



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2023 – 03:18 PM EDT

PDB ID : 4PTH
Title : Ensemble model for Escherichia coli dihydrofolate reductase at 100K
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 : 0.85 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : **FAILED**
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
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) : 2.35.1

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 0.85 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 699880 atoms, of which 315750 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
			Total	C	H	N	O	S			
1	1-A	159	2491	805	1221	217	241	7	0	0	0
1	2-A	159	2491	805	1221	217	241	7	0	0	0
1	3-A	159	2491	805	1221	217	241	7	0	0	0
1	4-A	159	2491	805	1221	217	241	7	0	0	0
1	5-A	159	2491	805	1221	217	241	7	0	0	0
1	6-A	159	2491	805	1221	217	241	7	0	0	0
1	7-A	159	2491	805	1221	217	241	7	0	0	0
1	8-A	159	2491	805	1221	217	241	7	0	0	0
1	9-A	159	2491	805	1221	217	241	7	0	0	0
1	10-A	159	2491	805	1221	217	241	7	0	0	0
1	11-A	159	2491	805	1221	217	241	7	0	0	0
1	12-A	159	2491	805	1221	217	241	7	0	0	0
1	13-A	159	2491	805	1221	217	241	7	0	0	0
1	14-A	159	2491	805	1221	217	241	7	0	0	0
1	15-A	159	2491	805	1221	217	241	7	0	0	0
1	16-A	159	2491	805	1221	217	241	7	0	0	0

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			
1	126-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	127-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	128-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	129-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	130-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	131-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	132-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	133-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	134-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	135-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	136-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	137-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	138-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	139-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	140-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	141-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	142-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	143-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	144-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	145-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	146-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	147-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	148-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	149-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	150-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	151-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	152-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	153-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	154-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	155-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	156-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	157-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	158-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	159-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	160-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	161-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	162-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	163-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	164-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	165-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	166-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	167-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	168-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	169-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	170-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	171-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	172-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	173-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	174-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	175-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	176-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	177-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	178-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	179-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	180-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	181-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	182-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	183-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	184-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	185-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	186-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	187-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	188-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	189-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	190-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	191-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	192-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	193-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	194-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	195-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	196-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	197-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	198-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	199-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	200-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	201-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	202-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	203-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	204-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	205-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	206-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	207-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	208-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	209-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	210-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	211-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	212-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	213-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	214-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	215-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	216-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	217-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	218-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	219-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	220-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	221-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	222-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	223-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	224-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	225-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	226-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...

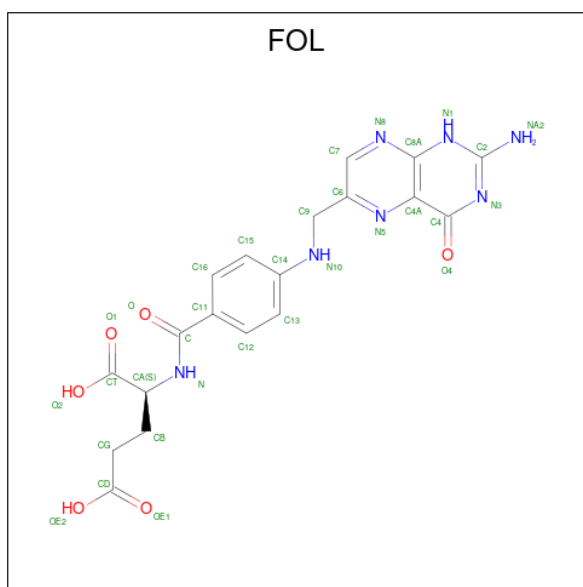
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	227-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	228-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	229-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	230-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	231-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	232-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	233-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	234-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	235-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	236-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	237-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	238-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	239-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	240-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	241-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	242-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	243-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	244-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	245-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	246-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	247-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	
			Total	C	H	N	O				S
1	248-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	249-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	250-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	9-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	10-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	11-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	12-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	13-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	14-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	15-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	16-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	17-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	18-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	19-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	20-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	21-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	22-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	23-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	24-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	25-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	26-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	27-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	28-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	29-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	30-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	31-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	32-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	33-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	34-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	35-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	36-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	37-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	38-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	39-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	40-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	41-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	42-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	43-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	44-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	45-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	46-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	47-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	48-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	49-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	50-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	51-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	52-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	53-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	54-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	55-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	56-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	57-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	58-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	59-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	60-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	61-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	62-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	63-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	64-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	65-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	66-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	67-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	68-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	69-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	70-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	71-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	72-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	73-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	74-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	75-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	76-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	77-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	78-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	79-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	80-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	81-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	82-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	83-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	84-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	85-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	86-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	87-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	88-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	89-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	90-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	91-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	92-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	93-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	94-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	95-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	96-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	97-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	98-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	99-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	100-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	101-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	102-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	103-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	104-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	105-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	106-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	107-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	108-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	109-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	110-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	111-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	112-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	113-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	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		
2	126-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	127-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	128-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	129-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	130-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	131-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	132-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	133-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	134-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	135-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	136-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	137-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	138-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	139-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	140-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	141-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	142-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	143-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	144-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	145-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	146-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	147-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	148-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	149-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	150-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	151-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	152-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	153-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	154-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	155-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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	177-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	178-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	179-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	180-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	181-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	182-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	183-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	184-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	185-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	186-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	187-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	188-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	189-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	190-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	191-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	192-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	193-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	194-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	195-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	196-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	197-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	198-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	199-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	200-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	201-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	202-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	203-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	204-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	205-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	206-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	207-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	208-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	209-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	210-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	211-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	212-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	213-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	214-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	215-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	216-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	217-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	218-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		

Continued on next page...

Continued from previous page...

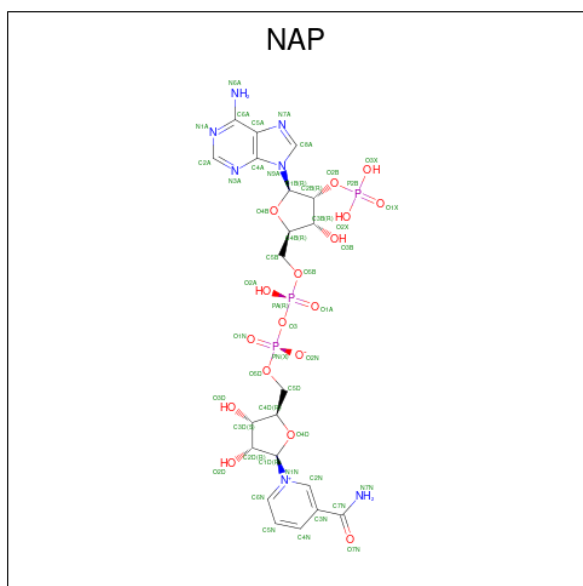
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	219-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	220-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	221-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	222-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	223-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	224-A	1	Total	C	H	N	O	0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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	23-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	24-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	25-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	26-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	27-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	28-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	29-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	30-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	31-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	32-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	33-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	34-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	35-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	36-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	37-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	38-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	39-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	40-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	41-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	42-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	43-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	44-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	45-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	46-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	47-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	48-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	49-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	50-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	51-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	52-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	53-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	54-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	55-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	56-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	57-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	58-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	59-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	60-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	61-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	62-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	63-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	64-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	
			Total	C	H	N	O			P
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
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
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
3	126-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	127-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	
			Total	C	H	N	O			P
3	128-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	129-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	130-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	131-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	132-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	133-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	134-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	135-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	136-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	137-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	138-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	139-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	140-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	141-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	142-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	143-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	144-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	145-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	146-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	147-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	148-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	
			Total	C	H	N	O			P
3	149-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	150-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	151-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	152-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	153-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	154-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	155-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	156-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	157-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	158-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	159-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	160-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	161-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	162-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	163-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	164-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	165-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	166-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	167-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	168-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	169-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	170-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	171-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	172-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	173-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	174-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	175-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	176-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	177-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	178-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	179-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	180-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	181-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	182-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	183-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	184-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	185-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	186-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	187-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	188-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	189-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	190-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	191-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	192-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	193-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	194-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	195-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	196-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	197-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	198-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	199-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	200-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	201-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	202-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	203-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	204-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	205-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	206-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	207-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	208-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	209-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	210-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	211-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	
			Total	C	H	N	O			P
3	212-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	213-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	214-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	215-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	216-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	217-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	218-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	219-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	220-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	221-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	222-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	223-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	224-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	225-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	226-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	227-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	228-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	229-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	230-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	231-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	232-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	233-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	234-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	235-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	236-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	237-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	238-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	239-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	240-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	241-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	242-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	243-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	244-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	245-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	246-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	247-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	248-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	249-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	250-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	2	Total	Mn	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	2-A	2	Total 2	Mn 2	0	0
4	3-A	2	Total 2	Mn 2	0	0
4	4-A	2	Total 2	Mn 2	0	0
4	5-A	2	Total 2	Mn 2	0	0
4	6-A	2	Total 2	Mn 2	0	0
4	7-A	2	Total 2	Mn 2	0	0
4	8-A	2	Total 2	Mn 2	0	0
4	9-A	2	Total 2	Mn 2	0	0
4	10-A	2	Total 2	Mn 2	0	0
4	11-A	2	Total 2	Mn 2	0	0
4	12-A	2	Total 2	Mn 2	0	0
4	13-A	2	Total 2	Mn 2	0	0
4	14-A	2	Total 2	Mn 2	0	0
4	15-A	2	Total 2	Mn 2	0	0
4	16-A	2	Total 2	Mn 2	0	0
4	17-A	2	Total 2	Mn 2	0	0
4	18-A	2	Total 2	Mn 2	0	0
4	19-A	2	Total 2	Mn 2	0	0
4	20-A	2	Total 2	Mn 2	0	0
4	21-A	2	Total 2	Mn 2	0	0
4	22-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	23-A	2	Total 2	Mn 2	0	0
4	24-A	2	Total 2	Mn 2	0	0
4	25-A	2	Total 2	Mn 2	0	0
4	26-A	2	Total 2	Mn 2	0	0
4	27-A	2	Total 2	Mn 2	0	0
4	28-A	2	Total 2	Mn 2	0	0
4	29-A	2	Total 2	Mn 2	0	0
4	30-A	2	Total 2	Mn 2	0	0
4	31-A	2	Total 2	Mn 2	0	0
4	32-A	2	Total 2	Mn 2	0	0
4	33-A	2	Total 2	Mn 2	0	0
4	34-A	2	Total 2	Mn 2	0	0
4	35-A	2	Total 2	Mn 2	0	0
4	36-A	2	Total 2	Mn 2	0	0
4	37-A	2	Total 2	Mn 2	0	0
4	38-A	2	Total 2	Mn 2	0	0
4	39-A	2	Total 2	Mn 2	0	0
4	40-A	2	Total 2	Mn 2	0	0
4	41-A	2	Total 2	Mn 2	0	0
4	42-A	2	Total 2	Mn 2	0	0
4	43-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	44-A	2	Total 2	Mn 2	0	0
4	45-A	2	Total 2	Mn 2	0	0
4	46-A	2	Total 2	Mn 2	0	0
4	47-A	2	Total 2	Mn 2	0	0
4	48-A	2	Total 2	Mn 2	0	0
4	49-A	2	Total 2	Mn 2	0	0
4	50-A	2	Total 2	Mn 2	0	0
4	51-A	2	Total 2	Mn 2	0	0
4	52-A	2	Total 2	Mn 2	0	0
4	53-A	2	Total 2	Mn 2	0	0
4	54-A	2	Total 2	Mn 2	0	0
4	55-A	2	Total 2	Mn 2	0	0
4	56-A	2	Total 2	Mn 2	0	0
4	57-A	2	Total 2	Mn 2	0	0
4	58-A	2	Total 2	Mn 2	0	0
4	59-A	2	Total 2	Mn 2	0	0
4	60-A	2	Total 2	Mn 2	0	0
4	61-A	2	Total 2	Mn 2	0	0
4	62-A	2	Total 2	Mn 2	0	0
4	63-A	2	Total 2	Mn 2	0	0
4	64-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	65-A	2	Total 2	Mn 2	0	0
4	66-A	2	Total 2	Mn 2	0	0
4	67-A	2	Total 2	Mn 2	0	0
4	68-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	71-A	2	Total 2	Mn 2	0	0
4	72-A	2	Total 2	Mn 2	0	0
4	73-A	2	Total 2	Mn 2	0	0
4	74-A	2	Total 2	Mn 2	0	0
4	75-A	2	Total 2	Mn 2	0	0
4	76-A	2	Total 2	Mn 2	0	0
4	77-A	2	Total 2	Mn 2	0	0
4	78-A	2	Total 2	Mn 2	0	0
4	79-A	2	Total 2	Mn 2	0	0
4	80-A	2	Total 2	Mn 2	0	0
4	81-A	2	Total 2	Mn 2	0	0
4	82-A	2	Total 2	Mn 2	0	0
4	83-A	2	Total 2	Mn 2	0	0
4	84-A	2	Total 2	Mn 2	0	0
4	85-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	86-A	2	Total 2	Mn 2	0	0
4	87-A	2	Total 2	Mn 2	0	0
4	88-A	2	Total 2	Mn 2	0	0
4	89-A	2	Total 2	Mn 2	0	0
4	90-A	2	Total 2	Mn 2	0	0
4	91-A	2	Total 2	Mn 2	0	0
4	92-A	2	Total 2	Mn 2	0	0
4	93-A	2	Total 2	Mn 2	0	0
4	94-A	2	Total 2	Mn 2	0	0
4	95-A	2	Total 2	Mn 2	0	0
4	96-A	2	Total 2	Mn 2	0	0
4	97-A	2	Total 2	Mn 2	0	0
4	98-A	2	Total 2	Mn 2	0	0
4	99-A	2	Total 2	Mn 2	0	0
4	100-A	2	Total 2	Mn 2	0	0
4	101-A	2	Total 2	Mn 2	0	0
4	102-A	2	Total 2	Mn 2	0	0
4	103-A	2	Total 2	Mn 2	0	0
4	104-A	2	Total 2	Mn 2	0	0
4	105-A	2	Total 2	Mn 2	0	0
4	106-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	107-A	2	Total 2	Mn 2	0	0
4	108-A	2	Total 2	Mn 2	0	0
4	109-A	2	Total 2	Mn 2	0	0
4	110-A	2	Total 2	Mn 2	0	0
4	111-A	2	Total 2	Mn 2	0	0
4	112-A	2	Total 2	Mn 2	0	0
4	113-A	2	Total 2	Mn 2	0	0
4	114-A	2	Total 2	Mn 2	0	0
4	115-A	2	Total 2	Mn 2	0	0
4	116-A	2	Total 2	Mn 2	0	0
4	117-A	2	Total 2	Mn 2	0	0
4	118-A	2	Total 2	Mn 2	0	0
4	119-A	2	Total 2	Mn 2	0	0
4	120-A	2	Total 2	Mn 2	0	0
4	121-A	2	Total 2	Mn 2	0	0
4	122-A	2	Total 2	Mn 2	0	0
4	123-A	2	Total 2	Mn 2	0	0
4	124-A	2	Total 2	Mn 2	0	0
4	125-A	2	Total 2	Mn 2	0	0
4	126-A	2	Total 2	Mn 2	0	0
4	127-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	128-A	2	Total 2	Mn 2	0	0
4	129-A	2	Total 2	Mn 2	0	0
4	130-A	2	Total 2	Mn 2	0	0
4	131-A	2	Total 2	Mn 2	0	0
4	132-A	2	Total 2	Mn 2	0	0
4	133-A	2	Total 2	Mn 2	0	0
4	134-A	2	Total 2	Mn 2	0	0
4	135-A	2	Total 2	Mn 2	0	0
4	136-A	2	Total 2	Mn 2	0	0
4	137-A	2	Total 2	Mn 2	0	0
4	138-A	2	Total 2	Mn 2	0	0
4	139-A	2	Total 2	Mn 2	0	0
4	140-A	2	Total 2	Mn 2	0	0
4	141-A	2	Total 2	Mn 2	0	0
4	142-A	2	Total 2	Mn 2	0	0
4	143-A	2	Total 2	Mn 2	0	0
4	144-A	2	Total 2	Mn 2	0	0
4	145-A	2	Total 2	Mn 2	0	0
4	146-A	2	Total 2	Mn 2	0	0
4	147-A	2	Total 2	Mn 2	0	0
4	148-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	149-A	2	Total 2	Mn 2	0	0
4	150-A	2	Total 2	Mn 2	0	0
4	151-A	2	Total 2	Mn 2	0	0
4	152-A	2	Total 2	Mn 2	0	0
4	153-A	2	Total 2	Mn 2	0	0
4	154-A	2	Total 2	Mn 2	0	0
4	155-A	2	Total 2	Mn 2	0	0
4	156-A	2	Total 2	Mn 2	0	0
4	157-A	2	Total 2	Mn 2	0	0
4	158-A	2	Total 2	Mn 2	0	0
4	159-A	2	Total 2	Mn 2	0	0
4	160-A	2	Total 2	Mn 2	0	0
4	161-A	2	Total 2	Mn 2	0	0
4	162-A	2	Total 2	Mn 2	0	0
4	163-A	2	Total 2	Mn 2	0	0
4	164-A	2	Total 2	Mn 2	0	0
4	165-A	2	Total 2	Mn 2	0	0
4	166-A	2	Total 2	Mn 2	0	0
4	167-A	2	Total 2	Mn 2	0	0
4	168-A	2	Total 2	Mn 2	0	0
4	169-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	170-A	2	Total 2	Mn 2	0	0
4	171-A	2	Total 2	Mn 2	0	0
4	172-A	2	Total 2	Mn 2	0	0
4	173-A	2	Total 2	Mn 2	0	0
4	174-A	2	Total 2	Mn 2	0	0
4	175-A	2	Total 2	Mn 2	0	0
4	176-A	2	Total 2	Mn 2	0	0
4	177-A	2	Total 2	Mn 2	0	0
4	178-A	2	Total 2	Mn 2	0	0
4	179-A	2	Total 2	Mn 2	0	0
4	180-A	2	Total 2	Mn 2	0	0
4	181-A	2	Total 2	Mn 2	0	0
4	182-A	2	Total 2	Mn 2	0	0
4	183-A	2	Total 2	Mn 2	0	0
4	184-A	2	Total 2	Mn 2	0	0
4	185-A	2	Total 2	Mn 2	0	0
4	186-A	2	Total 2	Mn 2	0	0
4	187-A	2	Total 2	Mn 2	0	0
4	188-A	2	Total 2	Mn 2	0	0
4	189-A	2	Total 2	Mn 2	0	0
4	190-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	191-A	2	Total 2	Mn 2	0	0
4	192-A	2	Total 2	Mn 2	0	0
4	193-A	2	Total 2	Mn 2	0	0
4	194-A	2	Total 2	Mn 2	0	0
4	195-A	2	Total 2	Mn 2	0	0
4	196-A	2	Total 2	Mn 2	0	0
4	197-A	2	Total 2	Mn 2	0	0
4	198-A	2	Total 2	Mn 2	0	0
4	199-A	2	Total 2	Mn 2	0	0
4	200-A	2	Total 2	Mn 2	0	0
4	201-A	2	Total 2	Mn 2	0	0
4	202-A	2	Total 2	Mn 2	0	0
4	203-A	2	Total 2	Mn 2	0	0
4	204-A	2	Total 2	Mn 2	0	0
4	205-A	2	Total 2	Mn 2	0	0
4	206-A	2	Total 2	Mn 2	0	0
4	207-A	2	Total 2	Mn 2	0	0
4	208-A	2	Total 2	Mn 2	0	0
4	209-A	2	Total 2	Mn 2	0	0
4	210-A	2	Total 2	Mn 2	0	0
4	211-A	2	Total 2	Mn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
4	212-A	2	2	2	0	0
4	213-A	2	2	2	0	0
4	214-A	2	2	2	0	0
4	215-A	2	2	2	0	0
4	216-A	2	2	2	0	0
4	217-A	2	2	2	0	0
4	218-A	2	2	2	0	0
4	219-A	2	2	2	0	0
4	220-A	2	2	2	0	0
4	221-A	2	2	2	0	0
4	222-A	2	2	2	0	0
4	223-A	2	2	2	0	0
4	224-A	2	2	2	0	0
4	225-A	2	2	2	0	0
4	226-A	2	2	2	0	0
4	227-A	2	2	2	0	0
4	228-A	2	2	2	0	0
4	229-A	2	2	2	0	0
4	230-A	2	2	2	0	0
4	231-A	2	2	2	0	0
4	232-A	2	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	233-A	2	Total 2	Mn 2	0	0
4	234-A	2	Total 2	Mn 2	0	0
4	235-A	2	Total 2	Mn 2	0	0
4	236-A	2	Total 2	Mn 2	0	0
4	237-A	2	Total 2	Mn 2	0	0
4	238-A	2	Total 2	Mn 2	0	0
4	239-A	2	Total 2	Mn 2	0	0
4	240-A	2	Total 2	Mn 2	0	0
4	241-A	2	Total 2	Mn 2	0	0
4	242-A	2	Total 2	Mn 2	0	0
4	243-A	2	Total 2	Mn 2	0	0
4	244-A	2	Total 2	Mn 2	0	0
4	245-A	2	Total 2	Mn 2	0	0
4	246-A	2	Total 2	Mn 2	0	0
4	247-A	2	Total 2	Mn 2	0	0
4	248-A	2	Total 2	Mn 2	0	0
4	249-A	2	Total 2	Mn 2	0	0
4	250-A	2	Total 2	Mn 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-A	180	Total 180	O 180	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2-A	171	Total 171	O 171	0	0
5	3-A	185	Total 185	O 185	0	0
5	4-A	189	Total 189	O 189	0	0
5	5-A	176	Total 176	O 176	0	0
5	6-A	189	Total 189	O 189	0	0
5	7-A	179	Total 179	O 179	0	0
5	8-A	196	Total 196	O 196	0	0
5	9-A	198	Total 198	O 198	0	0
5	10-A	197	Total 197	O 197	0	0
5	11-A	199	Total 199	O 199	0	0
5	12-A	191	Total 191	O 191	0	0
5	13-A	176	Total 176	O 176	0	0
5	14-A	191	Total 191	O 191	0	0
5	15-A	197	Total 197	O 197	0	0
5	16-A	183	Total 183	O 183	0	0
5	17-A	177	Total 177	O 177	0	0
5	18-A	170	Total 170	O 170	0	0
5	19-A	173	Total 173	O 173	0	0
5	20-A	179	Total 179	O 179	0	0
5	21-A	185	Total 185	O 185	0	0
5	22-A	195	Total 195	O 195	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	23-A	181	Total 181	O 181	0	0
5	24-A	172	Total 172	O 172	0	0
5	25-A	179	Total 179	O 179	0	0
5	26-A	196	Total 196	O 196	0	0
5	27-A	195	Total 195	O 195	0	0
5	28-A	193	Total 193	O 193	0	0
5	29-A	184	Total 184	O 184	0	0
5	30-A	185	Total 185	O 185	0	0
5	31-A	190	Total 190	O 190	0	0
5	32-A	175	Total 175	O 175	0	0
5	33-A	199	Total 199	O 199	0	0
5	34-A	196	Total 196	O 196	0	0
5	35-A	185	Total 185	O 185	0	0
5	36-A	191	Total 191	O 191	0	0
5	37-A	191	Total 191	O 191	0	0
5	38-A	183	Total 183	O 183	0	0
5	39-A	177	Total 177	O 177	0	0
5	40-A	183	Total 183	O 183	0	0
5	41-A	182	Total 182	O 182	0	0
5	42-A	176	Total 176	O 176	0	0
5	43-A	172	Total 172	O 172	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	44-A	181	Total 181	O 181	0	0
5	45-A	194	Total 194	O 194	0	0
5	46-A	198	Total 198	O 198	0	0
5	47-A	194	Total 194	O 194	0	0
5	48-A	177	Total 177	O 177	0	0
5	49-A	165	Total 165	O 165	0	0
5	50-A	172	Total 172	O 172	0	0
5	51-A	171	Total 171	O 171	0	0
5	52-A	175	Total 175	O 175	0	0
5	53-A	191	Total 191	O 191	0	0
5	54-A	185	Total 185	O 185	0	0
5	55-A	183	Total 183	O 183	0	0
5	56-A	186	Total 186	O 186	0	0
5	57-A	187	Total 187	O 187	0	0
5	58-A	193	Total 193	O 193	0	0
5	59-A	187	Total 187	O 187	0	0
5	60-A	178	Total 178	O 178	0	0
5	61-A	169	Total 169	O 169	0	0
5	62-A	169	Total 169	O 169	0	0
5	63-A	179	Total 179	O 179	0	0
5	64-A	180	Total 180	O 180	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	65-A	189	Total 189	O 189	0	0
5	66-A	194	Total 194	O 194	0	0
5	67-A	170	Total 170	O 170	0	0
5	68-A	174	Total 174	O 174	0	0
5	69-A	193	Total 193	O 193	0	0
5	70-A	199	Total 199	O 199	0	0
5	71-A	176	Total 176	O 176	0	0
5	72-A	172	Total 172	O 172	0	0
5	73-A	175	Total 175	O 175	0	0
5	74-A	185	Total 185	O 185	0	0
5	75-A	186	Total 186	O 186	0	0
5	76-A	183	Total 183	O 183	0	0
5	77-A	192	Total 192	O 192	0	0
5	78-A	192	Total 192	O 192	0	0
5	79-A	178	Total 178	O 178	0	0
5	80-A	181	Total 181	O 181	0	0
5	81-A	178	Total 178	O 178	0	0
5	82-A	188	Total 188	O 188	0	0
5	83-A	189	Total 189	O 189	0	0
5	84-A	189	Total 189	O 189	0	0
5	85-A	179	Total 179	O 179	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	86-A	185	Total 185	O 185	0	0
5	87-A	192	Total 192	O 192	0	0
5	88-A	187	Total 187	O 187	0	0
5	89-A	185	Total 185	O 185	0	0
5	90-A	182	Total 182	O 182	0	0
5	91-A	183	Total 183	O 183	0	0
5	92-A	182	Total 182	O 182	0	0
5	93-A	186	Total 186	O 186	0	0
5	94-A	175	Total 175	O 175	0	0
5	95-A	186	Total 186	O 186	0	0
5	96-A	188	Total 188	O 188	0	0
5	97-A	186	Total 186	O 186	0	0
5	98-A	180	Total 180	O 180	0	0
5	99-A	183	Total 183	O 183	0	0
5	100-A	172	Total 172	O 172	0	0
5	101-A	175	Total 175	O 175	0	0
5	102-A	183	Total 183	O 183	0	0
5	103-A	200	Total 200	O 200	0	0
5	104-A	185	Total 185	O 185	0	0
5	105-A	180	Total 180	O 180	0	0
5	106-A	189	Total 189	O 189	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	107-A	193	Total 193	O 193	0	0
5	108-A	185	Total 185	O 185	0	0
5	109-A	181	Total 181	O 181	0	0
5	110-A	212	Total 212	O 212	0	0
5	111-A	207	Total 207	O 207	0	0
5	112-A	206	Total 206	O 206	0	0
5	113-A	189	Total 189	O 189	0	0
5	114-A	173	Total 173	O 173	0	0
5	115-A	182	Total 182	O 182	0	0
5	116-A	189	Total 189	O 189	0	0
5	117-A	174	Total 174	O 174	0	0
5	118-A	180	Total 180	O 180	0	0
5	119-A	181	Total 181	O 181	0	0
5	120-A	179	Total 179	O 179	0	0
5	121-A	189	Total 189	O 189	0	0
5	122-A	201	Total 201	O 201	0	0
5	123-A	202	Total 202	O 202	0	0
5	124-A	198	Total 198	O 198	0	0
5	125-A	204	Total 204	O 204	0	0
5	126-A	192	Total 192	O 192	0	0
5	127-A	183	Total 183	O 183	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	128-A	184	Total 184	O 184	0	0
5	129-A	186	Total 186	O 186	0	0
5	130-A	196	Total 196	O 196	0	0
5	131-A	176	Total 176	O 176	0	0
5	132-A	187	Total 187	O 187	0	0
5	133-A	183	Total 183	O 183	0	0
5	134-A	182	Total 182	O 182	0	0
5	135-A	193	Total 193	O 193	0	0
5	136-A	185	Total 185	O 185	0	0
5	137-A	185	Total 185	O 185	0	0
5	138-A	181	Total 181	O 181	0	0
5	139-A	167	Total 167	O 167	0	0
5	140-A	173	Total 173	O 173	0	0
5	141-A	186	Total 186	O 186	0	0
5	142-A	206	Total 206	O 206	0	0
5	143-A	187	Total 187	O 187	0	0
5	144-A	178	Total 178	O 178	0	0
5	145-A	171	Total 171	O 171	0	0
5	146-A	174	Total 174	O 174	0	0
5	147-A	171	Total 171	O 171	0	0
5	148-A	176	Total 176	O 176	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	149-A	196	Total 196	O 196	0	0
5	150-A	185	Total 185	O 185	0	0
5	151-A	184	Total 184	O 184	0	0
5	152-A	179	Total 179	O 179	0	0
5	153-A	186	Total 186	O 186	0	0
5	154-A	184	Total 184	O 184	0	0
5	155-A	188	Total 188	O 188	0	0
5	156-A	176	Total 176	O 176	0	0
5	157-A	174	Total 174	O 174	0	0
5	158-A	181	Total 181	O 181	0	0
5	159-A	180	Total 180	O 180	0	0
5	160-A	186	Total 186	O 186	0	0
5	161-A	199	Total 199	O 199	0	0
5	162-A	199	Total 199	O 199	0	0
5	163-A	199	Total 199	O 199	0	0
5	164-A	181	Total 181	O 181	0	0
5	165-A	191	Total 191	O 191	0	0
5	166-A	189	Total 189	O 189	0	0
5	167-A	171	Total 171	O 171	0	0
5	168-A	171	Total 171	O 171	0	0
5	169-A	187	Total 187	O 187	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	170-A	186	Total 186	O 186	0	0
5	171-A	184	Total 184	O 184	0	0
5	172-A	185	Total 185	O 185	0	0
5	173-A	193	Total 193	O 193	0	0
5	174-A	184	Total 184	O 184	0	0
5	175-A	187	Total 187	O 187	0	0
5	176-A	186	Total 186	O 186	0	0
5	177-A	173	Total 173	O 173	0	0
5	178-A	185	Total 185	O 185	0	0
5	179-A	174	Total 174	O 174	0	0
5	180-A	173	Total 173	O 173	0	0
5	181-A	199	Total 199	O 199	0	0
5	182-A	192	Total 192	O 192	0	0
5	183-A	199	Total 199	O 199	0	0
5	184-A	187	Total 187	O 187	0	0
5	185-A	174	Total 174	O 174	0	0
5	186-A	169	Total 169	O 169	0	0
5	187-A	165	Total 165	O 165	0	0
5	188-A	180	Total 180	O 180	0	0
5	189-A	175	Total 175	O 175	0	0
5	190-A	181	Total 181	O 181	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	191-A	192	Total 192	O 192	0	0
5	192-A	191	Total 191	O 191	0	0
5	193-A	190	Total 190	O 190	0	0
5	194-A	193	Total 193	O 193	0	0
5	195-A	194	Total 194	O 194	0	0
5	196-A	186	Total 186	O 186	0	0
5	197-A	167	Total 167	O 167	0	0
5	198-A	174	Total 174	O 174	0	0
5	199-A	184	Total 184	O 184	0	0
5	200-A	190	Total 190	O 190	0	0
5	201-A	189	Total 189	O 189	0	0
5	202-A	171	Total 171	O 171	0	0
5	203-A	185	Total 185	O 185	0	0
5	204-A	188	Total 188	O 188	0	0
5	205-A	185	Total 185	O 185	0	0
5	206-A	186	Total 186	O 186	0	0
5	207-A	199	Total 199	O 199	0	0
5	208-A	186	Total 186	O 186	0	0
5	209-A	179	Total 179	O 179	0	0
5	210-A	179	Total 179	O 179	0	0
5	211-A	176	Total 176	O 176	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	212-A	175	Total O 175 175	0	0
5	213-A	180	Total O 180 180	0	0
5	214-A	181	Total O 181 181	0	0
5	215-A	191	Total O 191 191	0	0
5	216-A	185	Total O 185 185	0	0
5	217-A	204	Total O 204 204	0	0
5	218-A	191	Total O 191 191	0	0
5	219-A	176	Total O 176 176	0	0
5	220-A	185	Total O 185 185	0	0
5	221-A	179	Total O 179 179	0	0
5	222-A	173	Total O 173 173	0	0
5	223-A	180	Total O 180 180	0	0
5	224-A	178	Total O 178 178	0	0
5	225-A	187	Total O 187 187	0	0
5	226-A	189	Total O 189 189	0	0
5	227-A	187	Total O 187 187	0	0
5	228-A	184	Total O 184 184	0	0
5	229-A	183	Total O 183 183	0	0
5	230-A	193	Total O 193 193	0	0
5	231-A	198	Total O 198 198	0	0
5	232-A	183	Total O 183 183	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	233-A	180	Total 180	O 180	0	0
5	234-A	175	Total 175	O 175	0	0
5	235-A	201	Total 201	O 201	0	0
5	236-A	204	Total 204	O 204	0	0
5	237-A	193	Total 193	O 193	0	0
5	238-A	159	Total 159	O 159	0	0
5	239-A	164	Total 164	O 164	0	0
5	240-A	179	Total 179	O 179	0	0
5	241-A	183	Total 183	O 183	0	0
5	242-A	183	Total 183	O 183	0	0
5	243-A	194	Total 194	O 194	0	0
5	244-A	205	Total 205	O 205	0	0
5	245-A	198	Total 198	O 198	0	0
5	246-A	166	Total 166	O 166	0	0
5	247-A	171	Total 171	O 171	0	0
5	248-A	171	Total 171	O 171	0	0
5	249-A	191	Total 191	O 191	0	0
5	250-A	202	Total 202	O 202	0	0

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

3 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	33.96Å 44.82Å 98.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 0.85	Depositor
% Data completeness (in resolution range)	98.0 (49.00-0.85)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 0.85Å)	Xtrriage
Refinement program	PHENIX 1.8.4-1496	Depositor
R, R_{free}	0.126 , 0.144	Depositor
Wilson B-factor (Å ²)	7.7	Xtrriage
Anisotropy	0.182	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	699880	wwPDB-VP
Average B, all atoms (Å ²)	6.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.86% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

validation-pack failed to run properly - this section is therefore empty.

4.5 Carbohydrates [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.6 Ligand geometry [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.7 Other polymers [i](#)

validation-pack failed to run properly - this section is therefore 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 failed to run properly - this section is therefore empty.

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

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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