wwPDB X-ray Structure Validation Summary Report (i)

May 23, 2024 – 04:43 PM EDT

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

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

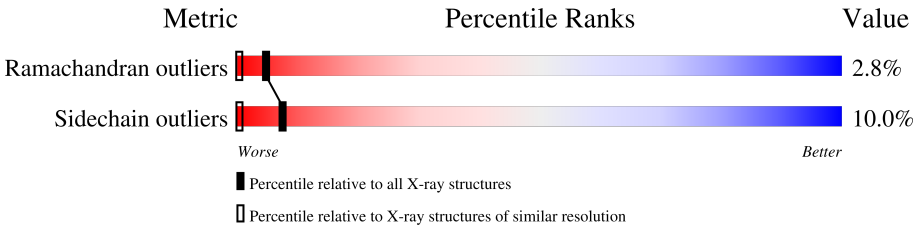
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 451154 atoms, of which 211088 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Dihydrofolate reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	2-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	3-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	4-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	5-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	6-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	7-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	8-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	9-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	10-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	11-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	12-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	13-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	14-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	15-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	16-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	18-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	19-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	20-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	21-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	22-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	23-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	24-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	25-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	26-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	27-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	28-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	29-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	30-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	31-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	32-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	33-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	34-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	35-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	36-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	37-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	39-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	40-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	41-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	42-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	43-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	44-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	45-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	46-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	47-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	48-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	49-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	50-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	51-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	52-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	53-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	54-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	55-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	56-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	57-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	58-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	59-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	60-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	61-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	62-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	63-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	64-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	65-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	66-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	67-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	68-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	69-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	70-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	71-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	72-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	73-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	74-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	75-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	76-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	77-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	78-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	79-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	80-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	81-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	82-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	83-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	84-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	85-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	86-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	87-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	88-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	89-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	90-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	91-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	92-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	93-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	94-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	95-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	96-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	97-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	98-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	99-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	100-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	101-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	102-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	103-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	104-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	105-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	106-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	107-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	108-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	109-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	110-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	111-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	112-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	113-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	114-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	115-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	116-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	117-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	118-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	119-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	120-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	121-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	122-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	123-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	124-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	125-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	126-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	127-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	128-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	129-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	130-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	131-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	132-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	133-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	134-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	135-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	136-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	137-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	138-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	139-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	140-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	141-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	142-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			

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

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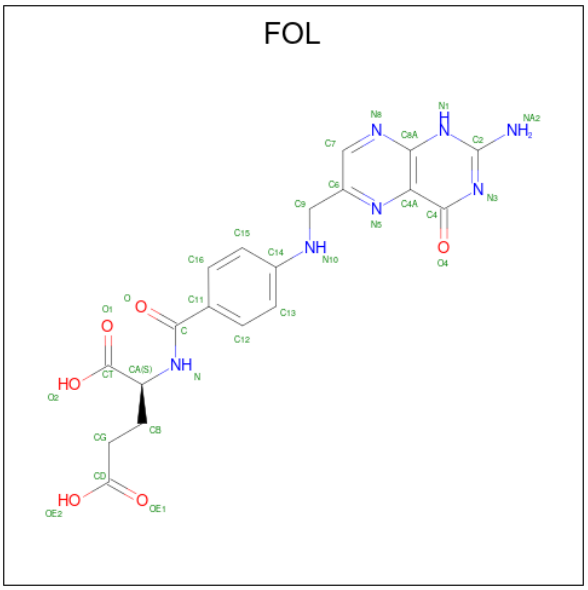
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	164-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	165-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	166-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	167-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239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

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



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	8-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	29-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	50-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	71-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	92-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
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		

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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		
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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	134-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
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		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	155-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	156-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	157-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	158-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	159-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	160-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	161-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	162-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	163-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	164-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	165-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	166-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	167-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	2	Total	Ca	0	0
			2	2		
3	2-A	2	Total	Ca	0	0
			2	2		
3	3-A	2	Total	Ca	0	0
			2	2		
3	4-A	2	Total	Ca	0	0
			2	2		
3	5-A	2	Total	Ca	0	0
			2	2		
3	6-A	2	Total	Ca	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	7-A	2	Total Ca 2 2	0	0
3	8-A	2	Total Ca 2 2	0	0
3	9-A	2	Total Ca 2 2	0	0
3	10-A	2	Total Ca 2 2	0	0
3	11-A	2	Total Ca 2 2	0	0
3	12-A	2	Total Ca 2 2	0	0
3	13-A	2	Total Ca 2 2	0	0
3	14-A	2	Total Ca 2 2	0	0
3	15-A	2	Total Ca 2 2	0	0
3	16-A	2	Total Ca 2 2	0	0
3	17-A	2	Total Ca 2 2	0	0
3	18-A	2	Total Ca 2 2	0	0
3	19-A	2	Total Ca 2 2	0	0
3	20-A	2	Total Ca 2 2	0	0
3	21-A	2	Total Ca 2 2	0	0
3	22-A	2	Total Ca 2 2	0	0
3	23-A	2	Total Ca 2 2	0	0
3	24-A	2	Total Ca 2 2	0	0
3	25-A	2	Total Ca 2 2	0	0
3	26-A	2	Total Ca 2 2	0	0
3	27-A	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	28-A	2	Total Ca 2 2	0	0
3	29-A	2	Total Ca 2 2	0	0
3	30-A	2	Total Ca 2 2	0	0
3	31-A	2	Total Ca 2 2	0	0
3	32-A	2	Total Ca 2 2	0	0
3	33-A	2	Total Ca 2 2	0	0
3	34-A	2	Total Ca 2 2	0	0
3	35-A	2	Total Ca 2 2	0	0
3	36-A	2	Total Ca 2 2	0	0
3	37-A	2	Total Ca 2 2	0	0
3	38-A	2	Total Ca 2 2	0	0
3	39-A	2	Total Ca 2 2	0	0
3	40-A	2	Total Ca 2 2	0	0
3	41-A	2	Total Ca 2 2	0	0
3	42-A	2	Total Ca 2 2	0	0
3	43-A	2	Total Ca 2 2	0	0
3	44-A	2	Total Ca 2 2	0	0
3	45-A	2	Total Ca 2 2	0	0
3	46-A	2	Total Ca 2 2	0	0
3	47-A	2	Total Ca 2 2	0	0
3	48-A	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	49-A	2	Total Ca 2 2	0	0
3	50-A	2	Total Ca 2 2	0	0
3	51-A	2	Total Ca 2 2	0	0
3	52-A	2	Total Ca 2 2	0	0
3	53-A	2	Total Ca 2 2	0	0
3	54-A	2	Total Ca 2 2	0	0
3	55-A	2	Total Ca 2 2	0	0
3	56-A	2	Total Ca 2 2	0	0
3	57-A	2	Total Ca 2 2	0	0
3	58-A	2	Total Ca 2 2	0	0
3	59-A	2	Total Ca 2 2	0	0
3	60-A	2	Total Ca 2 2	0	0
3	61-A	2	Total Ca 2 2	0	0
3	62-A	2	Total Ca 2 2	0	0
3	63-A	2	Total Ca 2 2	0	0
3	64-A	2	Total Ca 2 2	0	0
3	65-A	2	Total Ca 2 2	0	0
3	66-A	2	Total Ca 2 2	0	0
3	67-A	2	Total Ca 2 2	0	0
3	68-A	2	Total Ca 2 2	0	0
3	69-A	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	70-A	2	Total Ca 2 2	0	0
3	71-A	2	Total Ca 2 2	0	0
3	72-A	2	Total Ca 2 2	0	0
3	73-A	2	Total Ca 2 2	0	0
3	74-A	2	Total Ca 2 2	0	0
3	75-A	2	Total Ca 2 2	0	0
3	76-A	2	Total Ca 2 2	0	0
3	77-A	2	Total Ca 2 2	0	0
3	78-A	2	Total Ca 2 2	0	0
3	79-A	2	Total Ca 2 2	0	0
3	80-A	2	Total Ca 2 2	0	0
3	81-A	2	Total Ca 2 2	0	0
3	82-A	2	Total Ca 2 2	0	0
3	83-A	2	Total Ca 2 2	0	0
3	84-A	2	Total Ca 2 2	0	0
3	85-A	2	Total Ca 2 2	0	0
3	86-A	2	Total Ca 2 2	0	0
3	87-A	2	Total Ca 2 2	0	0
3	88-A	2	Total Ca 2 2	0	0
3	89-A	2	Total Ca 2 2	0	0
3	90-A	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	91-A	2	Total Ca 2 2	0	0
3	92-A	2	Total Ca 2 2	0	0
3	93-A	2	Total Ca 2 2	0	0
3	94-A	2	Total Ca 2 2	0	0
3	95-A	2	Total Ca 2 2	0	0
3	96-A	2	Total Ca 2 2	0	0
3	97-A	2	Total Ca 2 2	0	0
3	98-A	2	Total Ca 2 2	0	0
3	99-A	2	Total Ca 2 2	0	0
3	100-A	2	Total Ca 2 2	0	0
3	101-A	2	Total Ca 2 2	0	0
3	102-A	2	Total Ca 2 2	0	0
3	103-A	2	Total Ca 2 2	0	0
3	104-A	2	Total Ca 2 2	0	0
3	105-A	2	Total Ca 2 2	0	0
3	106-A	2	Total Ca 2 2	0	0
3	107-A	2	Total Ca 2 2	0	0
3	108-A	2	Total Ca 2 2	0	0
3	109-A	2	Total Ca 2 2	0	0
3	110-A	2	Total Ca 2 2	0	0
3	111-A	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	112-A	2	Total Ca 2 2	0	0
3	113-A	2	Total Ca 2 2	0	0
3	114-A	2	Total Ca 2 2	0	0
3	115-A	2	Total Ca 2 2	0	0
3	116-A	2	Total Ca 2 2	0	0
3	117-A	2	Total Ca 2 2	0	0
3	118-A	2	Total Ca 2 2	0	0
3	119-A	2	Total Ca 2 2	0	0
3	120-A	2	Total Ca 2 2	0	0
3	121-A	2	Total Ca 2 2	0	0
3	122-A	2	Total Ca 2 2	0	0
3	123-A	2	Total Ca 2 2	0	0
3	124-A	2	Total Ca 2 2	0	0
3	125-A	2	Total Ca 2 2	0	0
3	126-A	2	Total Ca 2 2	0	0
3	127-A	2	Total Ca 2 2	0	0
3	128-A	2	Total Ca 2 2	0	0
3	129-A	2	Total Ca 2 2	0	0
3	130-A	2	Total Ca 2 2	0	0
3	131-A	2	Total Ca 2 2	0	0
3	132-A	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	133-A	2	Total Ca 2 2	0	0
3	134-A	2	Total Ca 2 2	0	0
3	135-A	2	Total Ca 2 2	0	0
3	136-A	2	Total Ca 2 2	0	0
3	137-A	2	Total Ca 2 2	0	0
3	138-A	2	Total Ca 2 2	0	0
3	139-A	2	Total Ca 2 2	0	0
3	140-A	2	Total Ca 2 2	0	0
3	141-A	2	Total Ca 2 2	0	0
3	142-A	2	Total Ca 2 2	0	0
3	143-A	2	Total Ca 2 2	0	0
3	144-A	2	Total Ca 2 2	0	0
3	145-A	2	Total Ca 2 2	0	0
3	146-A	2	Total Ca 2 2	0	0
3	147-A	2	Total Ca 2 2	0	0
3	148-A	2	Total Ca 2 2	0	0
3	149-A	2	Total Ca 2 2	0	0
3	150-A	2	Total Ca 2 2	0	0
3	151-A	2	Total Ca 2 2	0	0
3	152-A	2	Total Ca 2 2	0	0
3	153-A	2	Total Ca 2 2	0	0

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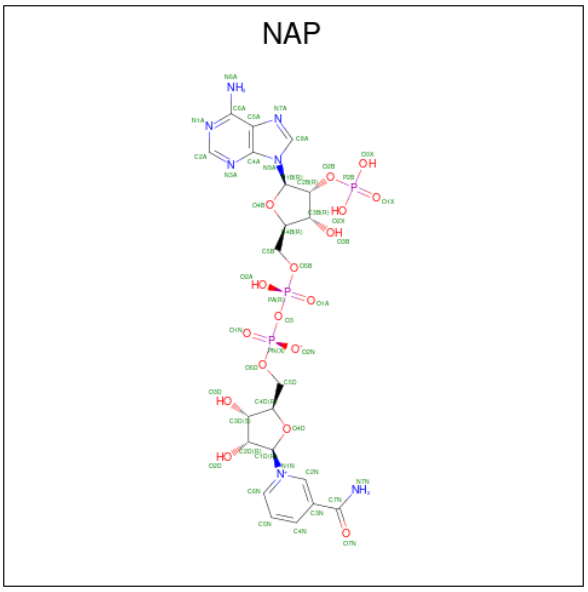
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	154-A	2	Total Ca 2 2	0	0
3	155-A	2	Total Ca 2 2	0	0
3	156-A	2	Total Ca 2 2	0	0
3	157-A	2	Total Ca 2 2	0	0
3	158-A	2	Total Ca 2 2	0	0
3	159-A	2	Total Ca 2 2	0	0
3	160-A	2	Total Ca 2 2	0	0
3	161-A	2	Total Ca 2 2	0	0
3	162-A	2	Total Ca 2 2	0	0
3	163-A	2	Total Ca 2 2	0	0
3	164-A	2	Total Ca 2 2	0	0
3	165-A	2	Total Ca 2 2	0	0
3	166-A	2	Total Ca 2 2	0	0
3	167-A	2	Total Ca 2 2	0	0

- Molecule 4 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
4	1-A	1	Total	C	H	N	O	P	0	0
			72	21	24	7	17	3		
4	2-A	1	Total	C	H	N	O	P	0	0
			72	21	24	7	17	3		
4	3-A	1	Total	C	H	N	O	P	0	0
			72	21	24	7	17	3		
4	4-A	1	Total	C	H	N	O	P	0	0
			72	21	24	7	17	3		
4	5-A	1	Total	C	H	N	O	P	0	0
			72	21	24	7	17	3		
4	6-A	1	Total	C	H	N	O	P	0	0
			72	21	24	7	17	3		
4	7-A	1	Total	C	H	N	O	P	0	0
			72	21	24	7	17	3		
4	8-A	1	Total	C	H	N	O	P	0	0
			72	21	24	7	17	3		
4	9-A	1	Total	C	H	N	O	P	0	0
			72	21	24	7	17	3		
4	10-A	1	Total	C	H	N	O	P	0	0
			72	21	24	7	17	3		
4	11-A	1	Total	C	H	N	O	P	0	0
			72	21	24	7	17	3		
4	12-A	1	Total	C	H	N	O	P	0	0
			72	21	24	7	17	3		
4	13-A	1	Total	C	H	N	O	P	0	0
			72	21	24	7	17	3		
4	14-A	1	Total	C	H	N	O	P	0	0
			72	21	24	7	17	3		

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

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

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

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

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

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

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

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

- Molecule 5 is water.

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

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

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

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

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

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

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

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

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

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	34.32Å 45.51Å 98.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.34 – 1.35	Depositor
% Data completeness (in resolution range)	91.6 (41.34-1.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 1.35Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement: 1.8.4_1496)	Depositor
R, R_{free}	0.118 , 0.153	Depositor
Wilson B-factor (Å^2)	11.2	Xtriage
Anisotropy	0.170	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	451154	wwPDB-VP
Average B, all atoms (Å^2)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, CA, FOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1-A	0.70	0/1302	0.91	3/1770 (0.2%)
1	2-A	0.71	0/1302	0.91	2/1770 (0.1%)
1	3-A	0.70	0/1302	1.01	4/1770 (0.2%)
1	4-A	0.76	2/1302 (0.2%)	0.97	5/1770 (0.3%)
1	5-A	0.73	0/1302	1.03	3/1770 (0.2%)
1	6-A	0.91	4/1302 (0.3%)	1.03	6/1770 (0.3%)
1	7-A	0.94	6/1302 (0.5%)	1.09	8/1770 (0.5%)
1	8-A	0.86	5/1302 (0.4%)	1.14	11/1770 (0.6%)
1	9-A	0.82	0/1302	1.00	6/1770 (0.3%)
1	10-A	0.66	0/1302	0.87	2/1770 (0.1%)
1	11-A	0.73	1/1302 (0.1%)	0.94	4/1770 (0.2%)
1	12-A	0.73	1/1302 (0.1%)	0.98	3/1770 (0.2%)
1	13-A	0.67	1/1302 (0.1%)	0.91	2/1770 (0.1%)
1	14-A	0.78	1/1302 (0.1%)	0.92	2/1770 (0.1%)
1	15-A	0.76	0/1302	0.94	1/1770 (0.1%)
1	16-A	0.72	0/1302	0.99	5/1770 (0.3%)
1	17-A	0.75	3/1302 (0.2%)	0.94	2/1770 (0.1%)
1	18-A	0.74	1/1302 (0.1%)	0.91	1/1770 (0.1%)
1	19-A	0.73	2/1302 (0.2%)	0.90	1/1770 (0.1%)
1	20-A	0.76	2/1302 (0.2%)	0.93	7/1770 (0.4%)
1	21-A	0.76	2/1302 (0.2%)	0.97	5/1770 (0.3%)
1	22-A	0.71	0/1302	0.99	4/1770 (0.2%)
1	23-A	0.75	0/1302	0.95	4/1770 (0.2%)
1	24-A	0.71	0/1302	0.95	3/1770 (0.2%)
1	25-A	0.72	0/1302	0.93	2/1770 (0.1%)
1	26-A	0.78	0/1302	0.95	4/1770 (0.2%)
1	27-A	0.78	0/1302	0.98	5/1770 (0.3%)
1	28-A	0.81	1/1239 (0.1%)	1.03	4/1688 (0.2%)
All	All	0.76	32/36393 (0.1%)	0.97	109/49478 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	1
1	2-A	0	1
1	3-A	0	1
1	4-A	0	3
1	5-A	0	3
1	6-A	0	2
1	7-A	0	5
1	8-A	0	4
1	9-A	0	5
1	10-A	0	5
1	11-A	0	2
1	12-A	0	3
1	13-A	0	3
1	14-A	0	3
1	15-A	0	1
1	16-A	0	3
1	17-A	0	4
1	18-A	0	2
1	19-A	0	2
1	20-A	0	2
1	21-A	0	2
1	22-A	0	1
1	23-A	0	3
1	24-A	0	2
1	25-A	0	3
1	26-A	0	3
1	27-A	0	1
1	28-A	0	3
1	29-A	0	1
1	30-A	0	1
1	31-A	0	2
1	32-A	0	4
1	33-A	0	6
1	34-A	0	3
1	35-A	0	2
1	36-A	0	4
1	37-A	0	2
1	38-A	0	2
1	39-A	0	1
1	40-A	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	41-A	0	4
1	42-A	0	2
1	43-A	0	1
1	44-A	0	2
1	45-A	0	2
1	46-A	0	3
1	47-A	0	1
1	48-A	0	2
1	49-A	0	4
1	50-A	0	4
1	51-A	0	3
1	52-A	0	4
1	53-A	0	4
1	57-A	0	1
1	61-A	0	1
1	62-A	0	1
1	63-A	0	1
1	66-A	0	3
1	67-A	0	1
1	68-A	0	2
1	69-A	0	1
1	70-A	0	1
1	71-A	0	2
1	72-A	0	4
1	73-A	0	2
1	74-A	0	1
1	75-A	0	1
1	78-A	0	1
1	79-A	0	2
1	80-A	0	2
1	81-A	0	2
1	82-A	0	1
1	83-A	0	1
1	84-A	0	1
1	85-A	0	1
1	86-A	0	2
1	88-A	0	1
1	89-A	0	2
1	90-A	0	2
1	91-A	0	1
1	94-A	0	1
1	95-A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	97-A	0	1
1	98-A	0	1
1	99-A	0	1
1	100-A	0	1
1	102-A	0	1
1	104-A	0	2
1	105-A	0	4
1	107-A	0	3
1	108-A	0	2
1	109-A	0	2
1	110-A	0	2
1	111-A	0	2
1	112-A	0	2
1	113-A	0	5
1	114-A	0	4
1	115-A	0	3
1	116-A	0	3
1	117-A	0	4
1	122-A	0	3
1	124-A	0	1
1	126-A	0	1
1	127-A	0	1
1	130-A	0	1
1	131-A	0	2
1	132-A	0	3
1	133-A	0	3
1	134-A	0	1
1	136-A	0	2
1	137-A	0	2
1	138-A	0	3
1	139-A	0	1
1	140-A	0	2
1	141-A	0	1
1	143-A	0	2
1	144-A	0	2
1	145-A	0	4
1	146-A	0	4
1	147-A	0	1
1	149-A	0	2
1	150-A	0	2
1	151-A	0	2
1	152-A	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	154-A	0	1
1	155-A	0	2
1	156-A	0	1
1	157-A	0	3
1	158-A	0	2
1	159-A	0	5
1	160-A	0	3
1	161-A	0	3
1	162-A	0	5
1	163-A	0	5
1	164-A	0	5
1	165-A	0	1
1	166-A	0	2
1	167-A	0	1
All	All	0	312

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	6-A	152	CYS	CB-SG	10.09	1.99	1.82
1	6-A	10	VAL	CB-CG2	-7.95	1.36	1.52
1	14-A	118	GLU	CB-CG	7.91	1.67	1.52
1	21-A	21	PRO	CA-C	7.22	1.67	1.52
1	8-A	101	GLU	CB-CG	-7.17	1.38	1.52

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	8-A	20	MET	C-N-CD	-13.50	90.90	120.60
1	5-A	129	GLU	C-N-CD	-13.17	91.63	120.60
1	8-A	16	MET	CG-SD-CE	10.75	117.40	100.20
1	4-A	129	GLU	C-N-CD	-10.24	98.06	120.60
1	16-A	129	GLU	C-N-CD	-9.63	99.41	120.60

There are no chirality outliers.

5 of 312 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	128	TYR	Peptide
1	2-A	20	MET	Peptide
1	3-A	129	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	4-A	127	ASP	Peptide
1	4-A	86	GLY	Peptide

4.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1268	1223	1223	0	0
1	2-A	1268	1223	1223	0	0
1	3-A	1268	1223	1223	0	0
1	4-A	1268	1223	1223	0	0
1	5-A	1268	1223	1223	0	0
1	6-A	1268	1223	1223	0	0
1	7-A	1268	1223	1223	0	0
1	8-A	1268	1223	1223	0	0
1	9-A	1268	1223	1223	0	0
1	10-A	1268	1223	1223	0	0
1	11-A	1268	1223	1223	0	0
1	12-A	1268	1223	1222	0	0
1	13-A	1268	1223	1223	0	0
1	14-A	1268	1223	1223	0	0
1	15-A	1268	1223	1223	0	0
1	16-A	1268	1223	1223	0	0
1	17-A	1268	1223	1223	0	0
1	18-A	1268	1223	1223	0	0
1	19-A	1268	1223	1223	0	0
1	20-A	1268	1223	1223	0	0
1	21-A	1268	1223	1223	0	0
1	22-A	1268	1223	1223	0	0
1	23-A	1268	1223	1223	0	0
1	24-A	1268	1223	1223	0	0
1	25-A	1268	1223	1223	0	0
1	26-A	1268	1223	1223	0	0
1	27-A	1268	1223	1222	0	0
1	28-A	1268	1223	1158	0	0
1	29-A	1268	1223	0	0	0
1	30-A	1268	1223	0	0	0
1	31-A	1268	1223	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	32-A	1268	1223	0	0	0
1	33-A	1268	1223	0	0	0
1	34-A	1268	1223	0	0	0
1	35-A	1268	1223	0	0	0
1	36-A	1268	1223	0	0	0
1	37-A	1268	1223	0	0	0
1	38-A	1268	1223	0	0	0
1	39-A	1268	1223	0	0	0
1	40-A	1268	1223	0	0	0
1	41-A	1268	1223	0	0	0
1	42-A	1268	1223	0	0	0
1	43-A	1268	1223	0	0	0
1	44-A	1268	1223	0	0	0
1	45-A	1268	1223	0	0	0
1	46-A	1268	1223	0	0	0
1	47-A	1268	1223	0	0	0
1	48-A	1268	1223	0	0	0
1	49-A	1268	1223	0	0	0
1	50-A	1268	1223	0	0	0
1	51-A	1268	1223	0	0	0
1	52-A	1268	1223	0	0	0
1	53-A	1268	1223	0	0	0
1	54-A	1268	1223	0	0	0
1	55-A	1268	1223	0	0	0
1	56-A	1268	1223	0	0	0
1	57-A	1268	1223	0	0	0
1	58-A	1268	1223	0	0	0
1	59-A	1268	1223	0	0	0
1	60-A	1268	1223	0	0	0
1	61-A	1268	1223	0	0	0
1	62-A	1268	1223	0	0	0
1	63-A	1268	1223	0	0	0
1	64-A	1268	1223	0	0	0
1	65-A	1268	1223	0	0	0
1	66-A	1268	1223	0	0	0
1	67-A	1268	1223	0	0	0
1	68-A	1268	1223	0	0	0
1	69-A	1268	1223	0	0	0
1	70-A	1268	1223	0	0	0
1	71-A	1268	1223	0	0	0
1	72-A	1268	1223	0	0	0
1	73-A	1268	1223	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	74-A	1268	1223	0	0	0
1	75-A	1268	1223	0	0	0
1	76-A	1268	1223	0	0	0
1	77-A	1268	1223	0	0	0
1	78-A	1268	1223	0	0	0
1	79-A	1268	1223	0	0	0
1	80-A	1268	1223	0	0	0
1	81-A	1268	1223	0	0	0
1	82-A	1268	1223	0	0	0
1	83-A	1268	1223	0	0	0
1	84-A	1268	1223	0	0	0
1	85-A	1268	1223	0	0	0
1	86-A	1268	1223	0	0	0
1	87-A	1268	1223	0	0	0
1	88-A	1268	1223	0	0	0
1	89-A	1268	1223	0	0	0
1	90-A	1268	1223	0	0	0
1	91-A	1268	1223	0	0	0
1	92-A	1268	1223	0	0	0
1	93-A	1268	1223	0	0	0
1	94-A	1268	1223	0	0	0
1	95-A	1268	1223	0	0	0
1	96-A	1268	1223	0	0	0
1	97-A	1268	1223	0	0	0
1	98-A	1268	1223	0	0	0
1	99-A	1268	1223	0	0	0
1	100-A	1268	1223	0	0	0
1	101-A	1268	1223	0	0	0
1	102-A	1268	1223	0	0	0
1	103-A	1268	1223	0	0	0
1	104-A	1268	1223	0	0	0
1	105-A	1268	1223	0	0	0
1	106-A	1268	1223	0	0	0
1	107-A	1268	1223	0	0	0
1	108-A	1268	1223	0	0	0
1	109-A	1268	1223	0	0	0
1	110-A	1268	1223	0	0	0
1	111-A	1268	1223	0	0	0
1	112-A	1268	1223	0	0	0
1	113-A	1268	1223	0	0	0
1	114-A	1268	1223	0	0	0
1	115-A	1268	1223	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	116-A	1268	1223	0	0	0
1	117-A	1268	1223	0	0	0
1	118-A	1268	1223	0	0	0
1	119-A	1268	1223	0	0	0
1	120-A	1268	1223	0	0	0
1	121-A	1268	1223	0	0	0
1	122-A	1268	1223	0	0	0
1	123-A	1268	1223	0	0	0
1	124-A	1268	1223	0	0	0
1	125-A	1268	1223	0	0	0
1	126-A	1268	1223	0	0	0
1	127-A	1268	1223	0	0	0
1	128-A	1268	1223	0	0	0
1	129-A	1268	1223	0	0	0
1	130-A	1268	1223	0	0	0
1	131-A	1268	1223	0	0	0
1	132-A	1268	1223	0	0	0
1	133-A	1268	1223	0	0	0
1	134-A	1268	1223	0	0	0
1	135-A	1268	1223	0	0	0
1	136-A	1268	1223	0	0	0
1	137-A	1268	1223	0	0	0
1	138-A	1268	1223	0	0	0
1	139-A	1268	1223	0	0	0
1	140-A	1268	1223	0	0	0
1	141-A	1268	1223	0	0	0
1	142-A	1268	1223	0	0	0
1	143-A	1268	1223	0	0	0
1	144-A	1268	1223	0	0	0
1	145-A	1268	1223	0	0	0
1	146-A	1268	1223	0	0	0
1	147-A	1268	1223	0	0	0
1	148-A	1268	1223	0	0	0
1	149-A	1268	1223	0	0	0
1	150-A	1268	1223	0	0	0
1	151-A	1268	1223	0	0	0
1	152-A	1268	1223	0	0	0
1	153-A	1268	1223	0	0	0
1	154-A	1268	1223	0	0	0
1	155-A	1268	1223	0	0	0
1	156-A	1268	1223	0	0	0
1	157-A	1268	1223	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	158-A	1268	1223	0	0	0
1	159-A	1268	1223	0	0	0
1	160-A	1268	1223	0	0	0
1	161-A	1268	1223	0	0	0
1	162-A	1268	1223	0	0	0
1	163-A	1268	1223	0	0	0
1	164-A	1268	1223	0	0	0
1	165-A	1268	1223	0	0	0
1	166-A	1268	1223	0	0	0
1	167-A	1268	1223	0	0	0
2	1-A	32	17	17	0	0
2	2-A	32	17	17	0	0
2	3-A	32	17	17	0	0
2	4-A	32	17	17	0	0
2	5-A	32	17	17	0	0
2	6-A	32	17	17	0	0
2	7-A	32	17	17	0	0
2	8-A	32	17	17	0	0
2	9-A	32	17	17	0	0
2	10-A	32	17	17	0	0
2	11-A	32	17	17	0	0
2	12-A	32	17	17	0	0
2	13-A	32	17	17	0	0
2	14-A	32	17	17	0	0
2	15-A	32	17	17	0	0
2	16-A	32	17	17	0	0
2	17-A	32	17	17	0	0
2	18-A	32	17	17	0	0
2	19-A	32	17	17	0	0
2	20-A	32	17	17	0	0
2	21-A	32	17	17	0	0
2	22-A	32	17	17	0	0
2	23-A	32	17	17	0	0
2	24-A	32	17	17	0	0
2	25-A	32	17	17	0	0
2	26-A	32	17	17	0	0
2	27-A	32	17	17	0	0
2	28-A	32	17	0	0	0
2	29-A	32	17	0	0	0
2	30-A	32	17	0	0	0
2	31-A	32	17	0	0	0
2	32-A	32	17	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	33-A	32	17	0	0	0
2	34-A	32	17	0	0	0
2	35-A	32	17	0	0	0
2	36-A	32	17	0	0	0
2	37-A	32	17	0	0	0
2	38-A	32	17	0	0	0
2	39-A	32	17	0	0	0
2	40-A	32	17	0	0	0
2	41-A	32	17	0	0	0
2	42-A	32	17	0	0	0
2	43-A	32	17	0	0	0
2	44-A	32	17	0	0	0
2	45-A	32	17	0	0	0
2	46-A	32	17	0	0	0
2	47-A	32	17	0	0	0
2	48-A	32	17	0	0	0
2	49-A	32	17	0	0	0
2	50-A	32	17	0	0	0
2	51-A	32	17	0	0	0
2	52-A	32	17	0	0	0
2	53-A	32	17	0	0	0
2	54-A	32	17	0	0	0
2	55-A	32	17	0	0	0
2	56-A	32	17	0	0	0
2	57-A	32	17	0	0	0
2	58-A	32	17	0	0	0
2	59-A	32	17	0	0	0
2	60-A	32	17	0	0	0
2	61-A	32	17	0	0	0
2	62-A	32	17	0	0	0
2	63-A	32	17	0	0	0
2	64-A	32	17	0	0	0
2	65-A	32	17	0	0	0
2	66-A	32	17	0	0	0
2	67-A	32	17	0	0	0
2	68-A	32	17	0	0	0
2	69-A	32	17	0	0	0
2	70-A	32	17	0	0	0
2	71-A	32	17	0	0	0
2	72-A	32	17	0	0	0
2	73-A	32	17	0	0	0
2	74-A	32	17	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	75-A	32	17	0	0	0
2	76-A	32	17	0	0	0
2	77-A	32	17	0	0	0
2	78-A	32	17	0	0	0
2	79-A	32	17	0	0	0
2	80-A	32	17	0	0	0
2	81-A	32	17	0	0	0
2	82-A	32	17	0	0	0
2	83-A	32	17	0	0	0
2	84-A	32	17	0	0	0
2	85-A	32	17	0	0	0
2	86-A	32	17	0	0	0
2	87-A	32	17	0	0	0
2	88-A	32	17	0	0	0
2	89-A	32	17	0	0	0
2	90-A	32	17	0	0	0
2	91-A	32	17	0	0	0
2	92-A	32	17	0	0	0
2	93-A	32	17	0	0	0
2	94-A	32	17	0	0	0
2	95-A	32	17	0	0	0
2	96-A	32	17	0	0	0
2	97-A	32	17	0	0	0
2	98-A	32	17	0	0	0
2	99-A	32	17	0	0	0
2	100-A	32	17	0	0	0
2	101-A	32	17	0	0	0
2	102-A	32	17	0	0	0
2	103-A	32	17	0	0	0
2	104-A	32	17	0	0	0
2	105-A	32	17	0	0	0
2	106-A	32	17	0	0	0
2	107-A	32	17	0	0	0
2	108-A	32	17	0	0	0
2	109-A	32	17	0	0	0
2	110-A	32	17	0	0	0
2	111-A	32	17	0	0	0
2	112-A	32	17	0	0	0
2	113-A	32	17	0	0	0
2	114-A	32	17	0	0	0
2	115-A	32	17	0	0	0
2	116-A	32	17	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	117-A	32	17	0	0	0
2	118-A	32	17	0	0	0
2	119-A	32	17	0	0	0
2	120-A	32	17	0	0	0
2	121-A	32	17	0	0	0
2	122-A	32	17	0	0	0
2	123-A	32	17	0	0	0
2	124-A	32	17	0	0	0
2	125-A	32	17	0	0	0
2	126-A	32	17	0	0	0
2	127-A	32	17	0	0	0
2	128-A	32	17	0	0	0
2	129-A	32	17	0	0	0
2	130-A	32	17	0	0	0
2	131-A	32	17	0	0	0
2	132-A	32	17	0	0	0
2	133-A	32	17	0	0	0
2	134-A	32	17	0	0	0
2	135-A	32	17	0	0	0
2	136-A	32	17	0	0	0
2	137-A	32	17	0	0	0
2	138-A	32	17	0	0	0
2	139-A	32	17	0	0	0
2	140-A	32	17	0	0	0
2	141-A	32	17	0	0	0
2	142-A	32	17	0	0	0
2	143-A	32	17	0	0	0
2	144-A	32	17	0	0	0
2	145-A	32	17	0	0	0
2	146-A	32	17	0	0	0
2	147-A	32	17	0	0	0
2	148-A	32	17	0	0	0
2	149-A	32	17	0	0	0
2	150-A	32	17	0	0	0
2	151-A	32	17	0	0	0
2	152-A	32	17	0	0	0
2	153-A	32	17	0	0	0
2	154-A	32	17	0	0	0
2	155-A	32	17	0	0	0
2	156-A	32	17	0	0	0
2	157-A	32	17	0	0	0
2	158-A	32	17	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	159-A	32	17	0	0	0
2	160-A	32	17	0	0	0
2	161-A	32	17	0	0	0
2	162-A	32	17	0	0	0
2	163-A	32	17	0	0	0
2	164-A	32	17	0	0	0
2	165-A	32	17	0	0	0
2	166-A	32	17	0	0	0
2	167-A	32	17	0	0	0
3	1-A	2	0	0	0	0
3	2-A	2	0	0	0	0
3	3-A	2	0	0	0	0
3	4-A	2	0	0	0	0
3	5-A	2	0	0	0	0
3	6-A	2	0	0	0	0
3	7-A	2	0	0	0	0
3	8-A	2	0	0	0	0
3	9-A	2	0	0	0	0
3	10-A	2	0	0	0	0
3	11-A	2	0	0	0	0
3	12-A	2	0	0	0	0
3	13-A	2	0	0	0	0
3	14-A	2	0	0	0	0
3	15-A	2	0	0	0	0
3	16-A	2	0	0	0	0
3	17-A	2	0	0	0	0
3	18-A	2	0	0	0	0
3	19-A	2	0	0	0	0
3	20-A	2	0	0	0	0
3	21-A	2	0	0	0	0
3	22-A	2	0	0	0	0
3	23-A	2	0	0	0	0
3	24-A	2	0	0	0	0
3	25-A	2	0	0	0	0
3	26-A	2	0	0	0	0
3	27-A	2	0	0	0	0
3	28-A	2	0	0	0	0
3	29-A	2	0	0	0	0
3	30-A	2	0	0	0	0
3	31-A	2	0	0	0	0
3	32-A	2	0	0	0	0
3	33-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	34-A	2	0	0	0	0
3	35-A	2	0	0	0	0
3	36-A	2	0	0	0	0
3	37-A	2	0	0	0	0
3	38-A	2	0	0	0	0
3	39-A	2	0	0	0	0
3	40-A	2	0	0	0	0
3	41-A	2	0	0	0	0
3	42-A	2	0	0	0	0
3	43-A	2	0	0	0	0
3	44-A	2	0	0	0	0
3	45-A	2	0	0	0	0
3	46-A	2	0	0	0	0
3	47-A	2	0	0	0	0
3	48-A	2	0	0	0	0
3	49-A	2	0	0	0	0
3	50-A	2	0	0	0	0
3	51-A	2	0	0	0	0
3	52-A	2	0	0	0	0
3	53-A	2	0	0	0	0
3	54-A	2	0	0	0	0
3	55-A	2	0	0	0	0
3	56-A	2	0	0	0	0
3	57-A	2	0	0	0	0
3	58-A	2	0	0	0	0
3	59-A	2	0	0	0	0
3	60-A	2	0	0	0	0
3	61-A	2	0	0	0	0
3	62-A	2	0	0	0	0
3	63-A	2	0	0	0	0
3	64-A	2	0	0	0	0
3	65-A	2	0	0	0	0
3	66-A	2	0	0	0	0
3	67-A	2	0	0	0	0
3	68-A	2	0	0	0	0
3	69-A	2	0	0	0	0
3	70-A	2	0	0	0	0
3	71-A	2	0	0	0	0
3	72-A	2	0	0	0	0
3	73-A	2	0	0	0	0
3	74-A	2	0	0	0	0
3	75-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	76-A	2	0	0	0	0
3	77-A	2	0	0	0	0
3	78-A	2	0	0	0	0
3	79-A	2	0	0	0	0
3	80-A	2	0	0	0	0
3	81-A	2	0	0	0	0
3	82-A	2	0	0	0	0
3	83-A	2	0	0	0	0
3	84-A	2	0	0	0	0
3	85-A	2	0	0	0	0
3	86-A	2	0	0	0	0
3	87-A	2	0	0	0	0
3	88-A	2	0	0	0	0
3	89-A	2	0	0	0	0
3	90-A	2	0	0	0	0
3	91-A	2	0	0	0	0
3	92-A	2	0	0	0	0
3	93-A	2	0	0	0	0
3	94-A	2	0	0	0	0
3	95-A	2	0	0	0	0
3	96-A	2	0	0	0	0
3	97-A	2	0	0	0	0
3	98-A	2	0	0	0	0
3	99-A	2	0	0	0	0
3	100-A	2	0	0	0	0
3	101-A	2	0	0	0	0
3	102-A	2	0	0	0	0
3	103-A	2	0	0	0	0
3	104-A	2	0	0	0	0
3	105-A	2	0	0	0	0
3	106-A	2	0	0	0	0
3	107-A	2	0	0	0	0
3	108-A	2	0	0	0	0
3	109-A	2	0	0	0	0
3	110-A	2	0	0	0	0
3	111-A	2	0	0	0	0
3	112-A	2	0	0	0	0
3	113-A	2	0	0	0	0
3	114-A	2	0	0	0	0
3	115-A	2	0	0	0	0
3	116-A	2	0	0	0	0
3	117-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	118-A	2	0	0	0	0
3	119-A	2	0	0	0	0
3	120-A	2	0	0	0	0
3	121-A	2	0	0	0	0
3	122-A	2	0	0	0	0
3	123-A	2	0	0	0	0
3	124-A	2	0	0	0	0
3	125-A	2	0	0	0	0
3	126-A	2	0	0	0	0
3	127-A	2	0	0	0	0
3	128-A	2	0	0	0	0
3	129-A	2	0	0	0	0
3	130-A	2	0	0	0	0
3	131-A	2	0	0	0	0
3	132-A	2	0	0	0	0
3	133-A	2	0	0	0	0
3	134-A	2	0	0	0	0
3	135-A	2	0	0	0	0
3	136-A	2	0	0	0	0
3	137-A	2	0	0	0	0
3	138-A	2	0	0	0	0
3	139-A	2	0	0	0	0
3	140-A	2	0	0	0	0
3	141-A	2	0	0	0	0
3	142-A	2	0	0	0	0
3	143-A	2	0	0	0	0
3	144-A	2	0	0	0	0
3	145-A	2	0	0	0	0
3	146-A	2	0	0	0	0
3	147-A	2	0	0	0	0
3	148-A	2	0	0	0	0
3	149-A	2	0	0	0	0
3	150-A	2	0	0	0	0
3	151-A	2	0	0	0	0
3	152-A	2	0	0	0	0
3	153-A	2	0	0	0	0
3	154-A	2	0	0	0	0
3	155-A	2	0	0	0	0
3	156-A	2	0	0	0	0
3	157-A	2	0	0	0	0
3	158-A	2	0	0	0	0
3	159-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	160-A	2	0	0	0	0
3	161-A	2	0	0	0	0
3	162-A	2	0	0	0	0
3	163-A	2	0	0	0	0
3	164-A	2	0	0	0	0
3	165-A	2	0	0	0	0
3	166-A	2	0	0	0	0
3	167-A	2	0	0	0	0
4	1-A	48	24	24	0	0
4	2-A	48	24	24	0	0
4	3-A	48	24	24	0	0
4	4-A	48	24	24	0	0
4	5-A	48	24	24	0	0
4	6-A	48	24	24	0	0
4	7-A	48	24	24	0	0
4	8-A	48	24	24	0	0
4	9-A	48	24	24	0	0
4	10-A	48	24	24	0	0
4	11-A	48	24	24	0	0
4	12-A	48	24	24	0	0
4	13-A	48	24	24	0	0
4	14-A	48	24	24	0	0
4	15-A	48	24	24	0	0
4	16-A	48	24	24	0	0
4	17-A	48	24	24	0	0
4	18-A	48	24	24	0	0
4	19-A	48	24	24	0	0
4	20-A	48	24	24	0	0
4	21-A	48	24	24	0	0
4	22-A	48	24	24	0	0
4	23-A	48	24	24	0	0
4	24-A	48	24	24	0	0
4	25-A	48	24	24	0	0
4	26-A	48	24	24	0	0
4	27-A	48	24	24	0	0
4	28-A	48	24	0	0	0
4	29-A	48	24	0	0	0
4	30-A	48	24	0	0	0
4	31-A	48	24	0	0	0
4	32-A	48	24	0	0	0
4	33-A	48	24	0	0	0
4	34-A	48	24	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	35-A	48	24	0	0	0
4	36-A	48	24	0	0	0
4	37-A	48	24	0	0	0
4	38-A	48	24	0	0	0
4	39-A	48	24	0	0	0
4	40-A	48	24	0	0	0
4	41-A	48	24	0	0	0
4	42-A	48	24	0	0	0
4	43-A	48	24	0	0	0
4	44-A	48	24	0	0	0
4	45-A	48	24	0	0	0
4	46-A	48	24	0	0	0
4	47-A	48	24	0	0	0
4	48-A	48	24	0	0	0
4	49-A	48	24	0	0	0
4	50-A	48	24	0	0	0
4	51-A	48	24	0	0	0
4	52-A	48	24	0	0	0
4	53-A	48	24	0	0	0
4	54-A	48	24	0	0	0
4	55-A	48	24	0	0	0
4	56-A	48	24	0	0	0
4	57-A	48	24	0	0	0
4	58-A	48	24	0	0	0
4	59-A	48	24	0	0	0
4	60-A	48	24	0	0	0
4	61-A	48	24	0	0	0
4	62-A	48	24	0	0	0
4	63-A	48	24	0	0	0
4	64-A	48	24	0	0	0
4	65-A	48	24	0	0	0
4	66-A	48	24	0	0	0
4	67-A	48	24	0	0	0
4	68-A	48	24	0	0	0
4	69-A	48	24	0	0	0
4	70-A	48	24	0	0	0
4	71-A	48	24	0	0	0
4	72-A	48	24	0	0	0
4	73-A	48	24	0	0	0
4	74-A	48	24	0	0	0
4	75-A	48	24	0	0	0
4	76-A	48	24	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	77-A	48	24	0	0	0
4	78-A	48	24	0	0	0
4	79-A	48	24	0	0	0
4	80-A	48	24	0	0	0
4	81-A	48	24	0	0	0
4	82-A	48	24	0	0	0
4	83-A	48	24	0	0	0
4	84-A	48	24	0	0	0
4	85-A	48	24	0	0	0
4	86-A	48	24	0	0	0
4	87-A	48	24	0	0	0
4	88-A	48	24	0	0	0
4	89-A	48	24	0	0	0
4	90-A	48	24	0	0	0
4	91-A	48	24	0	0	0
4	92-A	48	24	0	0	0
4	93-A	48	24	0	0	0
4	94-A	48	24	0	0	0
4	95-A	48	24	0	0	0
4	96-A	48	24	0	0	0
4	97-A	48	24	0	0	0
4	98-A	48	24	0	0	0
4	99-A	48	24	0	0	0
4	100-A	48	24	0	0	0
4	101-A	48	24	0	0	0
4	102-A	48	24	0	0	0
4	103-A	48	24	0	0	0
4	104-A	48	24	0	0	0
4	105-A	48	24	0	0	0
4	106-A	48	24	0	0	0
4	107-A	48	24	0	0	0
4	108-A	48	24	0	0	0
4	109-A	48	24	0	0	0
4	110-A	48	24	0	0	0
4	111-A	48	24	0	0	0
4	112-A	48	24	0	0	0
4	113-A	48	24	0	0	0
4	114-A	48	24	0	0	0
4	115-A	48	24	0	0	0
4	116-A	48	24	0	0	0
4	117-A	48	24	0	0	0
4	118-A	48	24	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	119-A	48	24	0	0	0
4	120-A	48	24	0	0	0
4	121-A	48	24	0	0	0
4	122-A	48	24	0	0	0
4	123-A	48	24	0	0	0
4	124-A	48	24	0	0	0
4	125-A	48	24	0	0	0
4	126-A	48	24	0	0	0
4	127-A	48	24	0	0	0
4	128-A	48	24	0	0	0
4	129-A	48	24	0	0	0
4	130-A	48	24	0	0	0
4	131-A	48	24	0	0	0
4	132-A	48	24	0	0	0
4	133-A	48	24	0	0	0
4	134-A	48	24	0	0	0
4	135-A	48	24	0	0	0
4	136-A	48	24	0	0	0
4	137-A	48	24	0	0	0
4	138-A	48	24	0	0	0
4	139-A	48	24	0	0	0
4	140-A	48	24	0	0	0
4	141-A	48	24	0	0	0
4	142-A	48	24	0	0	0
4	143-A	48	24	0	0	0
4	144-A	48	24	0	0	0
4	145-A	48	24	0	0	0
4	146-A	48	24	0	0	0
4	147-A	48	24	0	0	0
4	148-A	48	24	0	0	0
4	149-A	48	24	0	0	0
4	150-A	48	24	0	0	0
4	151-A	48	24	0	0	0
4	152-A	48	24	0	0	0
4	153-A	48	24	0	0	0
4	154-A	48	24	0	0	0
4	155-A	48	24	0	0	0
4	156-A	48	24	0	0	0
4	157-A	48	24	0	0	0
4	158-A	48	24	0	0	0
4	159-A	48	24	0	0	0
4	160-A	48	24	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	161-A	48	24	0	0	0
4	162-A	48	24	0	0	0
4	163-A	48	24	0	0	0
4	164-A	48	24	0	0	0
4	165-A	48	24	0	0	0
4	166-A	48	24	0	0	0
4	167-A	48	24	0	0	0
5	1-A	83	0	0	0	0
5	2-A	83	0	0	0	0
5	3-A	79	0	0	0	0
5	4-A	68	0	0	0	0
5	5-A	75	0	0	0	0
5	6-A	80	0	0	0	0
5	7-A	99	0	0	0	0
5	8-A	89	0	0	0	0
5	9-A	79	0	0	0	0
5	10-A	79	0	0	0	0
5	11-A	82	0	0	0	0
5	12-A	88	0	0	0	0
5	13-A	89	0	0	0	0
5	14-A	96	0	0	0	0
5	15-A	96	0	0	0	0
5	16-A	94	0	0	0	0
5	17-A	84	0	0	0	0
5	18-A	89	0	0	0	0
5	19-A	80	0	0	0	0
5	20-A	73	0	0	0	0
5	21-A	92	0	0	0	0
5	22-A	91	0	0	0	0
5	23-A	94	0	0	0	0
5	24-A	95	0	0	0	0
5	25-A	76	0	0	0	0
5	26-A	83	0	0	0	0
5	27-A	81	0	0	0	0
5	28-A	81	0	0	0	0
5	29-A	83	0	0	0	0
5	30-A	84	0	0	0	0
5	31-A	86	0	0	0	0
5	32-A	85	0	0	0	0
5	33-A	86	0	0	0	0
5	34-A	93	0	0	0	0
5	35-A	93	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	36-A	77	0	0	0	0
5	37-A	82	0	0	0	0
5	38-A	87	0	0	0	0
5	39-A	93	0	0	0	0
5	40-A	84	0	0	0	0
5	41-A	82	0	0	0	0
5	42-A	83	0	0	0	0
5	43-A	95	0	0	0	0
5	44-A	100	0	0	0	0
5	45-A	93	0	0	0	0
5	46-A	92	0	0	0	0
5	47-A	98	0	0	0	0
5	48-A	92	0	0	0	0
5	49-A	89	0	0	0	0
5	50-A	78	0	0	0	0
5	51-A	68	0	0	0	0
5	52-A	77	0	0	0	0
5	53-A	87	0	0	0	0
5	54-A	92	0	0	0	0
5	55-A	92	0	0	0	0
5	56-A	82	0	0	0	0
5	57-A	86	0	0	0	0
5	58-A	89	0	0	0	0
5	59-A	96	0	0	0	0
5	60-A	96	0	0	0	0
5	61-A	98	0	0	0	0
5	62-A	100	0	0	0	0
5	63-A	97	0	0	0	0
5	64-A	87	0	0	0	0
5	65-A	83	0	0	0	0
5	66-A	77	0	0	0	0
5	67-A	78	0	0	0	0
5	68-A	79	0	0	0	0
5	69-A	79	0	0	0	0
5	70-A	85	0	0	0	0
5	71-A	91	0	0	0	0
5	72-A	101	0	0	0	0
5	73-A	94	0	0	0	0
5	74-A	85	0	0	0	0
5	75-A	92	0	0	0	0
5	76-A	82	0	0	0	0
5	77-A	85	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	78-A	84	0	0	0	0
5	79-A	86	0	0	0	0
5	80-A	85	0	0	0	0
5	81-A	92	0	0	0	0
5	82-A	91	0	0	0	0
5	83-A	98	0	0	0	0
5	84-A	94	0	0	0	0
5	85-A	94	0	0	0	0
5	86-A	88	0	0	0	0
5	87-A	84	0	0	0	0
5	88-A	82	0	0	0	0
5	89-A	92	0	0	0	0
5	90-A	98	0	0	0	0
5	91-A	75	0	0	0	0
5	92-A	77	0	0	0	0
5	93-A	78	0	0	0	0
5	94-A	92	0	0	0	0
5	95-A	101	0	0	0	0
5	96-A	106	0	0	0	0
5	97-A	94	0	0	0	0
5	98-A	86	0	0	0	0
5	99-A	87	0	0	0	0
5	100-A	80	0	0	0	0
5	101-A	76	0	0	0	0
5	102-A	80	0	0	0	0
5	103-A	89	0	0	0	0
5	104-A	88	0	0	0	0
5	105-A	97	0	0	0	0
5	106-A	85	0	0	0	0
5	107-A	87	0	0	0	0
5	108-A	93	0	0	0	0
5	109-A	82	0	0	0	0
5	110-A	82	0	0	0	0
5	111-A	75	0	0	0	0
5	112-A	85	0	0	0	0
5	113-A	97	0	0	0	0
5	114-A	98	0	0	0	0
5	115-A	86	0	0	0	0
5	116-A	89	0	0	0	0
5	117-A	85	0	0	0	0
5	118-A	89	0	0	0	0
5	119-A	88	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	120-A	95	0	0	0	0
5	121-A	93	0	0	0	0
5	122-A	90	0	0	0	0
5	123-A	82	0	0	0	0
5	124-A	81	0	0	0	0
5	125-A	84	0	0	0	0
5	126-A	101	0	0	0	0
5	127-A	96	0	0	0	0
5	128-A	90	0	0	0	0
5	129-A	89	0	0	0	0
5	130-A	81	0	0	0	0
5	131-A	75	0	0	0	0
5	132-A	87	0	0	0	0
5	133-A	96	0	0	0	0
5	134-A	89	0	0	0	0
5	135-A	89	0	0	0	0
5	136-A	87	0	0	0	0
5	137-A	88	0	0	0	0
5	138-A	88	0	0	0	0
5	139-A	96	0	0	0	0
5	140-A	88	0	0	0	0
5	141-A	80	0	0	0	0
5	142-A	80	0	0	0	0
5	143-A	83	0	0	0	0
5	144-A	84	0	0	0	0
5	145-A	99	0	0	0	0
5	146-A	101	0	0	0	0
5	147-A	105	0	0	0	0
5	148-A	103	0	0	0	0
5	149-A	86	0	0	0	0
5	150-A	94	0	0	0	0
5	151-A	92	0	0	0	0
5	152-A	89	0	0	0	0
5	153-A	99	0	0	0	0
5	154-A	98	0	0	0	0
5	155-A	78	0	0	0	0
5	156-A	79	0	0	0	0
5	157-A	80	0	0	0	0
5	158-A	78	0	0	0	0
5	159-A	82	0	0	0	0
5	160-A	82	0	0	0	0
5	161-A	86	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	162-A	84	0	0	0	0
5	163-A	91	0	0	0	0
5	164-A	92	0	0	0	0
5	165-A	90	0	0	0	0
5	166-A	81	0	0	0	0
5	167-A	89	0	0	0	0
All	All	240066	211088	35284	0	0

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

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	5	0
1	2-A	157/159 (99%)	143 (91%)	11 (7%)	3 (2%)	8	0
1	3-A	157/159 (99%)	150 (96%)	4 (2%)	3 (2%)	8	0
1	4-A	157/159 (99%)	146 (93%)	6 (4%)	5 (3%)	4	0
1	5-A	157/159 (99%)	147 (94%)	4 (2%)	6 (4%)	3	0
1	6-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	5	0
1	7-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	8	0
1	8-A	157/159 (99%)	142 (90%)	11 (7%)	4 (2%)	5	0
1	9-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	5	0
1	10-A	157/159 (99%)	146 (93%)	3 (2%)	8 (5%)	2	0
1	11-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	3	0
1	12-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	5	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	13-A	157/159 (99%)	145 (92%)	10 (6%)	2 (1%)	12	1
1	14-A	157/159 (99%)	146 (93%)	8 (5%)	3 (2%)	8	0
1	15-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	5	0
1	16-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	4	0
1	17-A	157/159 (99%)	146 (93%)	5 (3%)	6 (4%)	3	0
1	18-A	157/159 (99%)	142 (90%)	10 (6%)	5 (3%)	4	0
1	19-A	157/159 (99%)	148 (94%)	4 (2%)	5 (3%)	4	0
1	20-A	157/159 (99%)	148 (94%)	8 (5%)	1 (1%)	25	6
1	21-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	5	0
1	22-A	157/159 (99%)	145 (92%)	9 (6%)	3 (2%)	8	0
1	23-A	157/159 (99%)	148 (94%)	5 (3%)	4 (2%)	5	0
1	24-A	157/159 (99%)	147 (94%)	4 (2%)	6 (4%)	3	0
1	25-A	157/159 (99%)	145 (92%)	6 (4%)	6 (4%)	3	0
1	26-A	157/159 (99%)	142 (90%)	9 (6%)	6 (4%)	3	0
1	27-A	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	5	0
1	28-A	151/159 (95%)	137 (91%)	7 (5%)	7 (5%)	2	0
All	All	4390/4452 (99%)	4065 (93%)	200 (5%)	125 (3%)	5	0

5 of 125 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	18	ASN
1	1-A	119	VAL
1	1-A	130	PRO
1	3-A	130	PRO
1	4-A	18	ASN

4.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	2-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	3-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	4-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	5-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	6-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	7-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	8-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	9-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	10-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	11-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	12-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	13-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	14-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	15-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	16-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	17-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	18-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	19-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	20-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	21-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	22-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	23-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	24-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	25-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	26-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	27-A	136/136 (100%)	117 (86%)	19 (14%)	3	0
1	28-A	129/136 (95%)	113 (88%)	16 (12%)	4	0
All	All	3801/3808 (100%)	3419 (90%)	382 (10%)	7	0

5 of 382 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	17-A	61	ILE
1	22-A	50	ILE
1	18-A	18	ASN
1	20-A	59	ASN
1	23-A	59	ASN

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

4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 668 ligands modelled in this entry, 334 are monoatomic - leaving 334 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FOL	11-A	201	-	34,34,34	1.04	3 (8%)	44,47,47	1.99	10 (22%)
2	FOL	33-A	201	-	34,34,34	1.16	3 (8%)	44,47,47	2.18	11 (25%)
2	FOL	18-A	201	-	34,34,34	1.08	3 (8%)	44,47,47	2.16	12 (27%)
2	FOL	21-A	201	-	34,34,34	1.32	3 (8%)	44,47,47	2.14	13 (29%)
2	FOL	27-A	201	-	34,34,34	1.23	3 (8%)	44,47,47	1.89	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FOL	29-A	201	-	34,34,34	1.08	2 (5%)	44,47,47	2.00	10 (22%)
4	NAP	5-A	204	-	45,52,52	1.76	10 (22%)	56,80,80	1.43	10 (17%)
4	NAP	31-A	204	-	45,52,52	1.83	11 (24%)	56,80,80	1.25	6 (10%)
4	NAP	22-A	204	-	45,52,52	1.87	11 (24%)	56,80,80	1.37	9 (16%)
4	NAP	8-A	204	-	45,52,52	1.72	11 (24%)	56,80,80	1.32	6 (10%)
2	FOL	23-A	201	-	34,34,34	1.07	4 (11%)	44,47,47	1.99	10 (22%)
4	NAP	21-A	204	-	45,52,52	1.81	10 (22%)	56,80,80	1.30	8 (14%)
4	NAP	29-A	204	-	45,52,52	1.83	11 (24%)	56,80,80	1.33	7 (12%)
4	NAP	10-A	204	-	45,52,52	1.82	9 (20%)	56,80,80	1.33	9 (16%)
2	FOL	3-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	1.91	8 (18%)
4	NAP	11-A	204	-	45,52,52	1.82	10 (22%)	56,80,80	1.33	8 (14%)
2	FOL	13-A	201	-	34,34,34	1.30	5 (14%)	44,47,47	2.60	16 (36%)
4	NAP	6-A	204	-	45,52,52	1.73	10 (22%)	56,80,80	1.28	6 (10%)
2	FOL	19-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	1.81	9 (20%)
2	FOL	24-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	2.12	13 (29%)
2	FOL	1-A	201	-	34,34,34	0.98	3 (8%)	44,47,47	1.89	11 (25%)
2	FOL	16-A	201	-	34,34,34	1.08	4 (11%)	44,47,47	1.98	7 (15%)
2	FOL	7-A	201	-	34,34,34	1.09	3 (8%)	44,47,47	1.88	10 (22%)
4	NAP	15-A	204	-	45,52,52	1.78	9 (20%)	56,80,80	1.44	11 (19%)
2	FOL	25-A	201	-	34,34,34	1.17	3 (8%)	44,47,47	2.27	13 (29%)
2	FOL	4-A	201	-	34,34,34	1.19	4 (11%)	44,47,47	2.01	11 (25%)
4	NAP	32-A	204	-	45,52,52	1.74	11 (24%)	56,80,80	1.25	5 (8%)
4	NAP	24-A	204	-	45,52,52	1.84	9 (20%)	56,80,80	1.29	8 (14%)
2	FOL	12-A	201	-	34,34,34	1.23	4 (11%)	44,47,47	1.85	7 (15%)
2	FOL	17-A	201	-	34,34,34	1.14	3 (8%)	44,47,47	1.73	6 (13%)
4	NAP	28-A	204	-	45,52,52	1.84	10 (22%)	56,80,80	1.34	7 (12%)
2	FOL	14-A	201	-	34,34,34	1.23	4 (11%)	44,47,47	2.47	14 (31%)
2	FOL	5-A	201	-	34,34,34	1.17	3 (8%)	44,47,47	1.96	12 (27%)
2	FOL	31-A	201	-	34,34,34	1.14	3 (8%)	44,47,47	2.08	14 (31%)
4	NAP	7-A	204	-	45,52,52	1.68	11 (24%)	56,80,80	1.26	5 (8%)
4	NAP	25-A	204	-	45,52,52	1.88	10 (22%)	56,80,80	1.39	8 (14%)
2	FOL	30-A	201	-	34,34,34	1.36	3 (8%)	44,47,47	1.97	8 (18%)
4	NAP	19-A	204	-	45,52,52	1.86	10 (22%)	56,80,80	1.36	9 (16%)
2	FOL	26-A	201	-	34,34,34	1.33	4 (11%)	44,47,47	2.18	15 (34%)
2	FOL	9-A	201	-	34,34,34	1.12	3 (8%)	44,47,47	1.81	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	FOL	20-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	1.70	6 (13%)
2	FOL	6-A	201	-	34,34,34	1.34	4 (11%)	44,47,47	2.03	12 (27%)
2	FOL	15-A	201	-	34,34,34	1.23	3 (8%)	44,47,47	2.14	11 (25%)
4	NAP	13-A	204	-	45,52,52	1.79	10 (22%)	56,80,80	1.30	10 (17%)
4	NAP	4-A	204	-	45,52,52	1.79	10 (22%)	56,80,80	1.35	9 (16%)
4	NAP	16-A	204	-	45,52,52	1.84	10 (22%)	56,80,80	1.29	9 (16%)
4	NAP	18-A	204	-	45,52,52	1.85	10 (22%)	56,80,80	1.48	10 (17%)
4	NAP	14-A	204	-	45,52,52	1.80	10 (22%)	56,80,80	1.37	10 (17%)
4	NAP	23-A	204	-	45,52,52	1.87	10 (22%)	56,80,80	1.53	10 (17%)
4	NAP	27-A	204	-	45,52,52	1.84	10 (22%)	56,80,80	1.34	8 (14%)
4	NAP	30-A	204	-	45,52,52	1.89	9 (20%)	56,80,80	1.30	8 (14%)
4	NAP	1-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	3-A	204	-	45,52,52	1.82	10 (22%)	56,80,80	1.37	8 (14%)
4	NAP	12-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.29	10 (17%)
2	FOL	10-A	201	-	34,34,34	1.09	3 (8%)	44,47,47	2.03	10 (22%)
2	FOL	32-A	201	-	34,34,34	1.08	4 (11%)	44,47,47	1.77	9 (20%)
4	NAP	20-A	204	-	45,52,52	1.84	9 (20%)	56,80,80	1.31	8 (14%)
4	NAP	17-A	204	-	45,52,52	1.83	9 (20%)	56,80,80	1.36	10 (17%)
2	FOL	22-A	201	-	34,34,34	1.12	3 (8%)	44,47,47	1.99	9 (20%)
4	NAP	9-A	204	-	45,52,52	1.73	11 (24%)	56,80,80	1.23	7 (12%)
2	FOL	28-A	201	-	34,34,34	1.25	3 (8%)	44,47,47	1.81	8 (18%)
4	NAP	26-A	204	-	45,52,52	1.83	10 (22%)	56,80,80	1.36	10 (17%)
4	NAP	2-A	204	-	45,52,52	1.76	9 (20%)	56,80,80	1.36	10 (17%)
2	FOL	2-A	201	-	34,34,34	1.16	3 (8%)	44,47,47	1.79	7 (15%)
2	FOL	8-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	1.91	7 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	11-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	33-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	18-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	21-A	201	-	-	3/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	27-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	29-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	5-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	31-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	22-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	8-A	204	-	-	0/31/67/67	0/5/5/5
2	FOL	23-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	21-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	29-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	10-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	3-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	11-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	13-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	6-A	204	-	-	0/31/67/67	0/5/5/5
2	FOL	19-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	24-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	1-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	16-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	7-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	15-A	204	-	-	6/31/67/67	0/5/5/5
2	FOL	25-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	4-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	32-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	24-A	204	-	-	0/31/67/67	0/5/5/5
2	FOL	12-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	17-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	28-A	204	-	-	4/31/67/67	0/5/5/5
2	FOL	14-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	5-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	31-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	7-A	204	-	-	0/31/67/67	0/5/5/5
4	NAP	25-A	204	-	-	0/31/67/67	0/5/5/5
2	FOL	30-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	19-A	204	-	-	3/31/67/67	0/5/5/5
2	FOL	26-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	9-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	20-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	6-A	201	-	-	5/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	15-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	13-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	4-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	16-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	18-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	14-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	23-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	27-A	204	-	-	4/31/67/67	0/5/5/5
4	NAP	30-A	204	-	-	0/31/67/67	0/5/5/5
4	NAP	1-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	3-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	12-A	204	-	-	3/31/67/67	0/5/5/5
2	FOL	10-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	32-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	20-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	17-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	22-A	201	-	-	8/22/22/22	0/3/3/3
4	NAP	9-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	28-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	26-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	2-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	2-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	8-A	201	-	-	0/22/22/22	0/3/3/3

The worst 5 of 428 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	25-A	204	NAP	O3B-C3B	-6.42	1.27	1.43
4	22-A	204	NAP	O3B-C3B	-6.37	1.28	1.43
4	26-A	204	NAP	O3B-C3B	-6.31	1.28	1.43
4	23-A	204	NAP	O3B-C3B	-6.27	1.28	1.43
4	30-A	204	NAP	O3B-C3B	-6.23	1.28	1.43

The worst 5 of 605 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	10-A	201	FOL	N8-C8A-N1	7.31	124.17	115.82
2	16-A	201	FOL	N8-C8A-N1	6.85	123.64	115.82
2	29-A	201	FOL	N8-C8A-N1	6.85	123.64	115.82
2	21-A	201	FOL	C8A-C4A-C4	-6.69	115.53	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	8-A	201	FOL	C4A-C4-N3	-6.68	114.29	123.43

There are no chirality outliers.

5 of 135 torsion outliers are listed below:

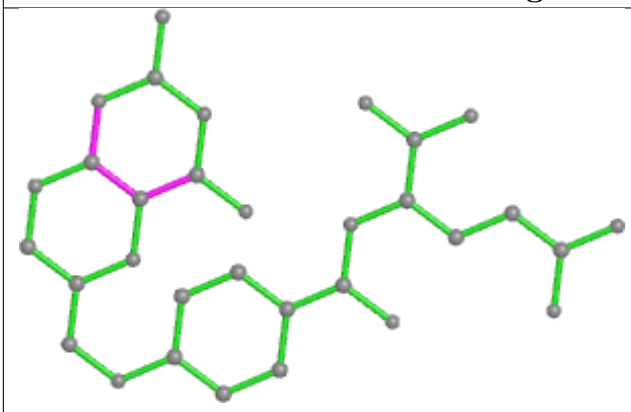
Mol	Chain	Res	Type	Atoms
2	7-A	201	FOL	CT-CA-CB-CG
2	14-A	201	FOL	CT-CA-CB-CG
2	22-A	201	FOL	N-CA-CB-CG
4	1-A	204	NAP	C5D-O5D-PN-O2N
4	2-A	204	NAP	O4D-C1D-N1N-C6N

There are no ring outliers.

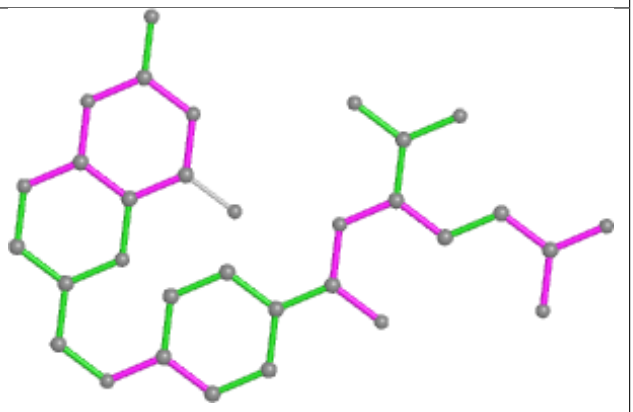
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

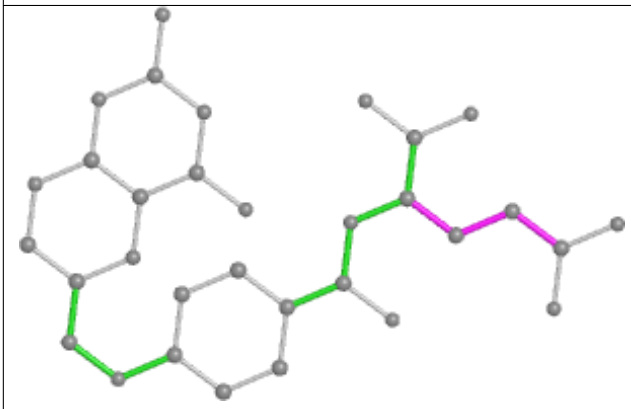
Ligand FOL A 201



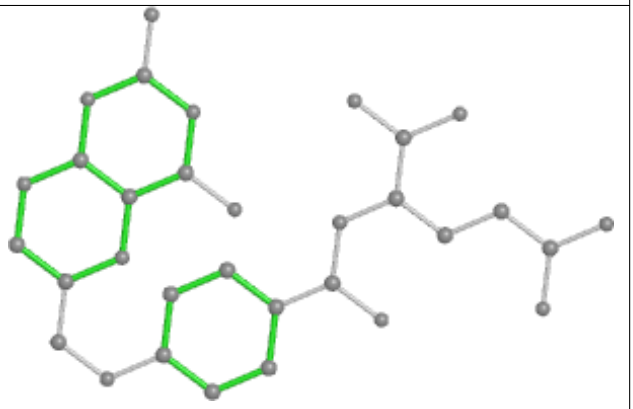
Bond lengths



Bond angles

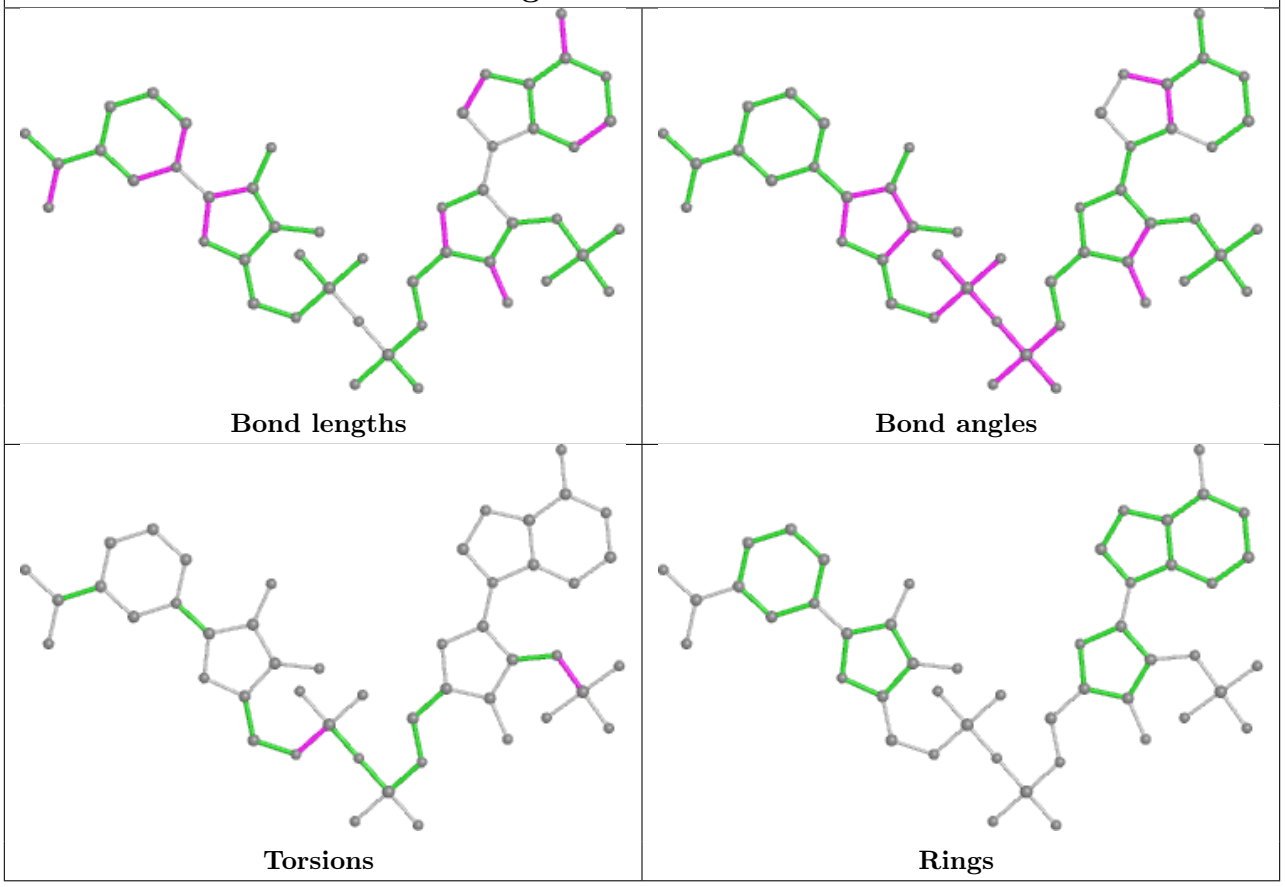


Torsions



Rings

Ligand NAP A 204



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

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.