



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:08 PM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : **NOT EXECUTED**
Mogul : **NOT EXECUTED**
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.05 Å.

There are no percentiles available for this entry.

MolProbity and EDS were not executed - the sequence quality summary graphics cannot be shown.

2 Entry composition

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

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

- Molecule 1 is a protein called Dihydrofolate reductase.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

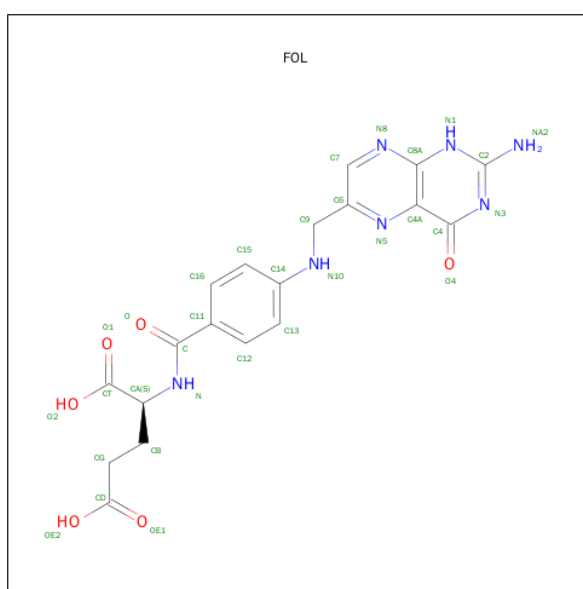
| Mol | Chain | Residues | Atoms | | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|------|-----|-----|---|---------|---------|-------|
| 1 | 101-A | 159 | Total | C | H | N | O | S | 0 | 0 | 0 |
| | | | 2491 | 805 | 1221 | 217 | 241 | 7 | | | |
| 1 | 102-A | 159 | Total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

Continued on next page...

Continued from previous page...

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

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

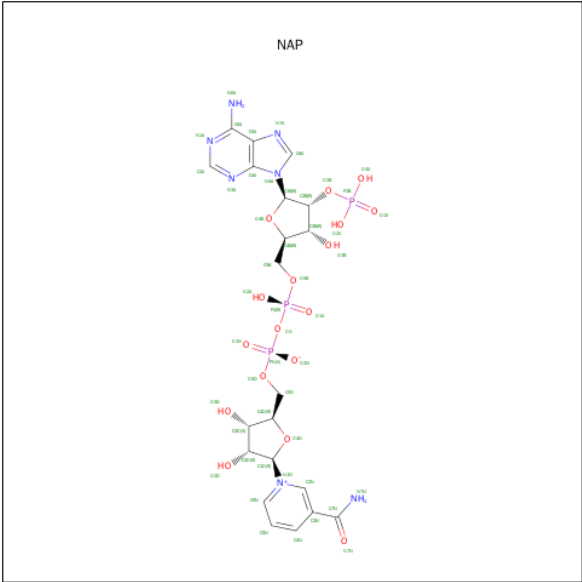
| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---------|---------|--------|--------|---------|---------|
| 2 | 92-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 93-A | 1 | Total 49 | C 19 | H 17 | N 7 | O 6 | 0 | 0 |
| 2 | 94-A | 1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

Continued on next page...

Continued from previous page...

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

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is water.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 5 | 118-A | 107 | Total 107 | O 107 | 0 | 0 |
| 5 | 119-A | 106 | Total 106 | O 106 | 0 | 0 |
| 5 | 120-A | 105 | Total 105 | O 105 | 0 | 0 |
| 5 | 121-A | 115 | Total 115 | O 115 | 0 | 0 |
| 5 | 122-A | 97 | Total 97 | O 97 | 0 | 0 |
| 5 | 123-A | 105 | Total 105 | O 105 | 0 | 0 |
| 5 | 124-A | 93 | Total 93 | O 93 | 0 | 0 |
| 5 | 125-A | 102 | Total 102 | O 102 | 0 | 0 |

MolProbity and EDS were not executed - this section will therefore be empty.

3 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

| Property | Value | Source |
|----------------------------------------------------------|-------------------------------------------------|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 34.30 Å 45.52 Å 98.71 Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.40 – 1.05 | Depositor |
| % Data completeness (in resolution range) | 98.2 (49.40-1.05) | Depositor |
| R_{merge} | 0.04 | Depositor |
| R_{sym} | (Not available) | Depositor |
| Refinement program | PHENIX 1.8.4-1496 | Depositor |
| R, R_{free} | 0.136 , 0.166 | Depositor |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 339833 | wwPDB-VP |
| Average B, all atoms (Å ²) | 11.0 | wwPDB-VP |

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity was not executed - this section will therefore be empty.

4.2 Too-close contacts [i](#)

MolProbity was not executed - this section will therefore be empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity was not executed - this section will therefore be empty.

4.3.2 Protein sidechains [i](#)

MolProbity was not executed - this section will therefore be empty.

4.3.3 RNA [i](#)

MolProbity was not executed - this section will therefore be empty.

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

validation-pack and Mogul were not executed - this section will therefore be empty.

4.5 Carbohydrates [i](#)

validation-pack and Mogul were not executed - this section will therefore be empty.

4.6 Ligand geometry [i](#)

validation-pack and Mogul were not executed - this section will therefore be empty.

4.7 Other polymers [i](#)

validation-pack and Mogul were not executed - this section will therefore be empty.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

5.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

5.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

5.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.