 117-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 97-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 123-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 71-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 121-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 8-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 167-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 47-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 67-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 15-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 206-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 73-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 194-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 205-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 236-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 151-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 85-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 226-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 75-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 128-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 41-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 230-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 163-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 192-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 172-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 168-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 183-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 135-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 1-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 237-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 62-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 46-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 103-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 31-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 100-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 146-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 173-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 105-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 36-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 59-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 188-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 24-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 118-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 83-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 209-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 132-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 197-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 70-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 79-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 222-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 227-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 148-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 109-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 9-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 40-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 181-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 2-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 77-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 214-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 216-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 187-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 221-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 147-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 248-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 64-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 115-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 124-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 180-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 78-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 178-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 231-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 235-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 141-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 99-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 130-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 142-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 35-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 18-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 165-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 139-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 133-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 159-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 74-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 199-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 93-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 229-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 101-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 112-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 84-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 150-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 7-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 69-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 88-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 193-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 28-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 203-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 250-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 45-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 160-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 53-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 191-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 11-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 110-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 37-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 153-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 212-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 25-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 134-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 19-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 131-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 218-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 42-A | 202 | NAP | C6N-N1N-C2N | -2.63 | 119.58 | 121.97 |
| 3 | 34-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 76-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 202-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 174-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 54-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 161-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 129-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 238-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 208-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 119-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 39-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 33-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 12-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 89-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 23-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 5-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 81-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 162-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 107-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 239-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 190-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 215-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 92-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 55-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 82-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 38-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 144-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 186-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 138-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 104-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 149-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 164-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 156-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 48-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 6-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 225-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 30-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 3-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 223-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 96-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 176-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 72-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 154-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 10-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 175-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 127-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 27-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 137-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 243-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 56-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 21-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 87-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 234-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 169-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 241-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 249-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 233-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 182-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 43-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 207-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 20-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 247-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 136-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 51-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 195-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 204-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 211-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 126-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 244-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 68-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 240-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 17-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 66-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 170-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 228-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 14-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 122-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 102-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 22-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 210-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 224-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 171-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 184-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 125-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 44-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 158-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 213-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 113-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 49-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 61-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 242-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 90-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 65-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 111-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 52-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 166-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 152-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 220-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 217-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 245-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 185-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 95-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 4-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 114-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 29-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 32-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 58-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 196-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 201-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 98-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 13-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 16-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 219-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 200-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 120-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 63-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 80-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 106-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 140-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 26-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 157-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 94-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 108-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 91-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 57-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 60-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 143-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 246-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 155-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 86-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 50-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 232-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 177-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 189-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 145-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 198-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 116-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 179-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 117-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 97-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 123-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 71-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 121-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 8-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 167-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 47-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 67-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 15-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 206-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 73-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 194-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 205-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 236-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 151-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 85-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 226-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 75-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 128-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 41-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 230-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 163-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 192-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 172-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 168-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 183-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 135-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 1-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 237-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 62-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 46-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 103-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 31-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 100-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 146-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 173-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 105-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 36-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 59-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 188-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 24-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 118-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 83-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 209-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 132-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 197-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 70-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 79-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 222-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 227-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 148-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 109-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 9-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 40-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 181-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 2-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 77-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 214-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 216-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 187-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 221-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 147-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 248-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 64-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 115-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 124-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 180-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 78-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 178-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 231-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 235-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 141-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 99-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 130-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 142-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 35-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 18-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 165-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 139-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 133-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 159-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 74-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 199-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 93-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 229-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 101-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 112-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 84-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 150-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 7-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 69-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 88-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 193-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 28-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 203-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 250-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 45-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 160-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 53-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 191-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 11-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 110-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 37-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 153-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 212-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 25-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 134-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 19-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 131-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 218-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 3 | 42-A | 202 | NAP | O5D-PN-O1N | 2.43 | 118.55 | 109.07 |
| 2 | 125-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 85-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 56-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 187-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 68-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 10-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 149-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 107-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 81-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 6-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 21-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 98-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 165-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 31-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 105-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 180-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 54-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 14-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 145-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 13-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 99-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 83-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 117-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 201-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 48-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 203-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 30-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 156-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 42-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 106-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 205-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 158-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 112-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 220-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 123-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 113-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 118-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 176-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 49-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 44-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 70-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 166-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 188-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 121-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 133-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 7-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 97-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 80-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 17-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 78-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 246-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 101-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 235-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 137-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 115-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 103-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 147-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 75-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 79-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 175-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 245-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 9-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 208-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 19-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 248-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 185-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 152-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 60-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 53-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 226-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 110-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 244-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 134-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 236-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 198-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 183-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 153-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 135-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 202-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 140-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 119-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 240-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 84-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 100-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 27-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 1-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 234-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 130-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 161-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 215-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 210-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 249-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 216-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 139-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 96-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 159-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 69-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 169-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 62-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 225-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 55-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 211-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 181-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 116-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 71-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 160-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 191-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 50-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 8-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 164-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 18-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 51-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 232-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 63-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 138-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 16-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 57-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 200-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 250-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 36-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 167-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 37-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 124-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 34-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 218-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 243-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 209-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 111-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 90-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 122-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 151-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 45-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 128-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 74-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 11-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 207-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 241-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 2-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 155-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 88-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 5-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 170-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 229-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 222-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 47-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 76-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 35-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 41-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 108-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 104-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 141-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 25-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 87-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 32-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 77-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 93-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 233-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 4-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 24-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 237-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 28-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 238-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 26-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 129-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 223-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 162-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 178-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 46-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 38-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 227-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 179-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 219-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 172-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 58-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 114-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 204-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 120-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 23-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 72-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 189-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 127-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 143-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 82-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 15-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 136-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 184-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 197-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 148-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 231-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 224-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 195-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 39-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 131-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 242-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 186-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 182-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 177-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 157-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 190-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|------|-------------|----------|
| 2 | 86-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 150-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 146-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 228-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 144-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 43-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 193-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 59-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 94-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 174-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 64-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 65-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 142-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 247-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 163-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 214-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 206-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 102-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 132-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 168-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 173-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 217-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 212-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 171-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 22-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 29-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 89-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 95-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 239-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 221-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 67-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 154-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 91-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 109-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 66-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 20-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 73-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 40-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 230-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 199-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 52-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 33-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 2 | 126-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 194-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 213-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 12-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 192-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 3-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 92-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 196-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 2 | 61-A | 201 | FOL | C7-N8-C8A | 2.39 | 119.10 | 116.69 |
| 3 | 34-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 76-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 202-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 174-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 54-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 161-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 129-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 238-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 208-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 119-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 39-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 33-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 12-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 89-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 23-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 5-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 81-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 162-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 107-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 239-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 190-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 215-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 92-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 55-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 82-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 38-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 144-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 186-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 138-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 104-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 149-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 164-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 156-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 48-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 6-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 225-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 30-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 3-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 223-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 96-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 176-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 72-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 154-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 10-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 175-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 127-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 27-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 137-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 243-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 56-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 21-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 87-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 234-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 169-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 241-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 249-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 233-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 182-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 43-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 207-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 20-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 247-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 136-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 51-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 195-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 204-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 211-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 126-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 244-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 68-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 240-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 17-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 66-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 170-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 228-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 14-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 122-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 102-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 22-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 210-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 224-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 171-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 184-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 125-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 44-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 158-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 213-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 113-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 49-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 61-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 242-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 90-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 65-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 111-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 52-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 166-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 152-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 220-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 217-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 245-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 185-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 95-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 4-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 114-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 29-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 32-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 58-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 196-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 201-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 98-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 13-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 16-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 219-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 200-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 120-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 63-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 80-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 106-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 140-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 26-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 157-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 94-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 108-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 91-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 57-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 60-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 143-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 246-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 155-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 86-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 50-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 232-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 177-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 189-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 145-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 198-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 116-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 179-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 117-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 97-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 123-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 71-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 121-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 8-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 167-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 47-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 67-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 15-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 206-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 73-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 194-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 205-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 236-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 151-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 85-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 226-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 75-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 128-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 41-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 230-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 163-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 192-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 172-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 168-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 183-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 135-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 1-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 237-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 62-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 46-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 103-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 31-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 100-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 146-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 173-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 105-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 36-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 59-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 188-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 24-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 118-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 83-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 209-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 132-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 197-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 70-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 79-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 222-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 227-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 148-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 109-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 9-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 40-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 181-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 2-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 77-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 214-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 216-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 187-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 221-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 147-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 3 | 248-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 64-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 115-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 124-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 180-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 78-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 178-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 231-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 235-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 141-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 99-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 130-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 142-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 35-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 18-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 165-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 139-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 133-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 159-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 74-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 199-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 93-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 229-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 101-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 112-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 84-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 150-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 7-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 69-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 88-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 193-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 28-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 203-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 250-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 45-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 160-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 53-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 191-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 11-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 110-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 37-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 153-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 212-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 25-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 134-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 19-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 131-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 218-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 42-A | 202 | NAP | C2N-C3N-C4N | 2.35 | 120.92 | 118.26 |
| 3 | 34-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 76-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 202-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 174-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 54-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 161-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 129-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 238-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 208-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 119-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 39-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 33-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 12-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 89-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 23-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 5-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 81-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 162-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 107-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 239-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 190-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 215-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 92-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 55-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 82-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 38-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 144-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 186-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 138-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 104-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 149-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 164-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 156-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 48-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 6-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 225-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 30-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 3-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 223-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 96-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 176-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 72-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 154-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 10-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 175-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 127-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 27-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 137-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 243-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 56-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 21-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 87-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 234-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 169-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 241-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 249-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 233-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 182-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 43-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 207-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 20-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 247-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 136-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 51-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 195-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 204-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 211-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 126-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 244-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 68-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 240-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 17-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 66-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 170-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 228-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 14-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 122-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 102-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 22-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 210-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 224-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 171-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 184-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 125-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 44-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 158-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 213-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 113-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 49-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 61-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 242-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 90-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 65-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 111-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 52-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 166-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 152-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 220-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 217-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 245-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 185-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 95-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 4-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 114-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 29-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 32-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 58-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 196-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 201-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 98-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 13-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 16-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 219-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 200-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 120-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 63-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 80-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 106-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 140-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 26-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 157-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 94-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 108-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 91-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 57-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 60-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 143-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 246-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 155-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 86-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 50-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 232-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 177-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 189-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 145-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 198-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 116-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 179-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 117-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 97-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 123-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 71-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 121-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 8-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 167-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 47-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 67-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 15-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 206-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 73-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 194-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 205-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 236-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 151-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 85-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 226-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 75-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 128-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 41-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 230-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 163-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 192-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 172-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 168-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 183-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 135-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 1-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 237-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 62-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 46-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 103-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 31-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 100-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 146-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 173-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 105-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 36-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 59-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 188-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 24-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 118-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 83-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 209-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 132-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 197-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 70-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 79-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 222-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 227-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 148-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 109-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 9-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 40-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 181-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 2-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 77-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 214-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 216-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 187-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 221-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 147-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 248-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 64-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 115-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 124-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 180-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 78-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 178-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 231-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 235-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 141-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 99-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 130-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 142-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 35-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 18-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 165-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 139-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 133-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 159-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 74-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 199-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 93-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 229-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 101-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 112-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 84-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 150-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 7-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 69-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 88-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 193-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 28-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 203-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 250-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 45-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 160-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 53-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 191-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 11-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 110-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 37-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 153-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 212-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 25-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 3 | 134-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 19-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 131-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 218-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 42-A | 202 | NAP | N3A-C2A-N1A | -2.34 | 125.02 | 128.68 |
| 3 | 34-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 76-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 202-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 174-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 54-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 161-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 129-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 238-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 208-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 119-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 39-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 33-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 12-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 89-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 23-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 5-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 81-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 162-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 107-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 239-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 190-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 215-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 92-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 55-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 82-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 38-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 144-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 186-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 138-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 104-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 149-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 164-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 156-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 48-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 6-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 225-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 30-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 3-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 223-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 96-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 176-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 72-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 154-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 10-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 175-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 127-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 27-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 137-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 243-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 56-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 21-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 87-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 234-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 169-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 241-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 249-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 233-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 182-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 43-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 207-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 20-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 247-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 136-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 51-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 195-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 204-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 211-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 126-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 244-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 68-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 240-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 17-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 66-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 170-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 228-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 14-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 122-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 102-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 22-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |

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Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 210-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 224-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 171-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 184-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 125-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 44-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 158-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 213-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 113-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 49-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 61-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 242-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 90-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 65-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 111-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 52-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 166-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 152-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 220-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 217-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 245-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 185-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 95-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 4-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 114-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 29-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 32-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 58-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 196-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 201-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 98-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 13-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 16-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 219-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 200-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 120-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 63-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 80-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 106-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 140-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 26-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 157-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 94-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 108-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 91-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 57-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 60-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 143-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 246-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 155-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 86-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 50-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 232-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 177-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 189-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 145-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 198-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 116-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 179-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 117-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 97-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 123-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 71-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 121-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 8-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 167-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 47-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 67-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 15-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 206-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 73-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 194-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 205-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 236-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 151-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 85-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 226-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 75-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 128-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 41-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 230-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 163-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 192-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 172-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 168-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 183-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 135-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 1-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 237-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 62-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 46-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 103-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 31-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 100-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 146-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 173-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 105-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 36-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 59-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 188-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 24-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 118-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 83-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 209-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 132-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 197-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 70-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 79-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 222-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 227-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 148-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 109-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 9-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 40-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 181-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 2-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 77-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 214-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 216-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 187-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 221-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 147-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 248-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 64-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 115-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 124-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 180-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 78-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 178-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 231-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 235-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 141-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 99-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 130-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 142-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 35-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 18-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 165-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 139-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 133-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 159-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 74-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 199-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 93-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 229-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 101-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 112-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 84-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 150-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 7-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 69-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 88-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 193-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 28-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 203-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 250-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 45-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 160-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 53-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 191-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 11-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 110-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 37-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 153-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 212-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 25-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 134-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 19-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|------|-------------|----------|
| 3 | 131-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 218-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |
| 3 | 42-A | 202 | NAP | O2A-PA-O1A | 2.23 | 123.29 | 112.24 |

All (40) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3 | 238-A | 202 | NAP | C3B |
| 3 | 119-A | 202 | NAP | C3B |
| 3 | 239-A | 202 | NAP | C3B |
| 3 | 55-A | 202 | NAP | C3B |
| 3 | 164-A | 202 | NAP | C3B |
| 3 | 30-A | 202 | NAP | C3B |
| 3 | 223-A | 202 | NAP | C3B |
| 3 | 96-A | 202 | NAP | C3B |
| 3 | 154-A | 202 | NAP | C3B |
| 3 | 213-A | 202 | NAP | C3B |
| 3 | 95-A | 202 | NAP | C3B |
| 3 | 29-A | 202 | NAP | C3B |
| 3 | 120-A | 202 | NAP | C3B |
| 3 | 63-A | 202 | NAP | C3B |
| 3 | 143-A | 202 | NAP | C3B |
| 3 | 179-A | 202 | NAP | C3B |
| 3 | 205-A | 202 | NAP | C3B |
| 3 | 236-A | 202 | NAP | C3B |
| 3 | 85-A | 202 | NAP | C3B |
| 3 | 41-A | 202 | NAP | C3B |
| 3 | 163-A | 202 | NAP | C3B |
| 3 | 192-A | 202 | NAP | C3B |
| 3 | 1-A | 202 | NAP | C3B |
| 3 | 237-A | 202 | NAP | C3B |
| 3 | 62-A | 202 | NAP | C3B |
| 3 | 103-A | 202 | NAP | C3B |
| 3 | 118-A | 202 | NAP | C3B |
| 3 | 132-A | 202 | NAP | C3B |
| 3 | 222-A | 202 | NAP | C3B |
| 3 | 109-A | 202 | NAP | C3B |
| 3 | 2-A | 202 | NAP | C3B |
| 3 | 178-A | 202 | NAP | C3B |
| 3 | 235-A | 202 | NAP | C3B |
| 3 | 141-A | 202 | NAP | C3B |
| 3 | 142-A | 202 | NAP | C3B |

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| Mol | Chain | Res | Type | Atom |
|-----|-------|-----|------|------|
| 3 | 18-A | 202 | NAP | C3B |
| 3 | 74-A | 202 | NAP | C3B |
| 3 | 45-A | 202 | NAP | C3B |
| 3 | 191-A | 202 | NAP | C3B |
| 3 | 212-A | 202 | NAP | C3B |

All (2000) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 125-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 125-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 34-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 34-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 76-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 76-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 202-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 202-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 85-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 85-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 174-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 174-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 56-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 56-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 54-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 54-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 187-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 187-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 68-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 68-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 10-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 10-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 149-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 149-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 161-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 161-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 107-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 107-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 81-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 81-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 129-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 129-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 6-A | 201 | FOL | CT-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 6-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 21-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 21-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 238-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 238-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 98-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 98-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 208-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 208-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 165-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 165-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 31-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 31-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 119-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 119-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 105-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 105-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 39-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 39-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 33-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 33-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 180-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 180-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 54-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 54-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 14-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 14-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 12-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 12-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 145-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 145-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 13-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 13-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 99-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 99-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 83-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 83-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 89-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 89-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 117-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 117-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 201-A | 201 | FOL | CT-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 201-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 23-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 23-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 5-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 5-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 48-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 48-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 203-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 203-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 81-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 81-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 30-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 30-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 156-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 156-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 162-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 162-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 107-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 107-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 42-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 42-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 239-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 239-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 190-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 190-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 106-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 106-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 205-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 205-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 158-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 158-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 112-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 112-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 215-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 215-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 220-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 220-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 92-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 92-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 55-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 55-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 123-A | 201 | FOL | CT-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 123-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 113-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 113-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 118-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 118-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 82-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 82-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 38-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 38-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 176-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 176-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 144-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 144-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 49-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 49-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 44-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 44-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 70-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 70-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 166-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 166-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 186-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 186-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 138-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 138-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 104-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 104-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 149-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 149-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 164-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 164-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 156-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 156-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 188-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 188-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 121-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 121-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 48-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 48-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 133-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 133-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 6-A | 202 | NAP | C5D-O5D-PN-O2N |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 6-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 7-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 7-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 225-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 225-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 30-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 30-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 97-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 97-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 3-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 3-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 80-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 80-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 223-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 223-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 17-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 17-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 96-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 96-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 78-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 78-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 246-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 246-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 101-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 101-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 176-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 176-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 72-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 72-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 235-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 235-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 154-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 154-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 10-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 10-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 175-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 175-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 127-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 127-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 27-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 27-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 137-A | 202 | NAP | C5D-O5D-PN-O2N |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 137-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 137-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 137-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 115-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 115-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 103-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 103-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 147-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 147-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 75-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 75-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 243-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 243-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 56-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 56-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 79-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 79-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 175-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 175-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 21-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 21-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 87-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 87-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 234-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 234-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 169-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 169-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 241-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 241-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 245-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 245-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 9-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 9-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 249-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 249-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 208-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 208-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 19-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 19-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 233-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 233-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 182-A | 202 | NAP | C5D-O5D-PN-O2N |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 182-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 43-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 43-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 207-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 207-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 20-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 20-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 248-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 248-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 247-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 247-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 185-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 185-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 136-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 136-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 152-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 152-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 60-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 60-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 51-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 51-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 53-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 53-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 226-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 226-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 195-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 195-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 204-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 204-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 110-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 110-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 211-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 211-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 126-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 126-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 244-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 244-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 134-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 134-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 236-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 236-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 198-A | 201 | FOL | CT-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 198-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 244-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 244-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 183-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 183-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 153-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 153-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 135-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 135-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 68-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 68-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 240-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 240-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 202-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 202-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 140-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 140-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 17-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 17-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 119-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 119-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 240-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 240-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 66-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 66-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 84-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 84-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 100-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 100-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 27-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 27-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 170-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 170-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 1-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 1-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 228-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 228-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 14-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 14-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 234-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 234-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 130-A | 201 | FOL | CT-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 130-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 161-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 161-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 122-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 122-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 102-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 102-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 215-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 215-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 210-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 210-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 22-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 22-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 249-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 249-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 216-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 216-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 139-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 139-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 96-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 96-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 210-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 210-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 224-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 224-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 171-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 171-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 184-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 184-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 125-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 125-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 159-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 159-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 44-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 44-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 158-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 158-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 69-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 69-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 213-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 213-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 169-A | 201 | FOL | CT-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 169-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 62-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 62-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 113-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 113-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 49-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 49-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 225-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 225-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 55-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 55-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 61-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 61-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 242-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 242-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 211-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 211-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 181-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 181-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 116-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 116-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 71-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 71-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 90-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 90-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 65-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 65-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 111-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 111-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 52-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 52-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 160-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 160-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 166-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 166-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 191-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 191-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 152-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 152-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 220-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 220-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 50-A | 201 | FOL | CT-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 50-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 8-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 8-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 164-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 164-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 217-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 217-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 18-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 18-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 51-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 51-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 245-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 245-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 185-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 185-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 95-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 95-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 232-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 232-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 4-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 4-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 114-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 114-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 29-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 29-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 32-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 32-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 58-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 58-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 63-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 63-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 196-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 196-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 138-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 138-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 16-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 16-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 57-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 57-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 200-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 200-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 201-A | 202 | NAP | C5D-O5D-PN-O2N |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 201-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 250-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 250-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 98-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 98-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 36-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 36-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 13-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 13-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 16-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 16-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 219-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 219-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 200-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 200-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 167-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 167-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 37-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 37-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 124-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 124-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 120-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 120-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 63-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 63-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 80-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 80-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 34-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 34-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 106-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 106-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 140-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 140-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 218-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 218-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 26-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 26-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 243-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 243-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 157-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 157-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 94-A | 202 | NAP | C5D-O5D-PN-O2N |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 94-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 108-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 108-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 91-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 91-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 209-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 209-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 57-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 57-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 111-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 111-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 60-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 60-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 90-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 90-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 143-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 143-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 246-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 246-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 155-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 155-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 122-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 122-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 151-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 151-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 86-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 86-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 50-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 50-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 45-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 45-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 232-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 232-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 128-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 128-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 74-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 74-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 11-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 11-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 177-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 177-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 207-A | 201 | FOL | CT-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 207-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 241-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 241-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 189-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 189-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 145-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 145-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 198-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 198-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 116-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 116-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 2-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 2-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 155-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 155-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 88-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 88-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 179-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 179-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 5-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 5-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 170-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 170-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 117-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 117-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 97-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 97-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 229-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 229-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 222-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 222-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 47-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 47-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 76-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 76-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 35-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 35-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 123-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 123-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 41-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 41-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 108-A | 201 | FOL | CT-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 108-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 71-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 71-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 104-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 104-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 121-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 121-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 8-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 8-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 167-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 167-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 47-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 47-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 67-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 67-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 141-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 141-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 15-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 15-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 25-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 25-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 87-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 87-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 32-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 32-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 206-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 206-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 73-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 73-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 194-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 194-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 77-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 77-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 205-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 205-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 236-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 236-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 151-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 151-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 93-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 93-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 85-A | 202 | NAP | C5D-O5D-PN-O2N |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 85-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 233-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 233-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 4-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 4-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 24-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 24-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 237-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 237-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 226-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 226-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 75-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 75-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 28-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 28-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 128-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 128-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 238-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 238-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 26-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 26-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 129-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 129-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 223-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 223-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 41-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 41-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 230-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 230-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 162-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 162-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 178-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 178-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 46-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 46-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 38-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 38-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 163-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 163-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 227-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 227-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 179-A | 201 | FOL | CT-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 179-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 192-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 192-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 219-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 219-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 172-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 172-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 172-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 172-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 58-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 58-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 168-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 168-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 183-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 183-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 114-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 114-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 204-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 204-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 120-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 120-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 23-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 23-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 72-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 72-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 135-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 135-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 189-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 189-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 127-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 127-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 143-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 143-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 1-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 1-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 237-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 237-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 62-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 62-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 46-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 46-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 82-A | 201 | FOL | CT-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 82-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 15-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 15-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 103-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 103-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 31-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 31-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 136-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 136-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 184-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 184-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 100-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 100-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 146-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 146-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 173-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 173-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 197-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 197-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 105-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 105-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 36-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 36-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 148-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 148-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 59-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 59-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 188-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 188-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 24-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 24-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 118-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 118-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 231-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 231-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 224-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 224-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 83-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 83-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 195-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 195-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 39-A | 201 | FOL | CT-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 39-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 131-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 131-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 209-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 209-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 242-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 242-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 132-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 132-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 197-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 197-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 186-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 186-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 182-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 182-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 70-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 70-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 79-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 79-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 177-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 177-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 222-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 222-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 227-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 227-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 148-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 148-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 157-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 157-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 190-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 190-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 109-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 109-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 9-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 9-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 40-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 40-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 181-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 181-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 2-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 2-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 77-A | 202 | NAP | C5D-O5D-PN-O2N |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 77-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 86-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 86-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 214-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 214-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 150-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 150-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 216-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 216-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 146-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 146-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 228-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 228-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 187-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 187-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 144-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 144-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 43-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 43-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 193-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 193-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 221-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 221-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 147-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 147-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 59-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 59-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 248-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 248-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 94-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 94-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 174-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 174-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 64-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 64-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 64-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 64-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 115-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 115-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 65-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 65-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 124-A | 202 | NAP | C5D-O5D-PN-O2N |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 124-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 142-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 142-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 247-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 247-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 180-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 180-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 78-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 78-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 163-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 163-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 214-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 214-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 178-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 178-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 206-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 206-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 102-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 102-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 231-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 231-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 235-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 235-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 141-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 141-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 132-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 132-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 168-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 168-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 99-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 99-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 173-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 173-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 130-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 130-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 142-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 142-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 217-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 217-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 212-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 212-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 171-A | 201 | FOL | CT-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 171-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 35-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 35-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 22-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 22-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 29-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 29-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 18-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 18-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 89-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 89-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 165-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 165-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 139-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 139-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 133-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 133-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 95-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 95-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 159-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 159-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 239-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 239-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 74-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 74-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 199-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 199-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 93-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 93-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 229-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 229-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 221-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 221-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 67-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 67-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 154-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 154-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 101-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 101-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 112-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 112-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 84-A | 202 | NAP | C5D-O5D-PN-O2N |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 84-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 91-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 91-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 109-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 109-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 66-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 66-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 20-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 20-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 150-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 150-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 7-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 7-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 69-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 69-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 88-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 88-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 193-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 193-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 73-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 73-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 28-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 28-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 40-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 40-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 203-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 203-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 230-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 230-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 250-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 250-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 199-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 199-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 52-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 52-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 45-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 45-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 160-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 160-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 53-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 53-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 33-A | 201 | FOL | CT-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 2 | 33-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 191-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 191-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 126-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 126-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 11-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 11-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 110-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 110-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 37-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 37-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 153-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 153-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 212-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 212-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 25-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 25-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 194-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 194-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 213-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 213-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 12-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 12-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 134-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 134-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 19-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 19-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 192-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 192-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 3-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 3-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 92-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 92-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 131-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 131-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 3 | 218-A | 202 | NAP | C5D-O5D-PN-O2N |
| 3 | 218-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 196-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 196-A | 201 | FOL | CA-CB-CG-CD |
| 2 | 61-A | 201 | FOL | CT-CA-CB-CG |
| 2 | 61-A | 201 | FOL | CA-CB-CG-CD |
| 3 | 42-A | 202 | NAP | C5D-O5D-PN-O2N |

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| Mol | Chain | Res | Type | Atoms |
|------------|--------------|------------|-------------|-----------------|
| 3 | 42-A | 202 | NAP | O4D-C1D-N1N-C6N |
| 2 | 125-A | 201 | FOL | N-CA-CB-CG |
| 2 | 85-A | 201 | FOL | N-CA-CB-CG |
| 2 | 56-A | 201 | FOL | N-CA-CB-CG |
| 2 | 187-A | 201 | FOL | N-CA-CB-CG |
| 2 | 68-A | 201 | FOL | N-CA-CB-CG |
| 2 | 10-A | 201 | FOL | N-CA-CB-CG |
| 2 | 149-A | 201 | FOL | N-CA-CB-CG |
| 2 | 107-A | 201 | FOL | N-CA-CB-CG |
| 2 | 81-A | 201 | FOL | N-CA-CB-CG |
| 2 | 6-A | 201 | FOL | N-CA-CB-CG |
| 2 | 21-A | 201 | FOL | N-CA-CB-CG |
| 2 | 98-A | 201 | FOL | N-CA-CB-CG |
| 2 | 165-A | 201 | FOL | N-CA-CB-CG |
| 2 | 31-A | 201 | FOL | N-CA-CB-CG |
| 2 | 105-A | 201 | FOL | N-CA-CB-CG |
| 2 | 180-A | 201 | FOL | N-CA-CB-CG |
| 2 | 54-A | 201 | FOL | N-CA-CB-CG |
| 2 | 14-A | 201 | FOL | N-CA-CB-CG |
| 2 | 145-A | 201 | FOL | N-CA-CB-CG |
| 2 | 13-A | 201 | FOL | N-CA-CB-CG |
| 2 | 99-A | 201 | FOL | N-CA-CB-CG |
| 2 | 83-A | 201 | FOL | N-CA-CB-CG |
| 2 | 117-A | 201 | FOL | N-CA-CB-CG |
| 2 | 201-A | 201 | FOL | N-CA-CB-CG |
| 2 | 48-A | 201 | FOL | N-CA-CB-CG |
| 2 | 203-A | 201 | FOL | N-CA-CB-CG |
| 2 | 30-A | 201 | FOL | N-CA-CB-CG |
| 2 | 156-A | 201 | FOL | N-CA-CB-CG |
| 2 | 42-A | 201 | FOL | N-CA-CB-CG |
| 2 | 106-A | 201 | FOL | N-CA-CB-CG |
| 2 | 205-A | 201 | FOL | N-CA-CB-CG |
| 2 | 158-A | 201 | FOL | N-CA-CB-CG |
| 2 | 112-A | 201 | FOL | N-CA-CB-CG |
| 2 | 220-A | 201 | FOL | N-CA-CB-CG |
| 2 | 123-A | 201 | FOL | N-CA-CB-CG |
| 2 | 113-A | 201 | FOL | N-CA-CB-CG |
| 2 | 118-A | 201 | FOL | N-CA-CB-CG |
| 2 | 176-A | 201 | FOL | N-CA-CB-CG |
| 2 | 49-A | 201 | FOL | N-CA-CB-CG |
| 2 | 44-A | 201 | FOL | N-CA-CB-CG |
| 2 | 70-A | 201 | FOL | N-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|------------|
| 2 | 166-A | 201 | FOL | N-CA-CB-CG |
| 2 | 188-A | 201 | FOL | N-CA-CB-CG |
| 2 | 121-A | 201 | FOL | N-CA-CB-CG |
| 2 | 133-A | 201 | FOL | N-CA-CB-CG |
| 2 | 7-A | 201 | FOL | N-CA-CB-CG |
| 2 | 97-A | 201 | FOL | N-CA-CB-CG |
| 2 | 80-A | 201 | FOL | N-CA-CB-CG |
| 2 | 17-A | 201 | FOL | N-CA-CB-CG |
| 2 | 78-A | 201 | FOL | N-CA-CB-CG |
| 2 | 246-A | 201 | FOL | N-CA-CB-CG |
| 2 | 101-A | 201 | FOL | N-CA-CB-CG |
| 2 | 235-A | 201 | FOL | N-CA-CB-CG |
| 2 | 137-A | 201 | FOL | N-CA-CB-CG |
| 2 | 115-A | 201 | FOL | N-CA-CB-CG |
| 2 | 103-A | 201 | FOL | N-CA-CB-CG |
| 2 | 147-A | 201 | FOL | N-CA-CB-CG |
| 2 | 75-A | 201 | FOL | N-CA-CB-CG |
| 2 | 79-A | 201 | FOL | N-CA-CB-CG |
| 2 | 175-A | 201 | FOL | N-CA-CB-CG |
| 2 | 245-A | 201 | FOL | N-CA-CB-CG |
| 2 | 9-A | 201 | FOL | N-CA-CB-CG |
| 2 | 208-A | 201 | FOL | N-CA-CB-CG |
| 2 | 19-A | 201 | FOL | N-CA-CB-CG |
| 2 | 248-A | 201 | FOL | N-CA-CB-CG |
| 2 | 185-A | 201 | FOL | N-CA-CB-CG |
| 2 | 152-A | 201 | FOL | N-CA-CB-CG |
| 2 | 60-A | 201 | FOL | N-CA-CB-CG |
| 2 | 53-A | 201 | FOL | N-CA-CB-CG |
| 2 | 226-A | 201 | FOL | N-CA-CB-CG |
| 2 | 110-A | 201 | FOL | N-CA-CB-CG |
| 2 | 244-A | 201 | FOL | N-CA-CB-CG |
| 2 | 134-A | 201 | FOL | N-CA-CB-CG |
| 2 | 236-A | 201 | FOL | N-CA-CB-CG |
| 2 | 198-A | 201 | FOL | N-CA-CB-CG |
| 2 | 183-A | 201 | FOL | N-CA-CB-CG |
| 2 | 153-A | 201 | FOL | N-CA-CB-CG |
| 2 | 135-A | 201 | FOL | N-CA-CB-CG |
| 2 | 202-A | 201 | FOL | N-CA-CB-CG |
| 2 | 140-A | 201 | FOL | N-CA-CB-CG |
| 2 | 119-A | 201 | FOL | N-CA-CB-CG |
| 2 | 240-A | 201 | FOL | N-CA-CB-CG |
| 2 | 84-A | 201 | FOL | N-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|------------|--------------|------------|-------------|--------------|
| 2 | 100-A | 201 | FOL | N-CA-CB-CG |
| 2 | 27-A | 201 | FOL | N-CA-CB-CG |
| 2 | 1-A | 201 | FOL | N-CA-CB-CG |
| 2 | 234-A | 201 | FOL | N-CA-CB-CG |
| 2 | 130-A | 201 | FOL | N-CA-CB-CG |
| 2 | 161-A | 201 | FOL | N-CA-CB-CG |
| 2 | 215-A | 201 | FOL | N-CA-CB-CG |
| 2 | 210-A | 201 | FOL | N-CA-CB-CG |
| 2 | 249-A | 201 | FOL | N-CA-CB-CG |
| 2 | 216-A | 201 | FOL | N-CA-CB-CG |
| 2 | 139-A | 201 | FOL | N-CA-CB-CG |
| 2 | 96-A | 201 | FOL | N-CA-CB-CG |
| 2 | 159-A | 201 | FOL | N-CA-CB-CG |
| 2 | 69-A | 201 | FOL | N-CA-CB-CG |
| 2 | 169-A | 201 | FOL | N-CA-CB-CG |
| 2 | 62-A | 201 | FOL | N-CA-CB-CG |
| 2 | 225-A | 201 | FOL | N-CA-CB-CG |
| 2 | 55-A | 201 | FOL | N-CA-CB-CG |
| 2 | 211-A | 201 | FOL | N-CA-CB-CG |
| 2 | 181-A | 201 | FOL | N-CA-CB-CG |
| 2 | 116-A | 201 | FOL | N-CA-CB-CG |
| 2 | 71-A | 201 | FOL | N-CA-CB-CG |
| 2 | 160-A | 201 | FOL | N-CA-CB-CG |
| 2 | 191-A | 201 | FOL | N-CA-CB-CG |
| 2 | 50-A | 201 | FOL | N-CA-CB-CG |
| 2 | 8-A | 201 | FOL | N-CA-CB-CG |
| 2 | 164-A | 201 | FOL | N-CA-CB-CG |
| 2 | 18-A | 201 | FOL | N-CA-CB-CG |
| 2 | 51-A | 201 | FOL | N-CA-CB-CG |
| 2 | 232-A | 201 | FOL | N-CA-CB-CG |
| 2 | 63-A | 201 | FOL | N-CA-CB-CG |
| 2 | 138-A | 201 | FOL | N-CA-CB-CG |
| 2 | 16-A | 201 | FOL | N-CA-CB-CG |
| 2 | 57-A | 201 | FOL | N-CA-CB-CG |
| 2 | 200-A | 201 | FOL | N-CA-CB-CG |
| 2 | 250-A | 201 | FOL | N-CA-CB-CG |
| 2 | 36-A | 201 | FOL | N-CA-CB-CG |
| 2 | 167-A | 201 | FOL | N-CA-CB-CG |
| 2 | 37-A | 201 | FOL | N-CA-CB-CG |
| 2 | 124-A | 201 | FOL | N-CA-CB-CG |
| 2 | 34-A | 201 | FOL | N-CA-CB-CG |
| 2 | 218-A | 201 | FOL | N-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|------------|
| 2 | 243-A | 201 | FOL | N-CA-CB-CG |
| 2 | 209-A | 201 | FOL | N-CA-CB-CG |
| 2 | 111-A | 201 | FOL | N-CA-CB-CG |
| 2 | 90-A | 201 | FOL | N-CA-CB-CG |
| 2 | 122-A | 201 | FOL | N-CA-CB-CG |
| 2 | 151-A | 201 | FOL | N-CA-CB-CG |
| 2 | 45-A | 201 | FOL | N-CA-CB-CG |
| 2 | 128-A | 201 | FOL | N-CA-CB-CG |
| 2 | 74-A | 201 | FOL | N-CA-CB-CG |
| 2 | 11-A | 201 | FOL | N-CA-CB-CG |
| 2 | 207-A | 201 | FOL | N-CA-CB-CG |
| 2 | 241-A | 201 | FOL | N-CA-CB-CG |
| 2 | 2-A | 201 | FOL | N-CA-CB-CG |
| 2 | 155-A | 201 | FOL | N-CA-CB-CG |
| 2 | 88-A | 201 | FOL | N-CA-CB-CG |
| 2 | 5-A | 201 | FOL | N-CA-CB-CG |
| 2 | 170-A | 201 | FOL | N-CA-CB-CG |
| 2 | 229-A | 201 | FOL | N-CA-CB-CG |
| 2 | 222-A | 201 | FOL | N-CA-CB-CG |
| 2 | 47-A | 201 | FOL | N-CA-CB-CG |
| 2 | 76-A | 201 | FOL | N-CA-CB-CG |
| 2 | 35-A | 201 | FOL | N-CA-CB-CG |
| 2 | 41-A | 201 | FOL | N-CA-CB-CG |
| 2 | 108-A | 201 | FOL | N-CA-CB-CG |
| 2 | 104-A | 201 | FOL | N-CA-CB-CG |
| 2 | 141-A | 201 | FOL | N-CA-CB-CG |
| 2 | 25-A | 201 | FOL | N-CA-CB-CG |
| 2 | 87-A | 201 | FOL | N-CA-CB-CG |
| 2 | 32-A | 201 | FOL | N-CA-CB-CG |
| 2 | 77-A | 201 | FOL | N-CA-CB-CG |
| 2 | 93-A | 201 | FOL | N-CA-CB-CG |
| 2 | 233-A | 201 | FOL | N-CA-CB-CG |
| 2 | 4-A | 201 | FOL | N-CA-CB-CG |
| 2 | 24-A | 201 | FOL | N-CA-CB-CG |
| 2 | 237-A | 201 | FOL | N-CA-CB-CG |
| 2 | 28-A | 201 | FOL | N-CA-CB-CG |
| 2 | 238-A | 201 | FOL | N-CA-CB-CG |
| 2 | 26-A | 201 | FOL | N-CA-CB-CG |
| 2 | 129-A | 201 | FOL | N-CA-CB-CG |
| 2 | 223-A | 201 | FOL | N-CA-CB-CG |
| 2 | 162-A | 201 | FOL | N-CA-CB-CG |
| 2 | 178-A | 201 | FOL | N-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|------------|
| 2 | 46-A | 201 | FOL | N-CA-CB-CG |
| 2 | 38-A | 201 | FOL | N-CA-CB-CG |
| 2 | 227-A | 201 | FOL | N-CA-CB-CG |
| 2 | 179-A | 201 | FOL | N-CA-CB-CG |
| 2 | 219-A | 201 | FOL | N-CA-CB-CG |
| 2 | 172-A | 201 | FOL | N-CA-CB-CG |
| 2 | 58-A | 201 | FOL | N-CA-CB-CG |
| 2 | 114-A | 201 | FOL | N-CA-CB-CG |
| 2 | 204-A | 201 | FOL | N-CA-CB-CG |
| 2 | 120-A | 201 | FOL | N-CA-CB-CG |
| 2 | 23-A | 201 | FOL | N-CA-CB-CG |
| 2 | 72-A | 201 | FOL | N-CA-CB-CG |
| 2 | 189-A | 201 | FOL | N-CA-CB-CG |
| 2 | 127-A | 201 | FOL | N-CA-CB-CG |
| 2 | 143-A | 201 | FOL | N-CA-CB-CG |
| 2 | 82-A | 201 | FOL | N-CA-CB-CG |
| 2 | 15-A | 201 | FOL | N-CA-CB-CG |
| 2 | 136-A | 201 | FOL | N-CA-CB-CG |
| 2 | 184-A | 201 | FOL | N-CA-CB-CG |
| 2 | 197-A | 201 | FOL | N-CA-CB-CG |
| 2 | 148-A | 201 | FOL | N-CA-CB-CG |
| 2 | 231-A | 201 | FOL | N-CA-CB-CG |
| 2 | 224-A | 201 | FOL | N-CA-CB-CG |
| 2 | 195-A | 201 | FOL | N-CA-CB-CG |
| 2 | 39-A | 201 | FOL | N-CA-CB-CG |
| 2 | 131-A | 201 | FOL | N-CA-CB-CG |
| 2 | 242-A | 201 | FOL | N-CA-CB-CG |
| 2 | 186-A | 201 | FOL | N-CA-CB-CG |
| 2 | 182-A | 201 | FOL | N-CA-CB-CG |
| 2 | 177-A | 201 | FOL | N-CA-CB-CG |
| 2 | 157-A | 201 | FOL | N-CA-CB-CG |
| 2 | 190-A | 201 | FOL | N-CA-CB-CG |
| 2 | 86-A | 201 | FOL | N-CA-CB-CG |
| 2 | 150-A | 201 | FOL | N-CA-CB-CG |
| 2 | 146-A | 201 | FOL | N-CA-CB-CG |
| 2 | 228-A | 201 | FOL | N-CA-CB-CG |
| 2 | 144-A | 201 | FOL | N-CA-CB-CG |
| 2 | 43-A | 201 | FOL | N-CA-CB-CG |
| 2 | 193-A | 201 | FOL | N-CA-CB-CG |
| 2 | 59-A | 201 | FOL | N-CA-CB-CG |
| 2 | 94-A | 201 | FOL | N-CA-CB-CG |
| 2 | 174-A | 201 | FOL | N-CA-CB-CG |

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| Mol | Chain | Res | Type | Atoms |
|------------|--------------|------------|-------------|--------------|
| 2 | 64-A | 201 | FOL | N-CA-CB-CG |
| 2 | 65-A | 201 | FOL | N-CA-CB-CG |
| 2 | 142-A | 201 | FOL | N-CA-CB-CG |
| 2 | 247-A | 201 | FOL | N-CA-CB-CG |
| 2 | 163-A | 201 | FOL | N-CA-CB-CG |
| 2 | 214-A | 201 | FOL | N-CA-CB-CG |
| 2 | 206-A | 201 | FOL | N-CA-CB-CG |
| 2 | 102-A | 201 | FOL | N-CA-CB-CG |
| 2 | 132-A | 201 | FOL | N-CA-CB-CG |
| 2 | 168-A | 201 | FOL | N-CA-CB-CG |
| 2 | 173-A | 201 | FOL | N-CA-CB-CG |
| 2 | 217-A | 201 | FOL | N-CA-CB-CG |
| 2 | 212-A | 201 | FOL | N-CA-CB-CG |
| 2 | 171-A | 201 | FOL | N-CA-CB-CG |
| 2 | 22-A | 201 | FOL | N-CA-CB-CG |
| 2 | 29-A | 201 | FOL | N-CA-CB-CG |
| 2 | 89-A | 201 | FOL | N-CA-CB-CG |
| 2 | 95-A | 201 | FOL | N-CA-CB-CG |
| 2 | 239-A | 201 | FOL | N-CA-CB-CG |
| 2 | 221-A | 201 | FOL | N-CA-CB-CG |
| 2 | 67-A | 201 | FOL | N-CA-CB-CG |
| 2 | 154-A | 201 | FOL | N-CA-CB-CG |
| 2 | 91-A | 201 | FOL | N-CA-CB-CG |
| 2 | 109-A | 201 | FOL | N-CA-CB-CG |
| 2 | 66-A | 201 | FOL | N-CA-CB-CG |
| 2 | 20-A | 201 | FOL | N-CA-CB-CG |
| 2 | 73-A | 201 | FOL | N-CA-CB-CG |
| 2 | 40-A | 201 | FOL | N-CA-CB-CG |
| 2 | 230-A | 201 | FOL | N-CA-CB-CG |
| 2 | 199-A | 201 | FOL | N-CA-CB-CG |
| 2 | 52-A | 201 | FOL | N-CA-CB-CG |
| 2 | 33-A | 201 | FOL | N-CA-CB-CG |
| 2 | 126-A | 201 | FOL | N-CA-CB-CG |
| 2 | 194-A | 201 | FOL | N-CA-CB-CG |
| 2 | 213-A | 201 | FOL | N-CA-CB-CG |
| 2 | 12-A | 201 | FOL | N-CA-CB-CG |
| 2 | 192-A | 201 | FOL | N-CA-CB-CG |
| 2 | 3-A | 201 | FOL | N-CA-CB-CG |
| 2 | 92-A | 201 | FOL | N-CA-CB-CG |
| 2 | 196-A | 201 | FOL | N-CA-CB-CG |
| 2 | 61-A | 201 | FOL | N-CA-CB-CG |
| 3 | 34-A | 202 | NAP | PA-O3-PN-O5D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 3 | 76-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 202-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 174-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 54-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 161-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 129-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 238-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 208-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 119-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 39-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 33-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 12-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 89-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 23-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 5-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 81-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 162-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 107-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 239-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 190-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 215-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 92-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 55-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 82-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 38-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 144-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 186-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 138-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 104-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 149-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 164-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 156-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 48-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 6-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 225-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 30-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 3-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 223-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 96-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 176-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 72-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 154-A | 202 | NAP | PA-O3-PN-O5D |

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| Mol | Chain | Res | Type | Atoms |
|------------|--------------|------------|-------------|--------------|
| 3 | 10-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 175-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 127-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 27-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 137-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 243-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 56-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 21-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 87-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 234-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 169-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 241-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 249-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 233-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 182-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 43-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 207-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 20-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 247-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 136-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 51-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 195-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 204-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 211-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 126-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 244-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 68-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 240-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 17-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 66-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 170-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 228-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 14-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 122-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 102-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 22-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 210-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 224-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 171-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 184-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 125-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 44-A | 202 | NAP | PA-O3-PN-O5D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 3 | 158-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 213-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 113-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 49-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 61-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 242-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 90-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 65-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 111-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 52-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 166-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 152-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 220-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 217-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 245-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 185-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 95-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 4-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 114-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 29-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 32-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 58-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 196-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 201-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 98-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 13-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 16-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 219-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 200-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 120-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 63-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 80-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 106-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 140-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 26-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 157-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 94-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 108-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 91-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 57-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 60-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 143-A | 202 | NAP | PA-O3-PN-O5D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 3 | 246-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 155-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 86-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 50-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 232-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 177-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 189-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 145-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 198-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 116-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 179-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 117-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 97-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 123-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 71-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 121-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 8-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 167-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 47-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 67-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 15-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 206-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 73-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 194-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 205-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 236-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 151-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 85-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 226-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 75-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 128-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 41-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 230-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 163-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 192-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 172-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 168-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 183-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 135-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 1-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 237-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 62-A | 202 | NAP | PA-O3-PN-O5D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|--------------|
| 3 | 46-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 103-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 31-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 100-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 146-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 173-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 105-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 36-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 59-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 188-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 24-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 118-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 83-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 209-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 132-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 197-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 70-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 79-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 222-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 227-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 148-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 109-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 9-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 40-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 181-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 2-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 77-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 214-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 216-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 187-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 221-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 147-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 248-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 64-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 115-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 124-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 180-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 78-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 178-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 231-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 235-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 141-A | 202 | NAP | PA-O3-PN-O5D |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 99-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 130-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 142-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 35-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 18-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 165-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 139-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 133-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 159-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 74-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 199-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 93-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 229-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 101-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 112-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 84-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 150-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 7-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 69-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 88-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 193-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 28-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 203-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 250-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 45-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 160-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 53-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 191-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 11-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 110-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 37-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 153-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 212-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 25-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 134-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 19-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 131-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 218-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 42-A | 202 | NAP | PA-O3-PN-O5D |
| 3 | 34-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 76-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 202-A | 202 | NAP | C2B-O2B-P2B-O3X |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 174-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 54-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 161-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 129-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 238-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 208-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 119-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 39-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 33-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 12-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 89-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 23-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 5-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 81-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 162-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 107-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 239-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 190-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 215-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 92-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 55-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 82-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 38-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 144-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 186-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 138-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 104-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 149-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 164-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 156-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 48-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 6-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 225-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 30-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 3-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 223-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 96-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 176-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 72-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 154-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 10-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 175-A | 202 | NAP | C2B-O2B-P2B-O3X |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 127-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 27-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 137-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 243-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 56-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 21-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 87-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 234-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 169-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 241-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 249-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 233-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 182-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 43-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 207-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 20-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 247-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 136-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 51-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 195-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 204-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 211-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 126-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 244-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 68-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 240-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 17-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 66-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 170-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 228-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 14-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 122-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 102-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 22-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 210-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 224-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 171-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 184-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 125-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 44-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 158-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 213-A | 202 | NAP | C2B-O2B-P2B-O3X |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 113-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 49-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 61-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 242-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 90-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 65-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 111-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 52-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 166-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 152-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 220-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 217-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 245-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 185-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 95-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 4-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 114-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 29-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 32-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 58-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 196-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 201-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 98-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 13-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 16-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 219-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 200-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 120-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 63-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 80-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 106-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 140-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 26-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 157-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 94-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 108-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 91-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 57-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 60-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 143-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 246-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 155-A | 202 | NAP | C2B-O2B-P2B-O3X |

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| Mol | Chain | Res | Type | Atoms |
|------------|--------------|------------|-------------|-----------------|
| 3 | 86-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 50-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 232-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 177-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 189-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 145-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 198-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 116-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 179-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 117-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 97-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 123-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 71-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 121-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 8-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 167-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 47-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 67-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 15-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 206-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 73-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 194-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 205-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 236-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 151-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 85-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 226-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 75-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 128-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 41-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 230-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 163-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 192-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 172-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 168-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 183-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 135-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 1-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 237-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 62-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 46-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 103-A | 202 | NAP | C2B-O2B-P2B-O3X |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 31-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 100-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 146-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 173-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 105-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 36-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 59-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 188-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 24-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 118-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 83-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 209-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 132-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 197-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 70-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 79-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 222-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 227-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 148-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 109-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 9-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 40-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 181-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 2-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 77-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 214-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 216-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 187-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 221-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 147-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 248-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 64-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 115-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 124-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 180-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 78-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 178-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 231-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 235-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 141-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 99-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 130-A | 202 | NAP | C2B-O2B-P2B-O3X |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 3 | 142-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 35-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 18-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 165-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 139-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 133-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 159-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 74-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 199-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 93-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 229-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 101-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 112-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 84-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 150-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 7-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 69-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 88-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 193-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 28-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 203-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 250-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 45-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 160-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 53-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 191-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 11-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 110-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 37-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 153-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 212-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 25-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 134-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 19-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 131-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 218-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 3 | 42-A | 202 | NAP | C2B-O2B-P2B-O3X |
| 2 | 125-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 85-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 56-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 187-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 68-A | 201 | FOL | C6-C9-N10-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|---------------|
| 2 | 10-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 149-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 107-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 81-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 6-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 21-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 98-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 165-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 31-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 105-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 180-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 54-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 14-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 145-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 13-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 99-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 83-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 117-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 201-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 48-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 203-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 30-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 156-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 42-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 106-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 205-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 158-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 112-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 220-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 123-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 113-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 118-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 176-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 49-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 44-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 70-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 166-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 188-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 121-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 133-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 7-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 97-A | 201 | FOL | C6-C9-N10-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|---------------|
| 2 | 80-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 17-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 78-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 246-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 101-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 235-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 137-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 115-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 103-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 147-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 75-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 79-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 175-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 245-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 9-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 208-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 19-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 248-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 185-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 152-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 60-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 53-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 226-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 110-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 244-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 134-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 236-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 198-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 183-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 153-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 135-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 202-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 140-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 119-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 240-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 84-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 100-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 27-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 1-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 234-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 130-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 161-A | 201 | FOL | C6-C9-N10-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|---------------|
| 2 | 215-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 210-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 249-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 216-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 139-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 96-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 159-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 69-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 169-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 62-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 225-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 55-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 211-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 181-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 116-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 71-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 160-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 191-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 50-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 8-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 164-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 18-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 51-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 232-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 63-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 138-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 16-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 57-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 200-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 250-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 36-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 167-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 37-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 124-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 34-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 218-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 243-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 209-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 111-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 90-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 122-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 151-A | 201 | FOL | C6-C9-N10-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|---------------|
| 2 | 45-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 128-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 74-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 11-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 207-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 241-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 2-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 155-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 88-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 5-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 170-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 229-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 222-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 47-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 76-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 35-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 41-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 108-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 104-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 141-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 25-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 87-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 32-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 77-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 93-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 233-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 4-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 24-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 237-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 28-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 238-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 26-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 129-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 223-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 162-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 178-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 46-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 38-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 227-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 179-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 219-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 172-A | 201 | FOL | C6-C9-N10-C14 |

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| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|---------------|
| 2 | 58-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 114-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 204-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 120-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 23-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 72-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 189-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 127-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 143-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 82-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 15-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 136-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 184-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 197-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 148-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 231-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 224-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 195-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 39-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 131-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 242-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 186-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 182-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 177-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 157-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 190-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 86-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 150-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 146-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 228-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 144-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 43-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 193-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 59-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 94-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 174-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 64-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 65-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 142-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 247-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 163-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 214-A | 201 | FOL | C6-C9-N10-C14 |

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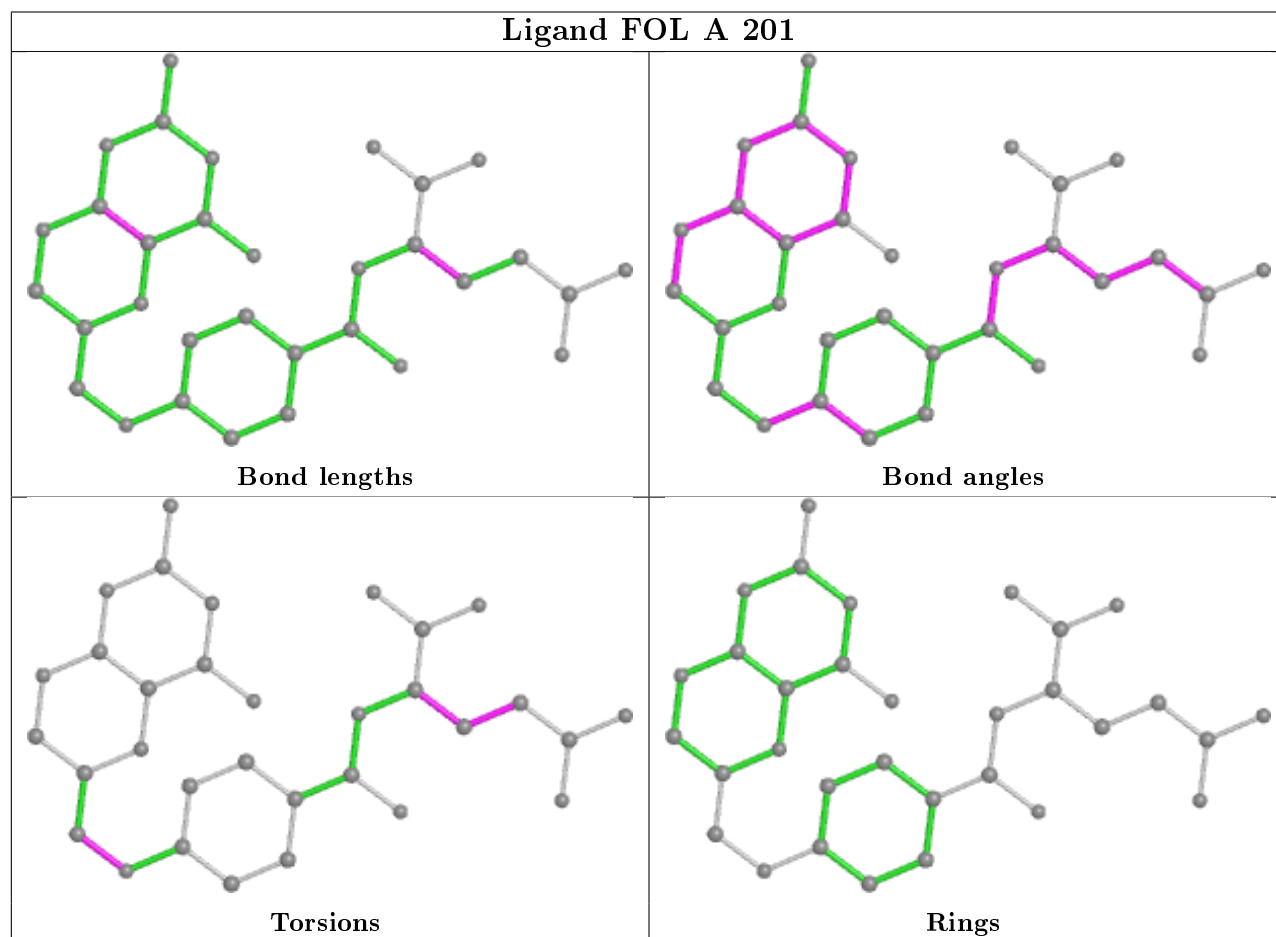
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|---------------|
| 2 | 206-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 102-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 132-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 168-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 173-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 217-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 212-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 171-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 22-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 29-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 89-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 95-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 239-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 221-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 67-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 154-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 91-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 109-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 66-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 20-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 73-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 40-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 230-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 199-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 52-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 33-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 126-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 194-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 213-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 12-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 192-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 3-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 92-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 196-A | 201 | FOL | C6-C9-N10-C14 |
| 2 | 61-A | 201 | FOL | C6-C9-N10-C14 |

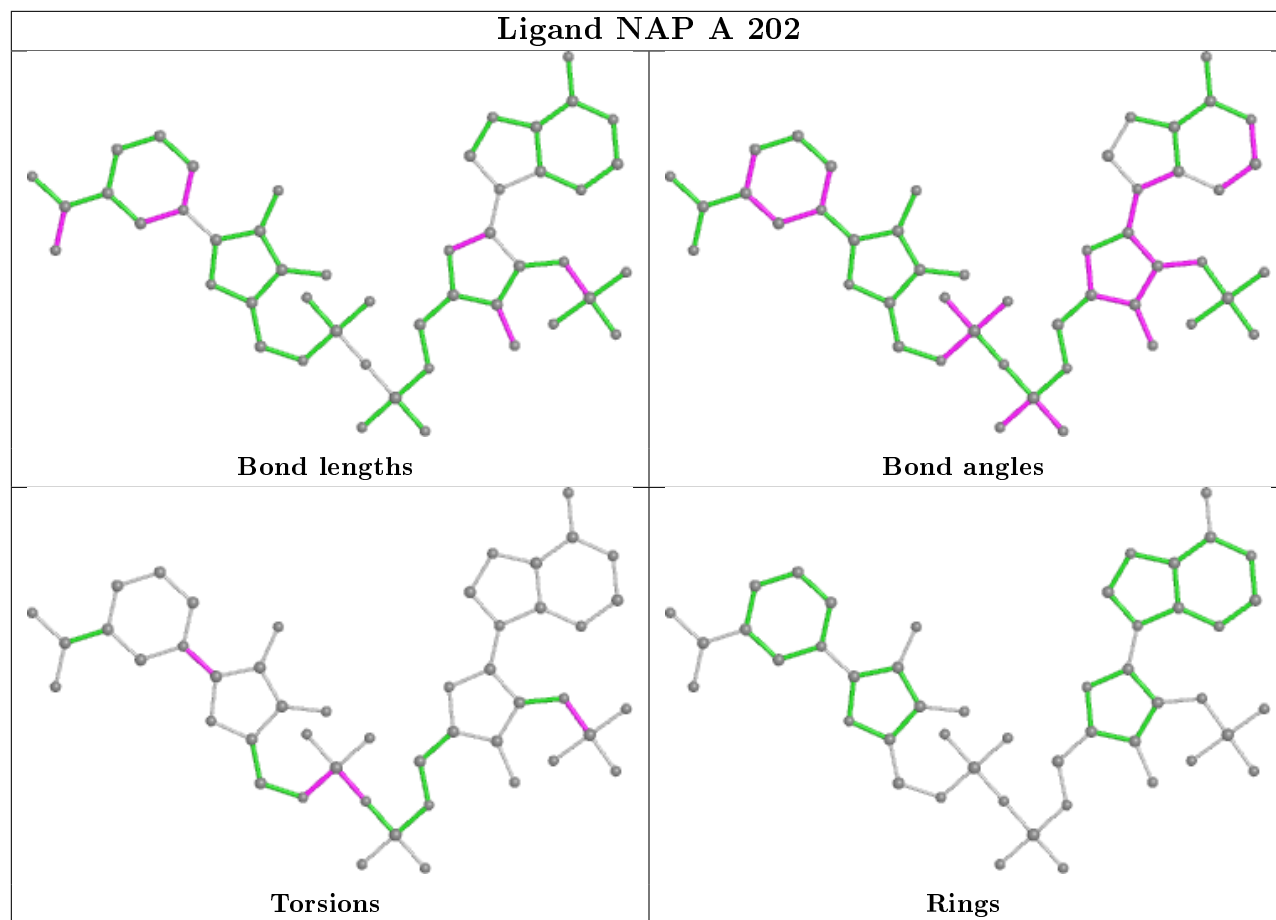
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.