



# wwPDB X-ray Structure Validation Summary 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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			

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

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

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

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

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

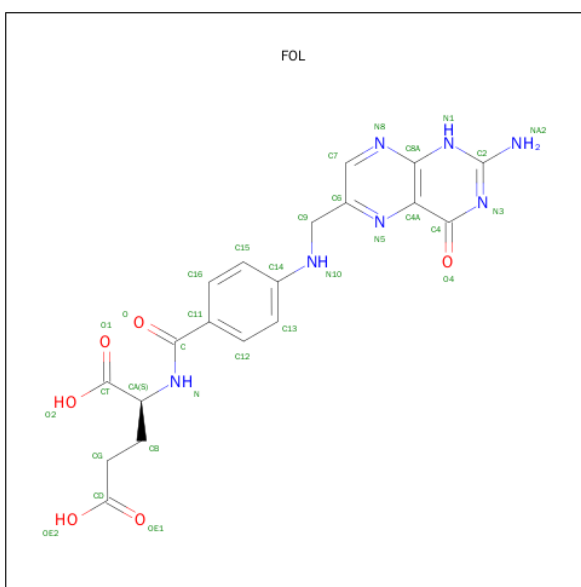
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	122-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	123-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	124-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	125-A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

- Molecule 2 is FOLIC ACID (three-letter code: FOL) (formula: C<sub>19</sub>H<sub>19</sub>N<sub>7</sub>O<sub>6</sub>).



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

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

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

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

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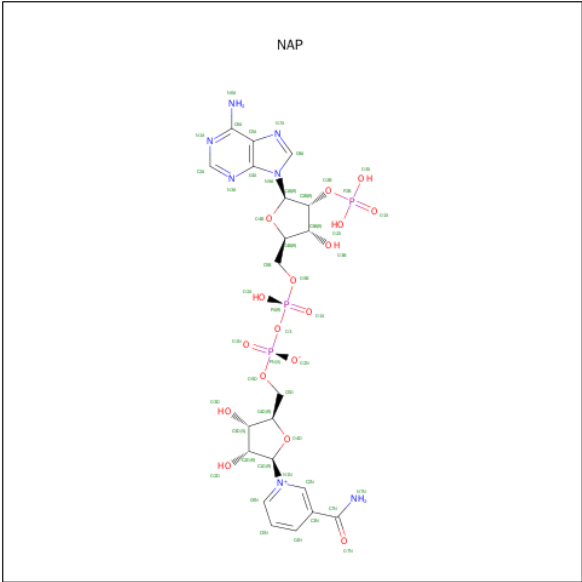
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	92-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	93-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	94-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	95-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	96-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	97-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	98-A	1	Total 49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

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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	120-A	1	Total	C	H	N	O	P	
			73	21	25	7	17	3	
3	121-A	1	Total	C	H	N	O	P	
			73	21	25	7	17	3	
3	122-A	1	Total	C	H	N	O	P	
			73	21	25	7	17	3	
3	123-A	1	Total	C	H	N	O	P	
			73	21	25	7	17	3	
3	124-A	1	Total	C	H	N	O	P	
			73	21	25	7	17	3	
3	125-A	1	Total	C	H	N	O	P	
			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	122-A	2	Total	Mn		
			2	2	0	0
4	110-A	2	Total	Mn		
			2	2	0	0
4	37-A	2	Total	Mn		
			2	2	0	0
4	80-A	2	Total	Mn		
			2	2	0	0
4	94-A	2	Total	Mn		
			2	2	0	0
4	60-A	2	Total	Mn		
			2	2	0	0
4	123-A	2	Total	Mn		
			2	2	0	0
4	44-A	2	Total	Mn		
			2	2	0	0
4	50-A	2	Total	Mn		
			2	2	0	0
4	104-A	2	Total	Mn		
			2	2	0	0
4	12-A	2	Total	Mn		
			2	2	0	0
4	114-A	2	Total	Mn		
			2	2	0	0
4	19-A	2	Total	Mn		
			2	2	0	0

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

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

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

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

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

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

- Molecule 5 is water.

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

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

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	76-A	93	Total 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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	118-A	107	Total 107	O 107	0	0
5	119-A	106	Total 106	O 106	0	0
5	120-A	105	Total 105	O 105	0	0
5	121-A	115	Total 115	O 115	0	0
5	122-A	97	Total 97	O 97	0	0
5	123-A	105	Total 105	O 105	0	0
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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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.