



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 08:42 AM UTC

PDB ID : 4P3Q / pdb_00004p3q
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	FAILED
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

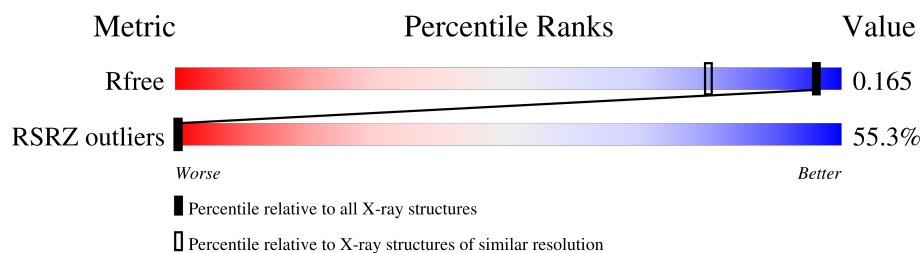
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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))
R_{free}	180053	1216 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CA	1-A	203	-	-	-	X

2 Entry composition

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 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	165-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	166-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	167-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0

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



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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 49	C 19	H 17	N 7	O 6	0	0
2	114-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	115-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	116-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	117-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	118-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	119-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	120-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	121-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	122-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	123-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	124-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	125-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	126-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	127-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	128-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	129-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	130-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	131-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	132-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	133-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	134-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	135-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	136-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	137-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	138-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	139-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	140-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	141-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	142-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	143-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	144-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	145-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	146-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	147-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	148-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	149-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	150-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	151-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	152-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	153-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	154-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

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

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

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

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

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

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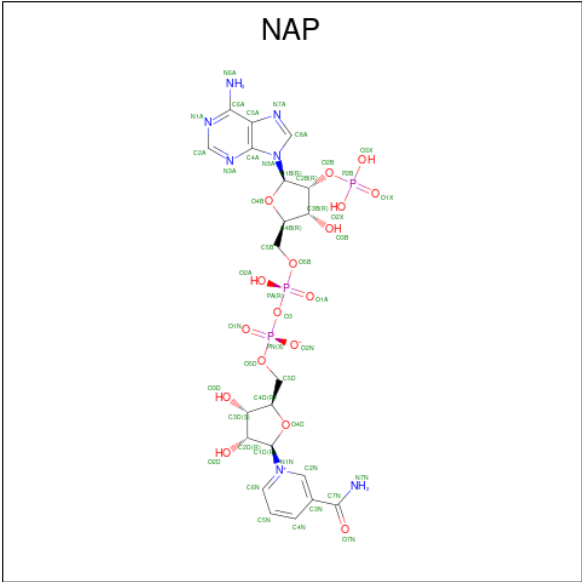
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	133-A	2	Total 2	Ca 2	0	0
3	134-A	2	Total 2	Ca 2	0	0
3	135-A	2	Total 2	Ca 2	0	0
3	136-A	2	Total 2	Ca 2	0	0
3	137-A	2	Total 2	Ca 2	0	0
3	138-A	2	Total 2	Ca 2	0	0
3	139-A	2	Total 2	Ca 2	0	0
3	140-A	2	Total 2	Ca 2	0	0
3	141-A	2	Total 2	Ca 2	0	0
3	142-A	2	Total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

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

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	1-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	2-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	3-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	4-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	5-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	6-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	7-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	8-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	9-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	10-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	11-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	12-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	13-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0
4	14-A	1	Total 72	C 21	H 24	N 7	O 17	P 3	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

3 Data and refinement statistics

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 41.34 – 1.35	Depositor EDS
% Data completeness (in resolution range)	91.6 (41.34-1.35) 87.6 (41.34-1.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.35Å)	Xtrriage
Refinement program	PHENIX (phenix.ensemble_refinement: 1.8.4_1496)	Depositor
R, R_{free}	0.118 , 0.153 0.134 , 0.165	Depositor DCC
R_{free} test set	1620 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	11.2	Xtrriage
Anisotropy	0.170	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.00 , 21.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	451154	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides 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
4	NAP	56-A	204	-	50,52,52	1.88	16 (32%)	71,80,80	2.69	16 (22%)
4	NAP	111-A	204	-	50,52,52	2.28	17 (34%)	71,80,80	1.72	16 (22%)
2	FOL	4-A	201	-	34,34,34	1.43	4 (11%)	43,47,47	1.50	8 (18%)
4	NAP	116-A	204	-	50,52,52	2.32	16 (32%)	71,80,80	1.75	17 (23%)
2	FOL	146-A	201	-	34,34,34	1.31	3 (8%)	43,47,47	1.13	2 (4%)
2	FOL	41-A	201	-	34,34,34	1.33	4 (11%)	43,47,47	1.57	5 (11%)
4	NAP	24-A	204	-	50,52,52	2.30	15 (30%)	71,80,80	1.68	16 (22%)
2	FOL	14-A	201	-	34,34,34	1.37	5 (14%)	43,47,47	1.91	10 (23%)
4	NAP	46-A	204	-	50,52,52	2.33	16 (32%)	71,80,80	1.71	16 (22%)
2	FOL	124-A	201	-	34,34,34	1.22	3 (8%)	43,47,47	1.59	8 (18%)
4	NAP	12-A	204	-	50,52,52	2.24	16 (32%)	71,80,80	1.68	17 (23%)
4	NAP	105-A	204	-	50,52,52	2.46	16 (32%)	71,80,80	1.67	15 (21%)
4	NAP	41-A	204	-	50,52,52	2.37	17 (34%)	71,80,80	1.78	16 (22%)
2	FOL	97-A	201	-	34,34,34	1.14	3 (8%)	43,47,47	1.45	5 (11%)
2	FOL	138-A	201	-	34,34,34	1.14	3 (8%)	43,47,47	1.79	8 (18%)
4	NAP	134-A	204	-	50,52,52	2.04	16 (32%)	71,80,80	1.50	14 (19%)
4	NAP	152-A	204	-	50,52,52	2.18	14 (28%)	71,80,80	1.69	14 (19%)
2	FOL	5-A	201	-	34,34,34	1.29	2 (5%)	43,47,47	1.55	8 (18%)
4	NAP	157-A	204	-	50,52,52	2.26	16 (32%)	71,80,80	1.40	10 (14%)
4	NAP	87-A	204	-	50,52,52	2.23	15 (30%)	71,80,80	1.65	15 (21%)
2	FOL	117-A	201	-	34,34,34	1.33	2 (5%)	43,47,47	1.15	5 (11%)
4	NAP	39-A	204	-	50,52,52	2.34	16 (32%)	71,80,80	1.75	18 (25%)
4	NAP	51-A	204	-	50,52,52	2.36	17 (34%)	71,80,80	1.78	15 (21%)
4	NAP	158-A	204	-	50,52,52	2.16	15 (30%)	71,80,80	1.49	10 (14%)
4	NAP	92-A	204	-	50,52,52	2.26	15 (30%)	71,80,80	1.70	17 (23%)
4	NAP	114-A	204	-	50,52,52	2.30	16 (32%)	71,80,80	1.67	16 (22%)
2	FOL	105-A	201	-	34,34,34	1.30	3 (8%)	43,47,47	1.79	8 (18%)
2	FOL	86-A	201	-	34,34,34	1.23	4 (11%)	43,47,47	1.51	6 (13%)
2	FOL	59-A	201	-	34,34,34	1.45	3 (8%)	43,47,47	1.63	7 (16%)
2	FOL	53-A	201	-	34,34,34	1.33	2 (5%)	43,47,47	1.39	6 (13%)
4	NAP	141-A	204	-	50,52,52	2.27	16 (32%)	71,80,80	1.66	15 (21%)
4	NAP	1-A	204	-	50,52,52	2.30	14 (28%)	71,80,80	1.76	17 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	93-A	204	-	50,52,52	2.30	15 (30%)	71,80,80	1.71	16 (22%)
2	FOL	88-A	201	-	34,34,34	1.12	3 (8%)	43,47,47	1.24	3 (6%)
4	NAP	59-A	204	-	50,52,52	2.13	14 (28%)	71,80,80	1.57	12 (16%)
2	FOL	70-A	201	-	34,34,34	1.37	3 (8%)	43,47,47	1.71	6 (13%)
2	FOL	30-A	201	-	34,34,34	1.41	3 (8%)	43,47,47	1.73	7 (16%)
4	NAP	113-A	204	-	50,52,52	2.26	14 (28%)	71,80,80	1.66	16 (22%)
4	NAP	10-A	204	-	50,52,52	2.28	15 (30%)	71,80,80	1.66	16 (22%)
4	NAP	153-A	204	-	50,52,52	2.29	16 (32%)	71,80,80	1.65	14 (19%)
4	NAP	89-A	204	-	50,52,52	2.26	16 (32%)	71,80,80	1.83	16 (22%)
4	NAP	45-A	204	-	50,52,52	2.36	16 (32%)	71,80,80	1.75	16 (22%)
4	NAP	73-A	204	-	50,52,52	2.26	17 (34%)	71,80,80	1.70	16 (22%)
2	FOL	64-A	201	-	34,34,34	1.22	3 (8%)	43,47,47	1.53	9 (20%)
2	FOL	3-A	201	-	34,34,34	1.25	3 (8%)	43,47,47	1.28	4 (9%)
4	NAP	147-A	204	-	50,52,52	2.30	17 (34%)	71,80,80	1.66	15 (21%)
2	FOL	46-A	201	-	34,34,34	1.25	3 (8%)	43,47,47	1.46	5 (11%)
2	FOL	12-A	201	-	34,34,34	1.43	3 (8%)	43,47,47	1.39	3 (6%)
4	NAP	21-A	204	-	50,52,52	2.31	15 (30%)	71,80,80	1.63	15 (21%)
2	FOL	33-A	201	-	34,34,34	1.40	4 (11%)	43,47,47	1.82	7 (16%)
4	NAP	53-A	204	-	50,52,52	2.28	14 (28%)	71,80,80	1.72	15 (21%)
2	FOL	80-A	201	-	34,34,34	1.34	3 (8%)	43,47,47	1.83	13 (30%)
2	FOL	134-A	201	-	34,34,34	1.43	3 (8%)	43,47,47	1.72	9 (20%)
2	FOL	115-A	201	-	34,34,34	1.26	3 (8%)	43,47,47	1.68	10 (23%)
2	FOL	113-A	201	-	34,34,34	1.36	3 (8%)	43,47,47	1.50	9 (20%)
2	FOL	152-A	201	-	34,34,34	1.43	3 (8%)	43,47,47	1.37	6 (13%)
2	FOL	153-A	201	-	34,34,34	1.26	2 (5%)	43,47,47	1.64	7 (16%)
2	FOL	50-A	201	-	34,34,34	1.34	3 (8%)	43,47,47	1.27	3 (6%)
4	NAP	80-A	204	-	50,52,52	2.38	15 (30%)	71,80,80	1.76	16 (22%)
2	FOL	167-A	201	-	34,34,34	1.33	3 (8%)	43,47,47	1.50	9 (20%)
2	FOL	142-A	201	-	34,34,34	1.20	3 (8%)	43,47,47	1.46	5 (11%)
4	NAP	34-A	204	-	50,52,52	2.09	14 (28%)	71,80,80	1.47	13 (18%)
4	NAP	57-A	204	-	50,52,52	1.95	17 (34%)	71,80,80	2.97	10 (14%)
2	FOL	101-A	201	-	34,34,34	1.24	3 (8%)	43,47,47	1.24	3 (6%)
2	FOL	20-A	201	-	34,34,34	1.35	3 (8%)	43,47,47	1.22	1 (2%)
2	FOL	162-A	201	-	34,34,34	1.35	3 (8%)	43,47,47	1.34	4 (9%)
4	NAP	160-A	204	-	50,52,52	2.29	17 (34%)	71,80,80	1.61	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	38-A	204	-	50,52,52	2.40	17 (34%)	71,80,80	1.68	19 (26%)
2	FOL	52-A	201	-	34,34,34	1.44	3 (8%)	43,47,47	1.81	8 (18%)
4	NAP	23-A	204	-	50,52,52	2.26	16 (32%)	71,80,80	1.76	16 (22%)
4	NAP	135-A	204	-	50,52,52	2.34	14 (28%)	71,80,80	1.68	15 (21%)
2	FOL	54-A	201	-	34,34,34	1.15	1 (2%)	43,47,47	1.34	5 (11%)
4	NAP	159-A	204	-	50,52,52	1.99	15 (30%)	71,80,80	1.49	14 (19%)
2	FOL	77-A	201	-	34,34,34	1.31	3 (8%)	43,47,47	1.44	4 (9%)
2	FOL	165-A	201	-	34,34,34	1.24	2 (5%)	43,47,47	1.60	7 (16%)
4	NAP	64-A	204	-	50,52,52	2.34	15 (30%)	71,80,80	1.64	15 (21%)
4	NAP	98-A	204	-	50,52,52	2.23	15 (30%)	71,80,80	1.68	16 (22%)
2	FOL	13-A	201	-	34,34,34	1.44	5 (14%)	43,47,47	2.07	12 (27%)
4	NAP	20-A	204	-	50,52,52	2.35	15 (30%)	71,80,80	1.68	15 (21%)
2	FOL	93-A	201	-	34,34,34	1.21	3 (8%)	43,47,47	1.58	9 (20%)
2	FOL	72-A	201	-	34,34,34	1.31	3 (8%)	43,47,47	1.54	5 (11%)
4	NAP	165-A	204	-	50,52,52	2.24	16 (32%)	71,80,80	1.72	14 (19%)
4	NAP	140-A	204	-	50,52,52	2.33	15 (30%)	71,80,80	1.72	15 (21%)
2	FOL	11-A	201	-	34,34,34	1.20	3 (8%)	43,47,47	1.44	6 (13%)
2	FOL	102-A	201	-	34,34,34	1.13	2 (5%)	43,47,47	1.40	7 (16%)
4	NAP	125-A	204	-	50,52,52	2.27	13 (26%)	71,80,80	1.66	15 (21%)
2	FOL	85-A	201	-	34,34,34	1.30	3 (8%)	43,47,47	1.47	5 (11%)
4	NAP	65-A	204	-	50,52,52	2.32	17 (34%)	71,80,80	1.67	16 (22%)
2	FOL	79-A	201	-	34,34,34	1.18	3 (8%)	43,47,47	1.29	5 (11%)
2	FOL	22-A	201	-	34,34,34	1.32	3 (8%)	43,47,47	1.30	4 (9%)
4	NAP	132-A	204	-	50,52,52	2.22	14 (28%)	71,80,80	1.41	11 (15%)
4	NAP	4-A	204	-	50,52,52	2.21	16 (32%)	71,80,80	1.78	16 (22%)
2	FOL	149-A	201	-	34,34,34	1.23	2 (5%)	43,47,47	1.79	6 (13%)
4	NAP	130-A	204	-	50,52,52	2.31	15 (30%)	71,80,80	1.79	15 (21%)
2	FOL	121-A	201	-	34,34,34	1.38	3 (8%)	43,47,47	1.22	3 (6%)
2	FOL	141-A	201	-	34,34,34	1.22	3 (8%)	43,47,47	1.38	6 (13%)
4	NAP	22-A	204	-	50,52,52	2.30	17 (34%)	71,80,80	1.67	16 (22%)
2	FOL	112-A	201	-	34,34,34	1.20	3 (8%)	43,47,47	1.53	4 (9%)
4	NAP	2-A	204	-	50,52,52	2.23	16 (32%)	71,80,80	1.78	16 (22%)
2	FOL	42-A	201	-	34,34,34	1.42	3 (8%)	43,47,47	1.57	9 (20%)
2	FOL	148-A	201	-	34,34,34	1.30	2 (5%)	43,47,47	1.38	4 (9%)
4	NAP	43-A	204	-	50,52,52	2.32	13 (26%)	71,80,80	1.67	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	19-A	201	-	34,34,34	1.38	3 (8%)	43,47,47	1.07	2 (4%)
2	FOL	119-A	201	-	34,34,34	1.32	3 (8%)	43,47,47	1.31	3 (6%)
4	NAP	112-A	204	-	50,52,52	2.29	15 (30%)	71,80,80	1.69	17 (23%)
4	NAP	77-A	204	-	50,52,52	2.23	15 (30%)	71,80,80	1.85	16 (22%)
4	NAP	17-A	204	-	50,52,52	2.34	14 (28%)	71,80,80	1.73	16 (22%)
4	NAP	156-A	204	-	50,52,52	2.29	16 (32%)	71,80,80	1.74	16 (22%)
4	NAP	6-A	204	-	50,52,52	2.28	17 (34%)	71,80,80	1.46	12 (16%)
2	FOL	159-A	201	-	34,34,34	1.29	3 (8%)	43,47,47	1.59	8 (18%)
2	FOL	132-A	201	-	34,34,34	1.52	5 (14%)	43,47,47	1.51	6 (13%)
2	FOL	38-A	201	-	34,34,34	1.09	2 (5%)	43,47,47	1.44	4 (9%)
2	FOL	16-A	201	-	34,34,34	1.30	2 (5%)	43,47,47	1.55	4 (9%)
4	NAP	30-A	204	-	50,52,52	2.48	17 (34%)	71,80,80	1.69	16 (22%)
4	NAP	118-A	204	-	50,52,52	1.95	15 (30%)	71,80,80	3.11	16 (22%)
4	NAP	109-A	204	-	50,52,52	2.17	16 (32%)	71,80,80	1.53	14 (19%)
4	NAP	142-A	204	-	50,52,52	2.24	15 (30%)	71,80,80	1.73	17 (23%)
2	FOL	69-A	201	-	34,34,34	1.32	3 (8%)	43,47,47	1.36	5 (11%)
2	FOL	2-A	201	-	34,34,34	1.39	3 (8%)	43,47,47	1.30	3 (6%)
4	NAP	149-A	204	-	50,52,52	2.22	15 (30%)	71,80,80	1.74	16 (22%)
4	NAP	35-A	204	-	50,52,52	2.37	15 (30%)	71,80,80	1.86	16 (22%)
4	NAP	136-A	204	-	50,52,52	2.31	15 (30%)	71,80,80	1.70	16 (22%)
4	NAP	107-A	204	-	50,52,52	2.53	17 (34%)	71,80,80	1.71	16 (22%)
2	FOL	18-A	201	-	34,34,34	1.23	3 (8%)	43,47,47	1.57	7 (16%)
2	FOL	58-A	201	-	34,34,34	1.32	4 (11%)	43,47,47	1.84	10 (23%)
2	FOL	130-A	201	-	34,34,34	1.20	2 (5%)	43,47,47	1.23	3 (6%)
4	NAP	61-A	204	-	50,52,52	2.31	15 (30%)	71,80,80	1.68	16 (22%)
4	NAP	119-A	204	-	50,52,52	2.33	16 (32%)	71,80,80	2.23	16 (22%)
2	FOL	37-A	201	-	34,34,34	1.28	3 (8%)	43,47,47	1.59	6 (13%)
4	NAP	70-A	204	-	50,52,52	2.34	14 (28%)	71,80,80	1.66	17 (23%)
4	NAP	72-A	204	-	50,52,52	2.31	17 (34%)	71,80,80	1.68	14 (19%)
2	FOL	65-A	201	-	34,34,34	1.43	4 (11%)	43,47,47	1.58	8 (18%)
2	FOL	8-A	201	-	34,34,34	1.40	3 (8%)	43,47,47	1.13	2 (4%)
4	NAP	151-A	204	-	50,52,52	2.30	16 (32%)	71,80,80	1.81	16 (22%)
2	FOL	89-A	201	-	34,34,34	1.33	3 (8%)	43,47,47	1.54	9 (20%)
4	NAP	14-A	204	-	50,52,52	2.31	16 (32%)	71,80,80	1.71	17 (23%)
2	FOL	104-A	201	-	34,34,34	1.13	2 (5%)	43,47,47	1.46	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	167-A	204	-	50,52,52	2.26	16 (32%)	71,80,80	1.68	16 (22%)
4	NAP	145-A	204	-	50,52,52	2.32	14 (28%)	71,80,80	1.79	15 (21%)
2	FOL	103-A	201	-	34,34,34	1.26	3 (8%)	43,47,47	1.38	5 (11%)
4	NAP	101-A	204	-	50,52,52	2.36	16 (32%)	71,80,80	1.78	17 (23%)
4	NAP	97-A	204	-	50,52,52	2.27	17 (34%)	71,80,80	1.64	16 (22%)
4	NAP	100-A	204	-	50,52,52	2.36	15 (30%)	71,80,80	1.74	16 (22%)
4	NAP	162-A	204	-	50,52,52	2.25	15 (30%)	71,80,80	1.66	15 (21%)
2	FOL	129-A	201	-	34,34,34	1.34	3 (8%)	43,47,47	1.83	12 (27%)
4	NAP	103-A	204	-	50,52,52	2.31	16 (32%)	71,80,80	1.75	14 (19%)
2	FOL	125-A	201	-	34,34,34	1.17	2 (5%)	43,47,47	1.40	6 (13%)
2	FOL	106-A	201	-	34,34,34	1.22	3 (8%)	43,47,47	1.94	8 (18%)
4	NAP	33-A	204	-	50,52,52	2.37	17 (34%)	71,80,80	1.56	15 (21%)
2	FOL	163-A	201	-	34,34,34	1.17	4 (11%)	43,47,47	1.45	6 (13%)
4	NAP	102-A	204	-	50,52,52	2.33	16 (32%)	71,80,80	1.71	15 (21%)
4	NAP	49-A	204	-	50,52,52	2.26	16 (32%)	71,80,80	1.94	20 (28%)
2	FOL	29-A	201	-	34,34,34	1.12	3 (8%)	43,47,47	1.44	5 (11%)
4	NAP	150-A	204	-	50,52,52	2.17	14 (28%)	71,80,80	1.72	18 (25%)
4	NAP	108-A	204	-	50,52,52	2.28	18 (36%)	71,80,80	1.71	13 (18%)
4	NAP	37-A	204	-	50,52,52	2.36	17 (34%)	71,80,80	1.64	16 (22%)
4	NAP	96-A	204	-	50,52,52	2.27	15 (30%)	71,80,80	1.59	15 (21%)
2	FOL	74-A	201	-	34,34,34	1.49	3 (8%)	43,47,47	1.35	5 (11%)
2	FOL	109-A	201	-	34,34,34	1.34	4 (11%)	43,47,47	1.50	6 (13%)
4	NAP	15-A	204	-	50,52,52	2.27	14 (28%)	71,80,80	1.78	16 (22%)
4	NAP	42-A	204	-	50,52,52	2.39	16 (32%)	71,80,80	1.86	16 (22%)
2	FOL	100-A	201	-	34,34,34	1.42	4 (11%)	43,47,47	1.53	6 (13%)
2	FOL	6-A	201	-	34,34,34	1.58	4 (11%)	43,47,47	1.59	6 (13%)
4	NAP	104-A	204	-	50,52,52	2.48	16 (32%)	71,80,80	1.84	17 (23%)
2	FOL	143-A	201	-	34,34,34	1.33	3 (8%)	43,47,47	1.31	3 (6%)
2	FOL	73-A	201	-	34,34,34	1.48	4 (11%)	43,47,47	1.46	4 (9%)
2	FOL	166-A	201	-	34,34,34	1.31	3 (8%)	43,47,47	1.09	2 (4%)
2	FOL	107-A	201	-	34,34,34	1.26	2 (5%)	43,47,47	1.31	3 (6%)
2	FOL	135-A	201	-	34,34,34	1.25	3 (8%)	43,47,47	1.33	6 (13%)
2	FOL	164-A	201	-	34,34,34	1.25	3 (8%)	43,47,47	1.23	2 (4%)
4	NAP	55-A	204	-	50,52,52	2.40	15 (30%)	71,80,80	1.74	16 (22%)
4	NAP	106-A	204	-	50,52,52	2.55	16 (32%)	71,80,80	1.70	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	79-A	204	-	50,52,52	2.31	17 (34%)	71,80,80	1.81	14 (19%)
4	NAP	146-A	204	-	50,52,52	2.31	16 (32%)	71,80,80	1.69	16 (22%)
4	NAP	44-A	204	-	50,52,52	2.36	16 (32%)	71,80,80	1.69	16 (22%)
4	NAP	131-A	204	-	50,52,52	2.24	13 (26%)	71,80,80	1.48	10 (14%)
2	FOL	17-A	201	-	34,34,34	1.25	3 (8%)	43,47,47	1.13	2 (4%)
2	FOL	140-A	201	-	34,34,34	1.22	3 (8%)	43,47,47	1.65	4 (9%)
2	FOL	154-A	201	-	34,34,34	1.31	3 (8%)	43,47,47	1.18	2 (4%)
4	NAP	85-A	204	-	50,52,52	2.26	16 (32%)	71,80,80	1.66	16 (22%)
4	NAP	74-A	204	-	50,52,52	2.25	15 (30%)	71,80,80	1.81	14 (19%)
4	NAP	84-A	204	-	50,52,52	2.12	14 (28%)	71,80,80	1.46	13 (18%)
2	FOL	94-A	201	-	34,34,34	1.29	3 (8%)	43,47,47	1.53	8 (18%)
2	FOL	92-A	201	-	34,34,34	1.39	4 (11%)	43,47,47	1.73	5 (11%)
2	FOL	27-A	201	-	34,34,34	1.32	3 (8%)	43,47,47	1.27	2 (4%)
2	FOL	32-A	201	-	34,34,34	1.36	4 (11%)	43,47,47	1.31	5 (11%)
2	FOL	90-A	201	-	34,34,34	1.16	3 (8%)	43,47,47	1.38	5 (11%)
4	NAP	69-A	204	-	50,52,52	2.35	14 (28%)	71,80,80	1.65	16 (22%)
4	NAP	71-A	204	-	50,52,52	2.30	17 (34%)	71,80,80	1.68	17 (23%)
4	NAP	75-A	204	-	50,52,52	2.31	14 (28%)	71,80,80	1.71	17 (23%)
2	FOL	60-A	201	-	34,34,34	1.27	4 (11%)	43,47,47	1.52	8 (18%)
2	FOL	91-A	201	-	34,34,34	1.28	3 (8%)	43,47,47	1.34	5 (11%)
2	FOL	83-A	201	-	34,34,34	1.53	3 (8%)	43,47,47	1.71	11 (25%)
2	FOL	47-A	201	-	34,34,34	1.37	3 (8%)	43,47,47	1.57	6 (13%)
2	FOL	35-A	201	-	34,34,34	1.23	2 (5%)	43,47,47	1.21	2 (4%)
2	FOL	123-A	201	-	34,34,34	1.30	3 (8%)	43,47,47	1.08	2 (4%)
4	NAP	60-A	204	-	50,52,52	2.38	16 (32%)	71,80,80	1.75	16 (22%)
4	NAP	110-A	204	-	50,52,52	2.32	16 (32%)	71,80,80	1.71	16 (22%)
2	FOL	40-A	201	-	34,34,34	1.36	4 (11%)	43,47,47	1.57	9 (20%)
4	NAP	54-A	204	-	50,52,52	2.15	15 (30%)	71,80,80	1.80	15 (21%)
4	NAP	78-A	204	-	50,52,52	2.21	15 (30%)	71,80,80	1.79	15 (21%)
4	NAP	122-A	204	-	50,52,52	2.34	15 (30%)	71,80,80	1.70	17 (23%)
4	NAP	123-A	204	-	50,52,52	2.31	16 (32%)	71,80,80	1.76	15 (21%)
4	NAP	8-A	204	-	50,52,52	2.20	16 (32%)	71,80,80	1.39	9 (12%)
2	FOL	15-A	201	-	34,34,34	1.41	3 (8%)	43,47,47	1.68	7 (16%)
2	FOL	139-A	201	-	34,34,34	1.30	3 (8%)	43,47,47	1.80	7 (16%)
4	NAP	66-A	204	-	50,52,52	2.27	16 (32%)	71,80,80	1.68	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	161-A	204	-	50,52,52	2.24	14 (28%)	71,80,80	1.70	16 (22%)
2	FOL	34-A	201	-	34,34,34	1.37	3 (8%)	43,47,47	1.77	10 (23%)
4	NAP	62-A	204	-	50,52,52	2.35	15 (30%)	71,80,80	1.69	16 (22%)
4	NAP	143-A	204	-	50,52,52	2.27	17 (34%)	71,80,80	1.68	15 (21%)
2	FOL	75-A	201	-	34,34,34	1.24	3 (8%)	43,47,47	1.45	4 (9%)
2	FOL	108-A	201	-	34,34,34	1.30	3 (8%)	43,47,47	1.52	8 (18%)
2	FOL	51-A	201	-	34,34,34	1.31	3 (8%)	43,47,47	1.10	3 (6%)
4	NAP	27-A	204	-	50,52,52	2.24	16 (32%)	71,80,80	1.76	16 (22%)
4	NAP	115-A	204	-	50,52,52	2.38	18 (36%)	71,80,80	1.78	17 (23%)
2	FOL	98-A	201	-	34,34,34	1.27	3 (8%)	43,47,47	1.31	5 (11%)
2	FOL	114-A	201	-	34,34,34	1.29	4 (11%)	43,47,47	1.52	4 (9%)
4	NAP	16-A	204	-	50,52,52	2.33	16 (32%)	71,80,80	1.67	16 (22%)
4	NAP	47-A	204	-	50,52,52	2.40	16 (32%)	71,80,80	1.70	16 (22%)
4	NAP	3-A	204	-	50,52,52	2.23	17 (34%)	71,80,80	1.77	15 (21%)
4	NAP	121-A	204	-	50,52,52	2.36	14 (28%)	71,80,80	1.63	14 (19%)
2	FOL	1-A	201	-	34,34,34	1.27	3 (8%)	43,47,47	1.33	6 (13%)
2	FOL	67-A	201	-	34,34,34	1.23	3 (8%)	43,47,47	1.45	5 (11%)
4	NAP	82-A	204	-	50,52,52	2.44	16 (32%)	71,80,80	1.47	10 (14%)
4	NAP	48-A	204	-	50,52,52	2.26	15 (30%)	71,80,80	1.76	15 (21%)
4	NAP	95-A	204	-	50,52,52	2.26	15 (30%)	71,80,80	1.68	15 (21%)
4	NAP	28-A	204	-	50,52,52	2.22	17 (34%)	71,80,80	1.78	15 (21%)
2	FOL	99-A	201	-	34,34,34	1.25	3 (8%)	43,47,47	1.49	6 (13%)
2	FOL	156-A	201	-	34,34,34	1.23	3 (8%)	43,47,47	1.63	5 (11%)
2	FOL	111-A	201	-	34,34,34	1.39	4 (11%)	43,47,47	1.31	6 (13%)
4	NAP	99-A	204	-	50,52,52	2.28	16 (32%)	71,80,80	1.74	15 (21%)
2	FOL	144-A	201	-	34,34,34	1.32	3 (8%)	43,47,47	1.87	10 (23%)
4	NAP	13-A	204	-	50,52,52	2.30	16 (32%)	71,80,80	1.67	16 (22%)
4	NAP	129-A	204	-	50,52,52	2.15	16 (32%)	71,80,80	1.80	14 (19%)
2	FOL	55-A	201	-	34,34,34	1.21	3 (8%)	43,47,47	1.31	3 (6%)
2	FOL	71-A	201	-	34,34,34	1.31	3 (8%)	43,47,47	1.33	3 (6%)
4	NAP	25-A	204	-	50,52,52	2.38	16 (32%)	71,80,80	1.81	15 (21%)
4	NAP	50-A	204	-	50,52,52	2.29	17 (34%)	71,80,80	1.71	16 (22%)
2	FOL	44-A	201	-	34,34,34	1.33	3 (8%)	43,47,47	1.38	5 (11%)
2	FOL	31-A	201	-	34,34,34	1.25	3 (8%)	43,47,47	1.68	9 (20%)
2	FOL	66-A	201	-	34,34,34	1.25	3 (8%)	43,47,47	1.41	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	61-A	201	-	34,34,34	1.20	2 (5%)	43,47,47	1.39	5 (11%)
2	FOL	56-A	201	-	34,34,34	1.34	3 (8%)	43,47,47	1.49	7 (16%)
4	NAP	29-A	204	-	50,52,52	2.30	16 (32%)	71,80,80	1.76	14 (19%)
4	NAP	117-A	204	-	50,52,52	2.23	16 (32%)	71,80,80	1.93	18 (25%)
2	FOL	62-A	201	-	34,34,34	1.31	3 (8%)	43,47,47	1.48	5 (11%)
2	FOL	48-A	201	-	34,34,34	1.30	2 (5%)	43,47,47	2.29	15 (34%)
4	NAP	9-A	204	-	50,52,52	2.07	16 (32%)	71,80,80	1.38	12 (16%)
2	FOL	78-A	201	-	34,34,34	1.26	3 (8%)	43,47,47	1.56	6 (13%)
2	FOL	122-A	201	-	34,34,34	1.24	2 (5%)	43,47,47	1.24	5 (11%)
2	FOL	116-A	201	-	34,34,34	1.19	3 (8%)	43,47,47	1.28	3 (6%)
2	FOL	137-A	201	-	34,34,34	1.36	3 (8%)	43,47,47	1.36	4 (9%)
4	NAP	76-A	204	-	50,52,52	2.34	17 (34%)	71,80,80	1.73	17 (23%)
4	NAP	164-A	204	-	50,52,52	2.25	15 (30%)	71,80,80	1.74	17 (23%)
2	FOL	21-A	201	-	34,34,34	1.47	3 (8%)	43,47,47	1.71	7 (16%)
4	NAP	26-A	204	-	50,52,52	2.35	15 (30%)	71,80,80	1.71	17 (23%)
2	FOL	157-A	201	-	34,34,34	1.42	3 (8%)	43,47,47	1.27	5 (11%)
2	FOL	24-A	201	-	34,34,34	1.25	3 (8%)	43,47,47	1.70	6 (13%)
2	FOL	131-A	201	-	34,34,34	1.29	3 (8%)	43,47,47	1.64	8 (18%)
4	NAP	86-A	204	-	50,52,52	2.25	16 (32%)	71,80,80	1.68	16 (22%)
4	NAP	154-A	204	-	50,52,52	2.18	16 (32%)	71,80,80	1.80	15 (21%)
4	NAP	94-A	204	-	50,52,52	2.26	17 (34%)	71,80,80	1.69	15 (21%)
4	NAP	127-A	204	-	50,52,52	2.21	14 (28%)	71,80,80	1.73	15 (21%)
4	NAP	11-A	204	-	50,52,52	2.28	15 (30%)	71,80,80	1.67	16 (22%)
2	FOL	133-A	201	-	34,34,34	1.37	3 (8%)	43,47,47	1.48	6 (13%)
2	FOL	160-A	201	-	34,34,34	1.40	3 (8%)	43,47,47	1.29	3 (6%)
2	FOL	118-A	201	-	34,34,34	1.42	3 (8%)	43,47,47	1.54	10 (23%)
2	FOL	145-A	201	-	34,34,34	1.25	3 (8%)	43,47,47	1.24	4 (9%)
2	FOL	84-A	201	-	34,34,34	1.24	3 (8%)	43,47,47	1.58	7 (16%)
2	FOL	128-A	201	-	34,34,34	1.09	3 (8%)	43,47,47	1.71	8 (18%)
2	FOL	87-A	201	-	34,34,34	1.20	3 (8%)	43,47,47	1.41	5 (11%)
4	NAP	124-A	204	-	50,52,52	2.26	14 (28%)	71,80,80	1.74	17 (23%)
2	FOL	82-A	201	-	34,34,34	1.37	5 (14%)	43,47,47	1.60	9 (20%)
2	FOL	9-A	201	-	34,34,34	1.43	3 (8%)	43,47,47	1.42	7 (16%)
4	NAP	90-A	204	-	50,52,52	2.23	16 (32%)	71,80,80	1.72	16 (22%)
4	NAP	7-A	204	-	50,52,52	2.27	17 (34%)	71,80,80	1.51	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	91-A	204	-	50,52,52	2.24	15 (30%)	71,80,80	1.70	16 (22%)
2	FOL	28-A	201	-	34,34,34	1.34	3 (8%)	43,47,47	1.18	3 (6%)
2	FOL	161-A	201	-	34,34,34	1.15	3 (8%)	43,47,47	1.37	5 (11%)
2	FOL	26-A	201	-	34,34,34	1.34	4 (11%)	43,47,47	1.77	13 (30%)
4	NAP	83-A	204	-	50,52,52	2.23	15 (30%)	71,80,80	1.40	11 (15%)
2	FOL	158-A	201	-	34,34,34	1.41	3 (8%)	43,47,47	1.52	9 (20%)
4	NAP	120-A	204	-	50,52,52	2.42	15 (30%)	71,80,80	1.66	15 (21%)
4	NAP	148-A	204	-	50,52,52	2.25	15 (30%)	71,80,80	1.77	16 (22%)
2	FOL	126-A	201	-	34,34,34	1.52	4 (11%)	43,47,47	2.32	12 (27%)
4	NAP	19-A	204	-	50,52,52	2.37	16 (32%)	71,80,80	1.69	16 (22%)
4	NAP	67-A	204	-	50,52,52	2.33	14 (28%)	71,80,80	1.71	13 (18%)
4	NAP	137-A	204	-	50,52,52	2.34	15 (30%)	71,80,80	1.74	16 (22%)
4	NAP	40-A	204	-	50,52,52	2.36	15 (30%)	71,80,80	1.72	17 (23%)
2	FOL	127-A	201	-	34,34,34	1.20	3 (8%)	43,47,47	1.76	10 (23%)
2	FOL	151-A	201	-	34,34,34	1.34	2 (5%)	43,47,47	1.26	4 (9%)
2	FOL	95-A	201	-	34,34,34	1.16	2 (5%)	43,47,47	1.49	6 (13%)
2	FOL	96-A	201	-	34,34,34	1.26	3 (8%)	43,47,47	1.38	3 (6%)
2	FOL	7-A	201	-	34,34,34	1.45	3 (8%)	43,47,47	1.34	5 (11%)
2	FOL	39-A	201	-	34,34,34	1.33	4 (11%)	43,47,47	1.81	9 (20%)
2	FOL	147-A	201	-	34,34,34	1.34	2 (5%)	43,47,47	1.42	5 (11%)
4	NAP	58-A	204	-	50,52,52	2.30	16 (32%)	71,80,80	1.45	9 (12%)
4	NAP	139-A	204	-	50,52,52	2.28	15 (30%)	71,80,80	1.74	17 (23%)
2	FOL	81-A	201	-	34,34,34	1.27	3 (8%)	43,47,47	1.71	7 (16%)
2	FOL	36-A	201	-	34,34,34	1.27	3 (8%)	43,47,47	1.22	4 (9%)
2	FOL	68-A	201	-	34,34,34	1.39	4 (11%)	43,47,47	1.40	5 (11%)
2	FOL	10-A	201	-	34,34,34	1.23	2 (5%)	43,47,47	1.56	7 (16%)
4	NAP	166-A	204	-	50,52,52	2.20	15 (30%)	71,80,80	1.70	15 (21%)
2	FOL	155-A	201	-	34,34,34	1.24	3 (8%)	43,47,47	1.48	9 (20%)
2	FOL	63-A	201	-	34,34,34	1.21	3 (8%)	43,47,47	1.66	9 (20%)
4	NAP	128-A	204	-	50,52,52	2.18	15 (30%)	71,80,80	1.85	14 (19%)
4	NAP	155-A	204	-	50,52,52	2.29	15 (30%)	71,80,80	1.61	15 (21%)
4	NAP	5-A	204	-	50,52,52	2.39	14 (28%)	71,80,80	1.75	15 (21%)
2	FOL	49-A	201	-	34,34,34	1.15	3 (8%)	43,47,47	1.32	5 (11%)
2	FOL	150-A	201	-	34,34,34	1.21	3 (8%)	43,47,47	1.07	2 (4%)
2	FOL	110-A	201	-	34,34,34	1.32	3 (8%)	43,47,47	1.87	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	45-A	201	-	34,34,34	1.34	3 (8%)	43,47,47	1.43	5 (11%)
4	NAP	138-A	204	-	50,52,52	2.26	15 (30%)	71,80,80	1.73	16 (22%)
2	FOL	25-A	201	-	34,34,34	1.28	3 (8%)	43,47,47	1.71	8 (18%)
4	NAP	18-A	204	-	50,52,52	2.39	15 (30%)	71,80,80	1.78	16 (22%)
4	NAP	126-A	204	-	50,52,52	2.36	16 (32%)	71,80,80	1.67	15 (21%)
4	NAP	32-A	204	-	50,52,52	2.35	17 (34%)	71,80,80	1.51	10 (14%)
4	NAP	163-A	204	-	50,52,52	2.22	15 (30%)	71,80,80	1.72	14 (19%)
2	FOL	120-A	201	-	34,34,34	1.27	2 (5%)	43,47,47	1.41	6 (13%)
2	FOL	43-A	201	-	34,34,34	1.25	2 (5%)	43,47,47	1.93	11 (25%)
4	NAP	81-A	204	-	50,52,52	2.41	15 (30%)	71,80,80	1.52	10 (14%)
4	NAP	144-A	204	-	50,52,52	2.30	15 (30%)	71,80,80	1.75	16 (22%)
2	FOL	76-A	201	-	34,34,34	1.44	3 (8%)	43,47,47	1.53	7 (16%)
4	NAP	88-A	204	-	50,52,52	2.24	15 (30%)	71,80,80	1.70	14 (19%)
2	FOL	57-A	201	-	34,34,34	1.52	4 (11%)	43,47,47	1.81	13 (30%)
4	NAP	36-A	204	-	50,52,52	2.35	16 (32%)	71,80,80	1.70	16 (22%)
4	NAP	133-A	204	-	50,52,52	2.21	15 (30%)	71,80,80	1.38	8 (11%)
4	NAP	68-A	204	-	50,52,52	2.31	17 (34%)	71,80,80	1.60	15 (21%)
4	NAP	63-A	204	-	50,52,52	2.26	16 (32%)	71,80,80	1.69	16 (22%)
4	NAP	52-A	204	-	50,52,52	2.31	15 (30%)	71,80,80	1.86	14 (19%)
2	FOL	136-A	201	-	34,34,34	1.24	3 (8%)	43,47,47	1.45	8 (18%)
2	FOL	23-A	201	-	34,34,34	1.32	4 (11%)	43,47,47	1.63	7 (16%)
4	NAP	31-A	204	-	50,52,52	2.32	16 (32%)	71,80,80	1.51	12 (16%)

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
4	NAP	56-A	204	-	-	9/35/67/67	0/5/5/5
4	NAP	111-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	4-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	116-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	146-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	41-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	24-A	204	-	-	1/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	14-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	46-A	204	-	-	5/35/67/67	0/5/5/5
2	FOL	124-A	201	-	-	6/22/22/22	0/3/3/3
4	NAP	12-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	105-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	41-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	97-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	138-A	201	-	-	6/22/22/22	0/3/3/3
4	NAP	134-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	152-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	5-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	157-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	87-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	117-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	39-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	51-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	158-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	92-A	204	-	-	1/35/67/67	0/5/5/5
4	NAP	114-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	105-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	86-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	59-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	53-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	141-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	1-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	93-A	204	-	-	1/35/67/67	0/5/5/5
2	FOL	88-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	59-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	70-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	30-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	113-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	10-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	153-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	89-A	204	-	-	1/35/67/67	0/5/5/5
4	NAP	45-A	204	-	-	2/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	73-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	64-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	3-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	147-A	204	-	-	0/35/67/67	0/5/5/5
2	FOL	46-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	12-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	21-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	33-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	53-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	80-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	134-A	201	-	-	8/22/22/22	0/3/3/3
2	FOL	115-A	201	-	-	8/22/22/22	0/3/3/3
2	FOL	113-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	152-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	153-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	50-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	80-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	167-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	142-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	34-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	57-A	204	-	-	5/35/67/67	0/5/5/5
2	FOL	101-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	20-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	162-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	160-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	38-A	204	-	-	1/35/67/67	0/5/5/5
2	FOL	52-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	23-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	135-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	54-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	159-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	77-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	165-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	64-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	98-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	13-A	201	-	-	2/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	20-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	93-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	72-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	165-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	140-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	11-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	102-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	125-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	85-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	65-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	79-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	22-A	201	-	-	8/22/22/22	0/3/3/3
4	NAP	132-A	204	-	-	5/35/67/67	0/5/5/5
4	NAP	4-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	149-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	130-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	121-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	141-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	22-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	112-A	201	-	-	9/22/22/22	0/3/3/3
4	NAP	2-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	42-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	148-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	43-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	19-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	119-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	112-A	204	-	-	4/35/67/67	0/5/5/5
4	NAP	77-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	17-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	156-A	204	-	-	1/35/67/67	0/5/5/5
4	NAP	6-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	159-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	132-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	38-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	16-A	201	-	-	0/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	30-A	204	-	-	1/35/67/67	0/5/5/5
4	NAP	118-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	109-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	142-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	69-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	2-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	149-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	35-A	204	-	-	0/35/67/67	0/5/5/5
4	NAP	136-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	107-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	18-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	58-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	130-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	61-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	119-A	204	-	-	7/35/67/67	0/5/5/5
2	FOL	37-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	70-A	204	-	-	1/35/67/67	0/5/5/5
4	NAP	72-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	65-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	8-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	151-A	204	-	-	0/35/67/67	0/5/5/5
2	FOL	89-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	14-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	104-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	167-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	145-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	103-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	101-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	97-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	100-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	162-A	204	-	-	4/35/67/67	0/5/5/5
2	FOL	129-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	103-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	125-A	201	-	-	8/22/22/22	0/3/3/3
2	FOL	106-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	33-A	204	-	-	6/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	163-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	102-A	204	-	-	4/35/67/67	0/5/5/5
4	NAP	49-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	29-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	150-A	204	-	-	1/35/67/67	0/5/5/5
4	NAP	108-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	37-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	96-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	74-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	109-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	15-A	204	-	-	8/35/67/67	0/5/5/5
4	NAP	42-A	204	-	-	5/35/67/67	0/5/5/5
2	FOL	100-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	6-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	104-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	143-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	73-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	166-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	107-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	135-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	164-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	55-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	106-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	79-A	204	-	-	1/35/67/67	0/5/5/5
4	NAP	146-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	44-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	131-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	17-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	140-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	154-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	85-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	74-A	204	-	-	1/35/67/67	0/5/5/5
4	NAP	84-A	204	-	-	5/35/67/67	0/5/5/5
2	FOL	94-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	92-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	27-A	201	-	-	2/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	32-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	90-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	69-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	71-A	204	-	-	1/35/67/67	0/5/5/5
4	NAP	75-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	60-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	91-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	83-A	201	-	-	10/22/22/22	0/3/3/3
2	FOL	47-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	35-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	123-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	60-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	110-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	40-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	54-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	78-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	122-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	123-A	204	-	-	1/35/67/67	0/5/5/5
4	NAP	8-A	204	-	-	0/35/67/67	0/5/5/5
2	FOL	15-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	139-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	66-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	161-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	34-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	62-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	143-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	75-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	108-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	51-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	27-A	204	-	-	4/35/67/67	0/5/5/5
4	NAP	115-A	204	-	-	0/35/67/67	0/5/5/5
2	FOL	98-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	114-A	201	-	-	9/22/22/22	0/3/3/3
4	NAP	16-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	47-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	3-A	204	-	-	2/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	121-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	1-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	67-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	82-A	204	-	-	4/35/67/67	0/5/5/5
4	NAP	48-A	204	-	-	4/35/67/67	0/5/5/5
4	NAP	95-A	204	-	-	5/35/67/67	0/5/5/5
4	NAP	28-A	204	-	-	6/35/67/67	0/5/5/5
2	FOL	99-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	156-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	111-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	99-A	204	-	-	1/35/67/67	0/5/5/5
2	FOL	144-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	13-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	129-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	55-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	71-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	25-A	204	-	-	0/35/67/67	0/5/5/5
4	NAP	50-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	44-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	31-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	66-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	61-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	56-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	29-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	117-A	204	-	-	4/35/67/67	0/5/5/5
2	FOL	62-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	48-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	9-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	78-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	122-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	116-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	137-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	76-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	164-A	204	-	-	2/35/67/67	0/5/5/5
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
4	NAP	26-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	157-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	24-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	131-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	86-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	154-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	94-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	127-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	11-A	204	-	-	1/35/67/67	0/5/5/5
2	FOL	133-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	160-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	118-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	145-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	84-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	128-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	87-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	124-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	82-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	9-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	90-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	7-A	204	-	-	1/35/67/67	0/5/5/5
4	NAP	91-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	28-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	161-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	26-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	83-A	204	-	-	1/35/67/67	0/5/5/5
2	FOL	158-A	201	-	-	7/22/22/22	0/3/3/3
4	NAP	120-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	148-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	126-A	201	-	-	8/22/22/22	0/3/3/3
4	NAP	19-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	67-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	137-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	40-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	127-A	201	-	-	4/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	151-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	95-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	96-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	7-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	39-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	147-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	58-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	139-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	81-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	36-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	68-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	10-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	166-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	155-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	63-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	128-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	155-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	5-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	49-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	150-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	110-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	45-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	138-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	25-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	18-A	204	-	-	0/35/67/67	0/5/5/5
4	NAP	126-A	204	-	-	1/35/67/67	0/5/5/5
4	NAP	32-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	163-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	120-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	43-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	81-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	144-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	76-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	88-A	204	-	-	3/35/67/67	0/5/5/5
2	FOL	57-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	36-A	204	-	-	1/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	133-A	204	-	-	2/35/67/67	0/5/5/5
4	NAP	68-A	204	-	-	3/35/67/67	0/5/5/5
4	NAP	63-A	204	-	-	8/35/67/67	0/5/5/5
4	NAP	52-A	204	-	-	2/35/67/67	0/5/5/5
2	FOL	136-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	23-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	31-A	204	-	-	1/35/67/67	0/5/5/5

The worst 5 of 3103 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	107-A	204	NAP	PA-O3	9.07	1.69	1.59
4	106-A	204	NAP	PA-O3	8.47	1.68	1.59
4	82-A	204	NAP	PA-O3	8.27	1.68	1.59
4	37-A	204	NAP	PN-O3	8.23	1.68	1.59
4	82-A	204	NAP	PN-O3	8.14	1.68	1.59

The worst 5 of 3538 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	118-A	204	NAP	O2N-PN-O3	-18.29	57.84	107.27
4	57-A	204	NAP	O2N-PN-O3	-17.51	59.95	107.27
4	56-A	204	NAP	O2N-PN-O3	-15.13	66.38	107.27
4	57-A	204	NAP	O2N-PN-O1N	13.10	173.38	112.44
4	118-A	204	NAP	O2N-PN-O1N	11.78	167.26	112.44

There are no chirality outliers.

5 of 919 torsion outliers are listed below:

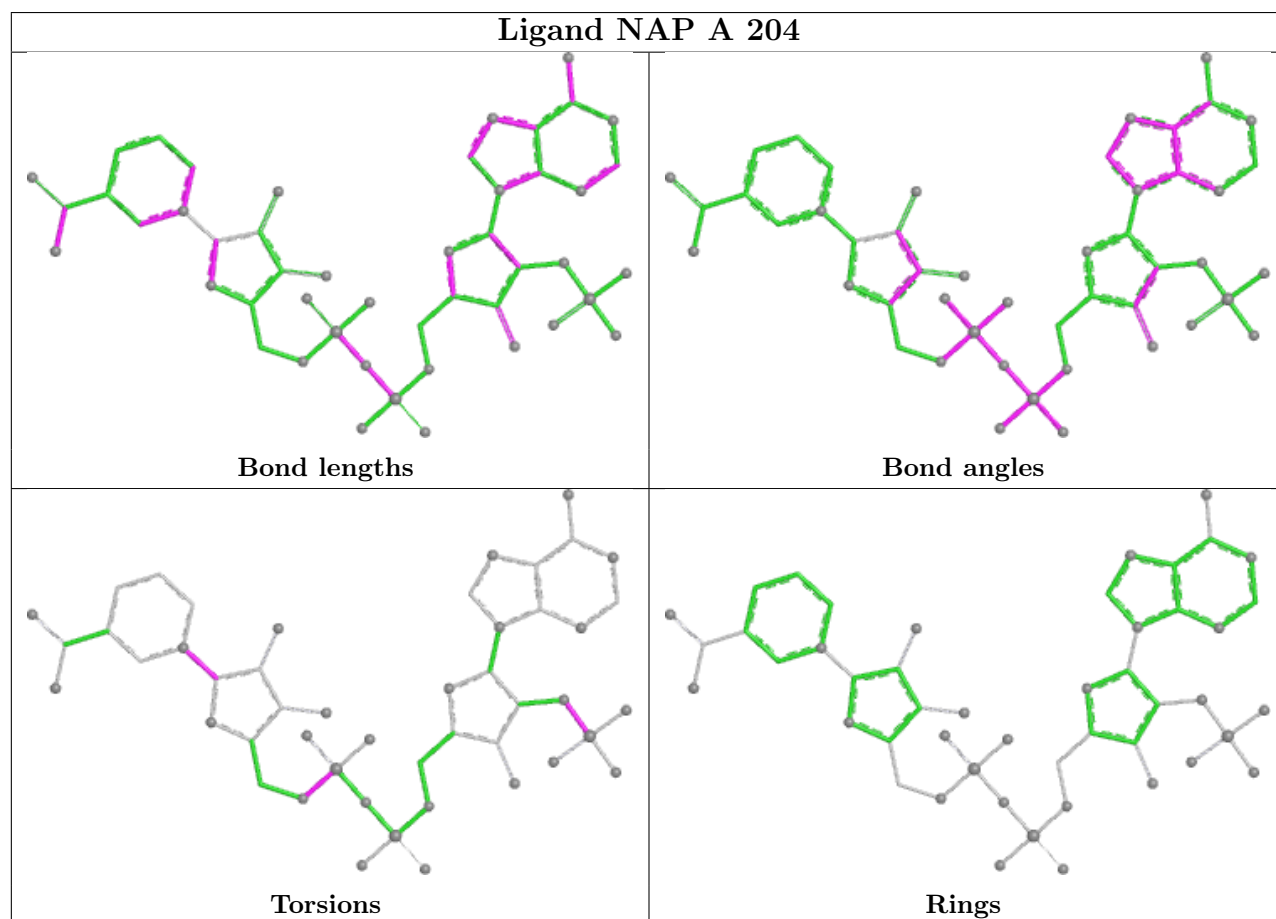
Mol	Chain	Res	Type	Atoms
2	14-A	201	FOL	CT-CA-CB-CG
2	22-A	201	FOL	N-CA-CB-CG
2	59-A	201	FOL	N-CA-CB-CG
2	60-A	201	FOL	N-CA-CB-CG
2	64-A	201	FOL	CA-CB-CG-CD

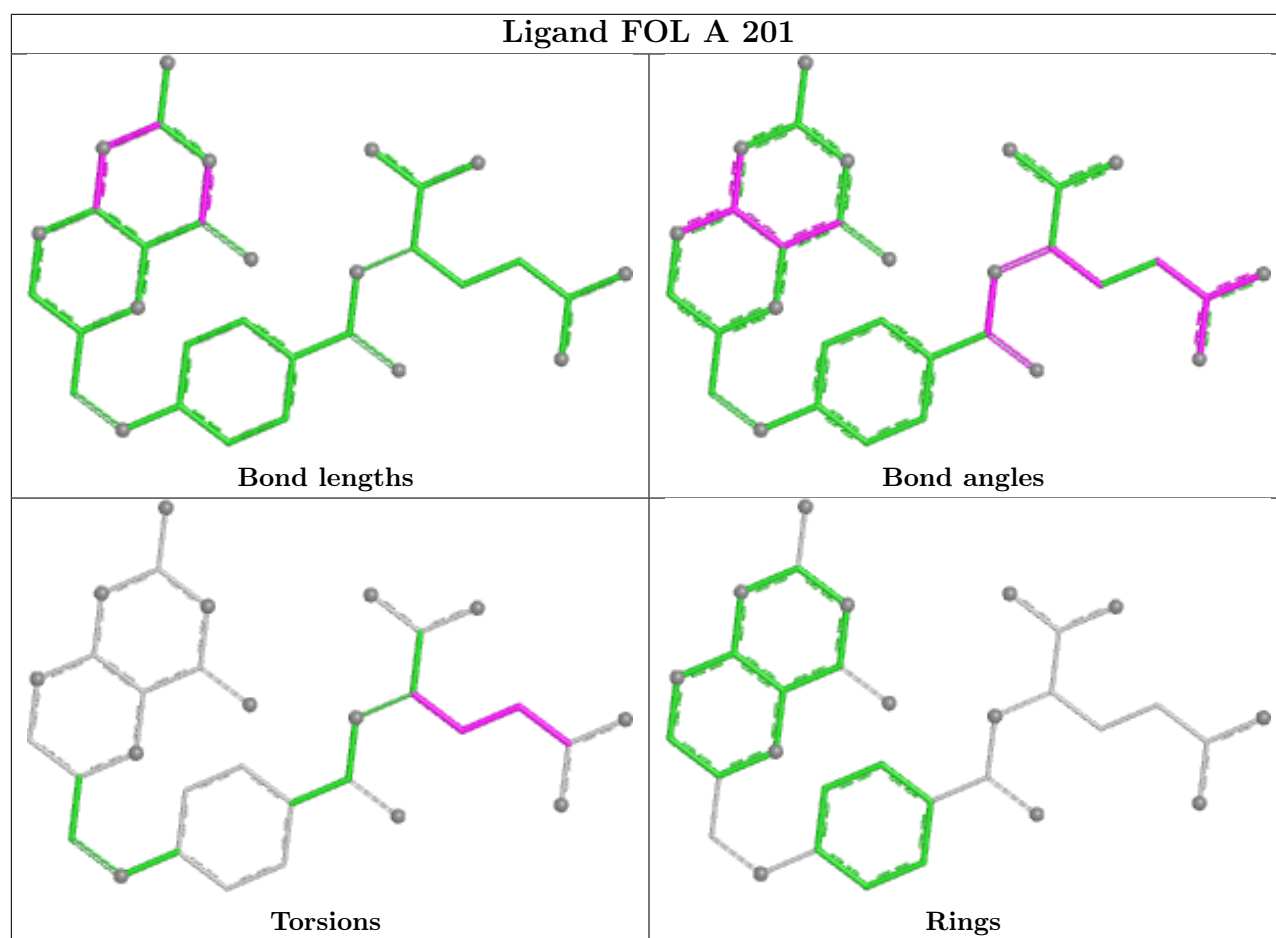
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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





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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	159/159 (100%)	2.58	88 (55%) 0 0	0, 0, 0, 0	159 (100%)
1	2-A	0/159	-	-	-	-
1	3-A	0/159	-	-	-	-
1	4-A	0/159	-	-	-	-
1	5-A	0/159	-	-	-	-
1	6-A	0/159	-	-	-	-
1	7-A	0/159	-	-	-	-
1	8-A	0/159	-	-	-	-
1	9-A	0/159	-	-	-	-
1	10-A	0/159	-	-	-	-
1	11-A	0/159	-	-	-	-
1	12-A	0/159	-	-	-	-
1	13-A	0/159	-	-	-	-
1	14-A	0/159	-	-	-	-
1	15-A	0/159	-	-	-	-
1	16-A	0/159	-	-	-	-
1	17-A	0/159	-	-	-	-
1	18-A	0/159	-	-	-	-
1	19-A	0/159	-	-	-	-
1	20-A	0/159	-	-	-	-
1	21-A	0/159	-	-	-	-
1	22-A	0/159	-	-	-	-
1	23-A	0/159	-	-	-	-
1	24-A	0/159	-	-	-	-
1	25-A	0/159	-	-	-	-
1	26-A	0/159	-	-	-	-
1	27-A	0/159	-	-	-	-
1	28-A	0/159	-	-	-	-
1	29-A	0/159	-	-	-	-
1	30-A	0/159	-	-	-	-
1	31-A	0/159	-	-	-	-
1	32-A	0/159	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	33-A	0/159	-	-	-	-
1	34-A	0/159	-	-	-	-
1	35-A	0/159	-	-	-	-
1	36-A	0/159	-	-	-	-
1	37-A	0/159	-	-	-	-
1	38-A	0/159	-	-	-	-
1	39-A	0/159	-	-	-	-
1	40-A	0/159	-	-	-	-
1	41-A	0/159	-	-	-	-
1	42-A	0/159	-	-	-	-
1	43-A	0/159	-	-	-	-
1	44-A	0/159	-	-	-	-
1	45-A	0/159	-	-	-	-
1	46-A	0/159	-	-	-	-
1	47-A	0/159	-	-	-	-
1	48-A	0/159	-	-	-	-
1	49-A	0/159	-	-	-	-
1	50-A	0/159	-	-	-	-
1	51-A	0/159	-	-	-	-
1	52-A	0/159	-	-	-	-
1	53-A	0/159	-	-	-	-
1	54-A	0/159	-	-	-	-
1	55-A	0/159	-	-	-	-
1	56-A	0/159	-	-	-	-
1	57-A	0/159	-	-	-	-
1	58-A	0/159	-	-	-	-
1	59-A	0/159	-	-	-	-
1	60-A	0/159	-	-	-	-
1	61-A	0/159	-	-	-	-
1	62-A	0/159	-	-	-	-
1	63-A	0/159	-	-	-	-
1	64-A	0/159	-	-	-	-
1	65-A	0/159	-	-	-	-
1	66-A	0/159	-	-	-	-
1	67-A	0/159	-	-	-	-
1	68-A	0/159	-	-	-	-
1	69-A	0/159	-	-	-	-
1	70-A	0/159	-	-	-	-
1	71-A	0/159	-	-	-	-
1	72-A	0/159	-	-	-	-
1	73-A	0/159	-	-	-	-
1	74-A	0/159	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	75-A	0/159	-	-	-	-
1	76-A	0/159	-	-	-	-
1	77-A	0/159	-	-	-	-
1	78-A	0/159	-	-	-	-
1	79-A	0/159	-	-	-	-
1	80-A	0/159	-	-	-	-
1	81-A	0/159	-	-	-	-
1	82-A	0/159	-	-	-	-
1	83-A	0/159	-	-	-	-
1	84-A	0/159	-	-	-	-
1	85-A	0/159	-	-	-	-
1	86-A	0/159	-	-	-	-
1	87-A	0/159	-	-	-	-
1	88-A	0/159	-	-	-	-
1	89-A	0/159	-	-	-	-
1	90-A	0/159	-	-	-	-
1	91-A	0/159	-	-	-	-
1	92-A	0/159	-	-	-	-
1	93-A	0/159	-	-	-	-
1	94-A	0/159	-	-	-	-
1	95-A	0/159	-	-	-	-
1	96-A	0/159	-	-	-	-
1	97-A	0/159	-	-	-	-
1	98-A	0/159	-	-	-	-
1	99-A	0/159	-	-	-	-
1	100-A	0/159	-	-	-	-
1	101-A	0/159	-	-	-	-
1	102-A	0/159	-	-	-	-
1	103-A	0/159	-	-	-	-
1	104-A	0/159	-	-	-	-
1	105-A	0/159	-	-	-	-
1	106-A	0/159	-	-	-	-
1	107-A	0/159	-	-	-	-
1	108-A	0/159	-	-	-	-
1	109-A	0/159	-	-	-	-
1	110-A	0/159	-	-	-	-
1	111-A	0/159	-	-	-	-
1	112-A	0/159	-	-	-	-
1	113-A	0/159	-	-	-	-
1	114-A	0/159	-	-	-	-
1	115-A	0/159	-	-	-	-
1	116-A	0/159	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	117-A	0/159	-	-	-	-
1	118-A	0/159	-	-	-	-
1	119-A	0/159	-	-	-	-
1	120-A	0/159	-	-	-	-
1	121-A	0/159	-	-	-	-
1	122-A	0/159	-	-	-	-
1	123-A	0/159	-	-	-	-
1	124-A	0/159	-	-	-	-
1	125-A	0/159	-	-	-	-
1	126-A	0/159	-	-	-	-
1	127-A	0/159	-	-	-	-
1	128-A	0/159	-	-	-	-
1	129-A	0/159	-	-	-	-
1	130-A	0/159	-	-	-	-
1	131-A	0/159	-	-	-	-
1	132-A	0/159	-	-	-	-
1	133-A	0/159	-	-	-	-
1	134-A	0/159	-	-	-	-
1	135-A	0/159	-	-	-	-
1	136-A	0/159	-	-	-	-
1	137-A	0/159	-	-	-	-
1	138-A	0/159	-	-	-	-
1	139-A	0/159	-	-	-	-
1	140-A	0/159	-	-	-	-
1	141-A	0/159	-	-	-	-
1	142-A	0/159	-	-	-	-
1	143-A	0/159	-	-	-	-
1	144-A	0/159	-	-	-	-
1	145-A	0/159	-	-	-	-
1	146-A	0/159	-	-	-	-
1	147-A	0/159	-	-	-	-
1	148-A	0/159	-	-	-	-
1	149-A	0/159	-	-	-	-
1	150-A	0/159	-	-	-	-
1	151-A	0/159	-	-	-	-
1	152-A	0/159	-	-	-	-
1	153-A	0/159	-	-	-	-
1	154-A	0/159	-	-	-	-
1	155-A	0/159	-	-	-	-
1	156-A	0/159	-	-	-	-
1	157-A	0/159	-	-	-	-
1	158-A	0/159	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	159-A	0/159	-	-	-	-
1	160-A	0/159	-	-	-	-
1	161-A	0/159	-	-	-	-
1	162-A	0/159	-	-	-	-
1	163-A	0/159	-	-	-	-
1	164-A	0/159	-	-	-	-
1	165-A	0/159	-	-	-	-
1	166-A	0/159	-	-	-	-
1	167-A	0/159	-	-	-	-
All	All	159/26553 (0%)	2.58	88 (55%) 0 0	0, 0, 0, 0	159 (100%)

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	128	TYR	8.2
1	1-A	21	PRO	7.8
1	1-A	18	ASN	7.8
1	1-A	16	MET	7.4
1	1-A	137	PHE	6.8

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

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

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	1-A	203	1/1	0.47	0.66	10,10,10,10	1
2	FOL	2-A	201	32/32	-	-	7,8,9,9	49
2	FOL	3-A	201	32/32	-	-	7,8,9,10	49
2	FOL	4-A	201	32/32	-	-	7,8,9,9	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FOL	5-A	201	32/32	-	-	7,8,9,9	49
2	FOL	6-A	201	32/32	-	-	7,7,9,9	49
2	FOL	7-A	201	32/32	-	-	7,8,9,9	49
2	FOL	8-A	201	32/32	-	-	7,8,9,9	49
2	FOL	9-A	201	32/32	-	-	7,8,9,9	49
2	FOL	10-A	201	32/32	-	-	7,8,9,9	49
2	FOL	11-A	201	32/32	-	-	7,8,9,9	49
2	FOL	12-A	201	32/32	-	-	7,8,9,9	49
2	FOL	13-A	201	32/32	-	-	7,7,9,9	49
2	FOL	14-A	201	32/32	-	-	7,8,9,10	49
2	FOL	15-A	201	32/32	-	-	7,8,9,9	49
2	FOL	16-A	201	32/32	-	-	7,7,9,9	49
2	FOL	17-A	201	32/32	-	-	7,8,9,9	49
2	FOL	18-A	201	32/32	-	-	7,8,9,9	49
2	FOL	19-A	201	32/32	-	-	7,8,9,9	49
2	FOL	20-A	201	32/32	-	-	7,8,9,9	49
2	FOL	21-A	201	32/32	-	-	7,8,9,9	49
2	FOL	22-A	201	32/32	-	-	7,8,9,9	49
2	FOL	23-A	201	32/32	-	-	7,8,9,9	49
2	FOL	24-A	201	32/32	-	-	7,8,9,9	49
2	FOL	25-A	201	32/32	-	-	7,8,9,10	49
2	FOL	26-A	201	32/32	-	-	7,8,9,10	49
2	FOL	27-A	201	32/32	-	-	7,8,9,9	49
2	FOL	28-A	201	32/32	-	-	7,8,9,9	49
2	FOL	29-A	201	32/32	-	-	7,8,9,9	49
2	FOL	30-A	201	32/32	-	-	7,7,9,9	49
2	FOL	31-A	201	32/32	-	-	7,8,9,9	49
2	FOL	32-A	201	32/32	-	-	7,8,9,9	49
2	FOL	33-A	201	32/32	-	-	7,8,9,9	49
2	FOL	34-A	201	32/32	-	-	7,8,9,9	49
2	FOL	35-A	201	32/32	-	-	7,8,9,9	49
2	FOL	36-A	201	32/32	-	-	7,8,9,9	49
2	FOL	37-A	201	32/32	-	-	7,8,9,9	49
2	FOL	38-A	201	32/32	-	-	7,8,9,9	49
2	FOL	39-A	201	32/32	-	-	7,8,9,9	49
2	FOL	40-A	201	32/32	-	-	7,8,9,9	49
2	FOL	41-A	201	32/32	-	-	7,8,9,10	49
2	FOL	42-A	201	32/32	-	-	7,8,9,9	49
2	FOL	43-A	201	32/32	-	-	7,7,9,9	49
2	FOL	44-A	201	32/32	-	-	7,8,9,9	49
2	FOL	45-A	201	32/32	-	-	7,8,9,9	49
2	FOL	46-A	201	32/32	-	-	7,8,9,9	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FOL	47-A	201	32/32	-	-	7,8,9,9	49
2	FOL	48-A	201	32/32	-	-	7,8,9,9	49
2	FOL	49-A	201	32/32	-	-	7,8,9,9	49
2	FOL	50-A	201	32/32	-	-	7,8,9,9	49
2	FOL	51-A	201	32/32	-	-	7,8,9,9	49
2	FOL	52-A	201	32/32	-	-	7,8,9,9	49
2	FOL	53-A	201	32/32	-	-	7,7,9,9	49
2	FOL	54-A	201	32/32	-	-	7,8,9,9	49
2	FOL	55-A	201	32/32	-	-	7,8,9,9	49
2	FOL	56-A	201	32/32	-	-	7,8,9,9	49
2	FOL	57-A	201	32/32	-	-	7,7,9,10	49
2	FOL	58-A	201	32/32	-	-	7,8,9,10	49
2	FOL	59-A	201	32/32	-	-	7,8,9,10	49
2	FOL	60-A	201	32/32	-	-	7,8,9,10	49
2	FOL	61-A	201	32/32	-	-	7,8,9,9	49
2	FOL	62-A	201	32/32	-	-	7,8,9,9	49
2	FOL	63-A	201	32/32	-	-	7,8,9,9	49
2	FOL	64-A	201	32/32	-	-	7,8,9,9	49
2	FOL	65-A	201	32/32	-	-	7,8,9,9	49
2	FOL	66-A	201	32/32	-	-	7,7,9,9	49
2	FOL	67-A	201	32/32	-	-	7,8,9,9	49
2	FOL	68-A	201	32/32	-	-	7,8,9,9	49
2	FOL	69-A	201	32/32	-	-	7,8,9,9	49
2	FOL	70-A	201	32/32	-	-	7,8,9,10	49
2	FOL	71-A	201	32/32	-	-	7,8,9,10	49
2	FOL	72-A	201	32/32	-	-	7,8,9,9	49
2	FOL	73-A	201	32/32	-	-	7,8,9,9	49
2	FOL	74-A	201	32/32	-	-	7,8,9,9	49
2	FOL	75-A	201	32/32	-	-	7,8,9,9	49
2	FOL	76-A	201	32/32	-	-	7,8,9,9	49
2	FOL	77-A	201	32/32	-	-	7,8,9,9	49
2	FOL	78-A	201	32/32	-	-	7,8,9,9	49
2	FOL	79-A	201	32/32	-	-	7,8,9,9	49
2	FOL	80-A	201	32/32	-	-	7,8,9,9	49
2	FOL	81-A	201	32/32	-	-	7,8,9,10	49
2	FOL	82-A	201	32/32	-	-	7,8,9,10	49
2	FOL	83-A	201	32/32	-	-	7,7,9,10	49
2	FOL	84-A	201	32/32	-	-	7,8,9,9	49
2	FOL	85-A	201	32/32	-	-	7,8,9,9	49
2	FOL	86-A	201	32/32	-	-	7,8,9,9	49
2	FOL	87-A	201	32/32	-	-	7,8,9,9	49
2	FOL	88-A	201	32/32	-	-	7,8,9,9	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FOL	89-A	201	32/32	-	-	7,8,9,9	49
2	FOL	90-A	201	32/32	-	-	7,8,9,9	49
2	FOL	91-A	201	32/32	-	-	7,8,9,9	49
2	FOL	92-A	201	32/32	-	-	7,8,9,9	49
2	FOL	93-A	201	32/32	-	-	7,7,9,9	49
2	FOL	94-A	201	32/32	-	-	7,8,9,9	49
2	FOL	95-A	201	32/32	-	-	7,7,9,9	49
2	FOL	96-A	201	32/32	-	-	7,8,9,9	49
2	FOL	97-A	201	32/32	-	-	7,8,9,9	49
2	FOL	98-A	201	32/32	-	-	7,8,9,9	49
2	FOL	99-A	201	32/32	-	-	7,8,9,9	49
2	FOL	100-A	201	32/32	-	-	7,8,9,9	49
2	FOL	101-A	201	32/32	-	-	7,8,9,9	49
2	FOL	102-A	201	32/32	-	-	7,8,9,9	49
2	FOL	103-A	201	32/32	-	-	7,8,9,9	49
2	FOL	104-A	201	32/32	-	-	7,8,9,9	49
2	FOL	105-A	201	32/32	-	-	7,7,9,9	49
2	FOL	106-A	201	32/32	-	-	7,8,9,9	49
2	FOL	107-A	201	32/32	-	-	7,8,9,9	49
2	FOL	108-A	201	32/32	-	-	7,8,9,9	49
2	FOL	109-A	201	32/32	-	-	7,8,9,9	49
2	FOL	110-A	201	32/32	-	-	7,8,9,9	49
2	FOL	111-A	201	32/32	-	-	7,8,9,9	49
2	FOL	112-A	201	32/32	-	-	7,8,9,9	49
2	FOL	113-A	201	32/32	-	-	7,8,9,9	49
2	FOL	114-A	201	32/32	-	-	7,8,9,9	49
2	FOL	115-A	201	32/32	-	-	7,8,9,9	49
2	FOL	116-A	201	32/32	-	-	7,8,9,9	49
2	FOL	117-A	201	32/32	-	-	7,8,9,9	49
2	FOL	118-A	201	32/32	-	-	7,8,9,9	49
2	FOL	119-A	201	32/32	-	-	7,8,9,9	49
2	FOL	120-A	201	32/32	-	-	7,8,9,9	49
2	FOL	121-A	201	32/32	-	-	7,8,9,9	49
2	FOL	122-A	201	32/32	-	-	7,8,9,9	49
2	FOL	123-A	201	32/32	-	-	7,8,9,9	49
2	FOL	124-A	201	32/32	-	-	7,8,9,9	49
2	FOL	125-A	201	32/32	-	-	7,8,9,9	49
2	FOL	126-A	201	32/32	-	-	7,7,9,9	49
2	FOL	127-A	201	32/32	-	-	7,8,9,9	49
2	FOL	128-A	201	32/32	-	-	7,8,9,10	49
2	FOL	129-A	201	32/32	-	-	7,7,9,9	49
2	FOL	130-A	201	32/32	-	-	7,8,9,9	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FOL	131-A	201	32/32	-	-	7,8,9,9	49
2	FOL	132-A	201	32/32	-	-	7,8,9,9	49
2	FOL	133-A	201	32/32	-	-	7,8,9,9	49
2	FOL	134-A	201	32/32	-	-	7,8,9,9	49
2	FOL	135-A	201	32/32	-	-	7,8,9,9	49
2	FOL	136-A	201	32/32	-	-	7,8,9,9	49
2	FOL	137-A	201	32/32	-	-	7,8,9,9	49
2	FOL	138-A	201	32/32	-	-	7,7,9,9	49
2	FOL	139-A	201	32/32	-	-	7,8,9,9	49
2	FOL	140-A	201	32/32	-	-	7,8,9,9	49
2	FOL	141-A	201	32/32	-	-	7,8,9,10	49
2	FOL	142-A	201	32/32	-	-	7,8,9,9	49
2	FOL	143-A	201	32/32	-	-	7,8,9,9	49
2	FOL	144-A	201	32/32	-	-	7,8,9,9	49
2	FOL	145-A	201	32/32	-	-	7,8,9,9	49
2	FOL	146-A	201	32/32	-	-	7,8,9,9	49
2	FOL	147-A	201	32/32	-	-	7,8,9,9	49
2	FOL	148-A	201	32/32	-	-	7,7,9,9	49
2	FOL	149-A	201	32/32	-	-	7,8,9,9	49
2	FOL	150-A	201	32/32	-	-	7,8,9,9	49
2	FOL	151-A	201	32/32	-	-	7,8,9,9	49
2	FOL	152-A	201	32/32	-	-	7,7,9,9	49
2	FOL	153-A	201	32/32	-	-	7,8,9,9	49
2	FOL	154-A	201	32/32	-	-	7,8,9,9	49
2	FOL	155-A	201	32/32	-	-	7,8,9,9	49
2	FOL	156-A	201	32/32	-	-	7,8,9,9	49
2	FOL	157-A	201	32/32	-	-	7,8,9,9	49
2	FOL	158-A	201	32/32	-	-	7,8,9,9	49
2	FOL	159-A	201	32/32	-	-	7,8,9,9	49
2	FOL	160-A	201	32/32	-	-	7,8,9,9	49
2	FOL	161-A	201	32/32	-	-	7,7,9,9	49
2	FOL	162-A	201	32/32	-	-	7,8,9,9	49
2	FOL	163-A	201	32/32	-	-	7,7,9,9	49
2	FOL	164-A	201	32/32	-	-	7,8,9,9	49
2	FOL	165-A	201	32/32	-	-	7,7,9,9	49
2	FOL	166-A	201	32/32	-	-	7,8,9,9	49
2	FOL	167-A	201	32/32	-	-	7,8,9,9	49
2	FOL	1-A	201	32/32	0.69	0.16	7,7,9,9	49
3	CA	2-A	202	1/1	-	-	10,10,10,10	1
3	CA	3-A	202	1/1	-	-	10,10,10,10	1
3	CA	4-A	202	1/1	-	-	10,10,10,10	1
3	CA	5-A	202	1/1	-	-	10,10,10,10	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	6-A	202	1/1	-	-	10,10,10,10	1
3	CA	7-A	202	1/1	-	-	10,10,10,10	1
3	CA	8-A	202	1/1	-	-	10,10,10,10	1
3	CA	9-A	202	1/1	-	-	10,10,10,10	1
3	CA	10-A	202	1/1	-	-	10,10,10,10	1
3	CA	11-A	202	1/1	-	-	10,10,10,10	1
3	CA	12-A	202	1/1	-	-	10,10,10,10	1
3	CA	13-A	202	1/1	-	-	10,10,10,10	1
3	CA	14-A	202	1/1	-	-	10,10,10,10	1
3	CA	15-A	202	1/1	-	-	10,10,10,10	1
3	CA	16-A	202	1/1	-	-	10,10,10,10	1
3	CA	17-A	202	1/1	-	-	10,10,10,10	1
3	CA	18-A	202	1/1	-	-	10,10,10,10	1
3	CA	19-A	202	1/1	-	-	10,10,10,10	1
3	CA	20-A	202	1/1	-	-	10,10,10,10	1
3	CA	21-A	202	1/1	-	-	10,10,10,10	1
3	CA	22-A	202	1/1	-	-	10,10,10,10	1
3	CA	23-A	202	1/1	-	-	10,10,10,10	1
3	CA	24-A	202	1/1	-	-	10,10,10,10	1
3	CA	25-A	202	1/1	-	-	10,10,10,10	1
3	CA	26-A	202	1/1	-	-	10,10,10,10	1
3	CA	27-A	202	1/1	-	-	10,10,10,10	1
3	CA	28-A	202	1/1	-	-	10,10,10,10	1
3	CA	29-A	202	1/1	-	-	10,10,10,10	1
3	CA	30-A	202	1/1	-	-	10,10,10,10	1
3	CA	31-A	202	1/1	-	-	10,10,10,10	1
3	CA	32-A	202	1/1	-	-	10,10,10,10	1
3	CA	33-A	202	1/1	-	-	10,10,10,10	1
3	CA	34-A	202	1/1	-	-	10,10,10,10	1
3	CA	35-A	202	1/1	-	-	10,10,10,10	1
3	CA	36-A	202	1/1	-	-	10,10,10,10	1
3	CA	37-A	202	1/1	-	-	10,10,10,10	1
3	CA	38-A	202	1/1	-	-	10,10,10,10	1
3	CA	39-A	202	1/1	-	-	10,10,10,10	1
3	CA	40-A	202	1/1	-	-	10,10,10,10	1
3	CA	41-A	202	1/1	-	-	10,10,10,10	1
3	CA	42-A	202	1/1	-	-	10,10,10,10	1
3	CA	43-A	202	1/1	-	-	10,10,10,10	1
3	CA	44-A	202	1/1	-	-	10,10,10,10	1
3	CA	45-A	202	1/1	-	-	10,10,10,10	1
3	CA	46-A	202	1/1	-	-	10,10,10,10	1
3	CA	47-A	202	1/1	-	-	10,10,10,10	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	48-A	202	1/1	-	-	10,10,10,10	1
3	CA	49-A	202	1/1	-	-	10,10,10,10	1
3	CA	50-A	202	1/1	-	-	10,10,10,10	1
3	CA	51-A	202	1/1	-	-	10,10,10,10	1
3	CA	52-A	202	1/1	-	-	10,10,10,10	1
3	CA	53-A	202	1/1	-	-	10,10,10,10	1
3	CA	54-A	202	1/1	-	-	10,10,10,10	1
3	CA	55-A	202	1/1	-	-	10,10,10,10	1
3	CA	56-A	202	1/1	-	-	10,10,10,10	1
3	CA	57-A	202	1/1	-	-	10,10,10,10	1
3	CA	58-A	202	1/1	-	-	10,10,10,10	1
3	CA	59-A	202	1/1	-	-	10,10,10,10	1
3	CA	60-A	202	1/1	-	-	10,10,10,10	1
3	CA	61-A	202	1/1	-	-	10,10,10,10	1
3	CA	62-A	202	1/1	-	-	10,10,10,10	1
3	CA	63-A	202	1/1	-	-	10,10,10,10	1
3	CA	64-A	202	1/1	-	-	10,10,10,10	1
3	CA	65-A	202	1/1	-	-	10,10,10,10	1
3	CA	66-A	202	1/1	-	-	10,10,10,10	1
3	CA	67-A	202	1/1	-	-	10,10,10,10	1
3	CA	68-A	202	1/1	-	-	10,10,10,10	1
3	CA	69-A	202	1/1	-	-	10,10,10,10	1
3	CA	70-A	202	1/1	-	-	10,10,10,10	1
3	CA	71-A	202	1/1	-	-	10,10,10,10	1
3	CA	72-A	202	1/1	-	-	10,10,10,10	1
3	CA	73-A	202	1/1	-	-	10,10,10,10	1
3	CA	74-A	202	1/1	-	-	10,10,10,10	1
3	CA	75-A	202	1/1	-	-	10,10,10,10	1
3	CA	76-A	202	1/1	-	-	10,10,10,10	1
3	CA	77-A	202	1/1	-	-	10,10,10,10	1
3	CA	78-A	202	1/1	-	-	10,10,10,10	1
3	CA	79-A	202	1/1	-	-	10,10,10,10	1
3	CA	80-A	202	1/1	-	-	10,10,10,10	1
3	CA	81-A	202	1/1	-	-	10,10,10,10	1
3	CA	82-A	202	1/1	-	-	10,10,10,10	1
3	CA	83-A	202	1/1	-	-	10,10,10,10	1
3	CA	84-A	202	1/1	-	-	10,10,10,10	1
3	CA	85-A	202	1/1	-	-	10,10,10,10	1
3	CA	86-A	202	1/1	-	-	10,10,10,10	1
3	CA	87-A	202	1/1	-	-	10,10,10,10	1
3	CA	88-A	202	1/1	-	-	10,10,10,10	1
3	CA	89-A	202	1/1	-	-	10,10,10,10	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	90-A	202	1/1	-	-	10,10,10,10	1
3	CA	91-A	202	1/1	-	-	10,10,10,10	1
3	CA	92-A	202	1/1	-	-	10,10,10,10	1
3	CA	93-A	202	1/1	-	-	10,10,10,10	1
3	CA	94-A	202	1/1	-	-	10,10,10,10	1
3	CA	95-A	202	1/1	-	-	10,10,10,10	1
3	CA	96-A	202	1/1	-	-	10,10,10,10	1
3	CA	97-A	202	1/1	-	-	10,10,10,10	1
3	CA	98-A	202	1/1	-	-	10,10,10,10	1
3	CA	99-A	202	1/1	-	-	10,10,10,10	1
3	CA	100-A	202	1/1	-	-	10,10,10,10	1
3	CA	101-A	202	1/1	-	-	10,10,10,10	1
3	CA	102-A	202	1/1	-	-	10,10,10,10	1
3	CA	103-A	202	1/1	-	-	10,10,10,10	1
3	CA	104-A	202	1/1	-	-	10,10,10,10	1
3	CA	105-A	202	1/1	-	-	10,10,10,10	1
3	CA	106-A	202	1/1	-	-	10,10,10,10	1
3	CA	107-A	202	1/1	-	-	10,10,10,10	1
3	CA	108-A	202	1/1	-	-	10,10,10,10	1
3	CA	109-A	202	1/1	-	-	10,10,10,10	1
3	CA	110-A	202	1/1	-	-	10,10,10,10	1
3	CA	111-A	202	1/1	-	-	10,10,10,10	1
3	CA	112-A	202	1/1	-	-	10,10,10,10	1
3	CA	113-A	202	1/1	-	-	10,10,10,10	1
3	CA	114-A	202	1/1	-	-	10,10,10,10	1
3	CA	115-A	202	1/1	-	-	10,10,10,10	1
3	CA	116-A	202	1/1	-	-	10,10,10,10	1
3	CA	117-A	202	1/1	-	-	10,10,10,10	1
3	CA	118-A	202	1/1	-	-	10,10,10,10	1
3	CA	119-A	202	1/1	-	-	10,10,10,10	1
3	CA	120-A	202	1/1	-	-	10,10,10,10	1
3	CA	121-A	202	1/1	-	-	10,10,10,10	1
3	CA	122-A	202	1/1	-	-	10,10,10,10	1
3	CA	123-A	202	1/1	-	-	10,10,10,10	1
3	CA	124-A	202	1/1	-	-	10,10,10,10	1
3	CA	125-A	202	1/1	-	-	10,10,10,10	1
3	CA	126-A	202	1/1	-	-	10,10,10,10	1
3	CA	127-A	202	1/1	-	-	10,10,10,10	1
3	CA	128-A	202	1/1	-	-	10,10,10,10	1
3	CA	129-A	202	1/1	-	-	10,10,10,10	1
3	CA	130-A	202	1/1	-	-	10,10,10,10	1
3	CA	131-A	202	1/1	-	-	10,10,10,10	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	132-A	202	1/1	-	-	10,10,10,10	1
3	CA	133-A	202	1/1	-	-	10,10,10,10	1
3	CA	134-A	202	1/1	-	-	10,10,10,10	1
3	CA	135-A	202	1/1	-	-	10,10,10,10	1
3	CA	136-A	202	1/1	-	-	10,10,10,10	1
3	CA	137-A	202	1/1	-	-	10,10,10,10	1
3	CA	138-A	202	1/1	-	-	10,10,10,10	1
3	CA	139-A	202	1/1	-	-	10,10,10,10	1
3	CA	140-A	202	1/1	-	-	10,10,10,10	1
3	CA	141-A	202	1/1	-	-	10,10,10,10	1
3	CA	142-A	202	1/1	-	-	10,10,10,10	1
3	CA	143-A	202	1/1	-	-	10,10,10,10	1
3	CA	144-A	202	1/1	-	-	10,10,10,10	1
3	CA	145-A	202	1/1	-	-	10,10,10,10	1
3	CA	146-A	202	1/1	-	-	10,10,10,10	1
3	CA	147-A	202	1/1	-	-	10,10,10,10	1
3	CA	148-A	202	1/1	-	-	10,10,10,10	1
3	CA	149-A	202	1/1	-	-	10,10,10,10	1
3	CA	150-A	202	1/1	-	-	10,10,10,10	1
3	CA	151-A	202	1/1	-	-	10,10,10,10	1
3	CA	152-A	202	1/1	-	-	10,10,10,10	1
3	CA	153-A	202	1/1	-	-	10,10,10,10	1
3	CA	154-A	202	1/1	-	-	10,10,10,10	1
3	CA	155-A	202	1/1	-	-	10,10,10,10	1
3	CA	156-A	202	1/1	-	-	10,10,10,10	1
3	CA	157-A	202	1/1	-	-	10,10,10,10	1
3	CA	158-A	202	1/1	-	-	10,10,10,10	1
3	CA	159-A	202	1/1	-	-	10,10,10,10	1
3	CA	160-A	202	1/1	-	-	10,10,10,10	1
3	CA	161-A	202	1/1	-	-	10,10,10,10	1
3	CA	162-A	202	1/1	-	-	10,10,10,10	1
3	CA	163-A	202	1/1	-	-	10,10,10,10	1
3	CA	164-A	202	1/1	-	-	10,10,10,10	1
3	CA	165-A	202	1/1	-	-	10,10,10,10	1
3	CA	166-A	202	1/1	-	-	10,10,10,10	1
3	CA	167-A	202	1/1	-	-	10,10,10,10	1
3	CA	1-A	202	1/1	0.92	0.07	10,10,10,10	1
3	CA	2-A	203	1/1	-	-	11,11,11,11	1
3	CA	3-A	203	1/1	-	-	10,10,10,10	1
3	CA	4-A	203	1/1	-	-	10,10,10,10	1
3	CA	5-A	203	1/1	-	-	10,10,10,10	1
3	CA	6-A	203	1/1	-	-	10,10,10,10	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	7-A	203	1/1	-	-	10,10,10,10	1
3	CA	8-A	203	1/1	-	-	11,11,11,11	1
3	CA	9-A	203	1/1	-	-	11,11,11,11	1
3	CA	10-A	203	1/1	-	-	11,11,11,11	1
3	CA	11-A	203	1/1	-	-	11,11,11,11	1
3	CA	12-A	203	1/1	-	-	11,11,11,11	1
3	CA	13-A	203	1/1	-	-	10,10,10,10	1
3	CA	14-A	203	1/1	-	-	11,11,11,11	1
3	CA	15-A	203	1/1	-	-	11,11,11,11	1
3	CA	16-A	203	1/1	-	-	10,10,10,10	1
3	CA	17-A	203	1/1	-	-	10,10,10,10	1
3	CA	18-A	203	1/1	-	-	10,10,10,10	1
3	CA	19-A	203	1/1	-	-	10,10,10,10	1
3	CA	20-A	203	1/1	-	-	10,10,10,10	1
3	CA	21-A	203	1/1	-	-	10,10,10,10	1
3	CA	22-A	203	1/1	-	-	9,9,9,9	1
3	CA	23-A	203	1/1	-	-	9,9,9,9	1
3	CA	24-A	203	1/1	-	-	9,9,9,9	1
3	CA	25-A	203	1/1	-	-	10,10,10,10	1
3	CA	26-A	203	1/1	-	-	9,9,9,9	1
3	CA	27-A	203	1/1	-	-	9,9,9,9	1
3	CA	28-A	203	1/1	-	-	10,10,10,10	1
3	CA	29-A	203	1/1	-	-	9,9,9,9	1
3	CA	30-A	203	1/1	-	-	10,10,10,10	1
3	CA	31-A	203	1/1	-	-	10,10,10,10	1
3	CA	32-A	203	1/1	-	-	10,10,10,10	1
3	CA	33-A	203	1/1	-	-	10,10,10,10	1
3	CA	34-A	203	1/1	-	-	10,10,10,10	1
3	CA	35-A	203	1/1	-	-	10,10,10,10	1
3	CA	36-A	203	1/1	-	-	10,10,10,10	1
3	CA	37-A	203	1/1	-	-	10,10,10,10	1
3	CA	38-A	203	1/1	-	-	10,10,10,10	1
3	CA	39-A	203	1/1	-	-	10,10,10,10	1
3	CA	40-A	203	1/1	-	-	10,10,10,10	1
3	CA	41-A	203	1/1	-	-	10,10,10,10	1
3	CA	42-A	203	1/1	-	-	11,11,11,11	1
3	CA	43-A	203	1/1	-	-	10,10,10,10	1
3	CA	44-A	203	1/1	-	-	10,10,10,10	1
3	CA	45-A	203	1/1	-	-	10,10,10,10	1
3	CA	46-A	203	1/1	-	-	10,10,10,10	1
3	CA	47-A	203	1/1	-	-	10,10,10,10	1
3	CA	48-A	203	1/1	-	-	10,10,10,10	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	49-A	203	1/1	-	-	9,9,9,9	1
3	CA	50-A	203	1/1	-	-	9,9,9,9	1
3	CA	51-A	203	1/1	-	-	9,9,9,9	1
3	CA	52-A	203	1/1	-	-	9,9,9,9	1
3	CA	53-A	203	1/1	-	-	9,9,9,9	1
3	CA	54-A	203	1/1	-	-	9,9,9,9	1
3	CA	55-A	203	1/1	-	-	9,9,9,9	1
3	CA	56-A	203	1/1	-	-	9,9,9,9	1
3	CA	57-A	203	1/1	-	-	9,9,9,9	1
3	CA	58-A	203	1/1	-	-	9,9,9,9	1
3	CA	59-A	203	1/1	-	-	9,9,9,9	1
3	CA	60-A	203	1/1	-	-	9,9,9,9	1
3	CA	61-A	203	1/1	-	-	9,9,9,9	1
3	CA	62-A	203	1/1	-	-	10,10,10,10	1
3	CA	63-A	203	1/1	-	-	10,10,10,10	1
3	CA	64-A	203	1/1	-	-	10,10,10,10	1
3	CA	65-A	203	1/1	-	-	10,10,10,10	1
3	CA	66-A	203	1/1	-	-	10,10,10,10	1
3	CA	67-A	203	1/1	-	-	10,10,10,10	1
3	CA	68-A	203	1/1	-	-	9,9,9,9	1
3	CA	69-A	203	1/1	-	-	10,10,10,10	1
3	CA	70-A	203	1/1	-	-	9,9,9,9	1
3	CA	71-A	203	1/1	-	-	9,9,9,9	1
3	CA	72-A	203	1/1	-	-	9,9,9,9	1
3	CA	73-A	203	1/1	-	-	9,9,9,9	1
3	CA	74-A	203	1/1	-	-	9,9,9,9	1
3	CA	75-A	203	1/1	-	-	9,9,9,9	1
3	CA	76-A	203	1/1	-	-	8,8,8,8	1
3	CA	77-A	203	1/1	-	-	9,9,9,9	1
3	CA	78-A	203	1/1	-	-	8,8,8,8	1
3	CA	79-A	203	1/1	-	-	8,8,8,8	1
3	CA	80-A	203	1/1	-	-	9,9,9,9	1
3	CA	81-A	203	1/1	-	-	10,10,10,10	1
3	CA	82-A	203	1/1	-	-	10,10,10,10	1
3	CA	83-A	203	1/1	-	-	10,10,10,10	1
3	CA	84-A	203	1/1	-	-	10,10,10,10	1
3	CA	85-A	203	1/1	-	-	10,10,10,10	1
3	CA	86-A	203	1/1	-	-	10,10,10,10	1
3	CA	87-A	203	1/1	-	-	10,10,10,10	1
3	CA	88-A	203	1/1	-	-	10,10,10,10	1
3	CA	89-A	203	1/1	-	-	10,10,10,10	1
3	CA	90-A	203	1/1	-	-	10,10,10,10	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	91-A	203	1/1	-	-	10,10,10,10	1
3	CA	92-A	203	1/1	-	-	10,10,10,10	1
3	CA	93-A	203	1/1	-	-	10,10,10,10	1
3	CA	94-A	203	1/1	-	-	11,11,11,11	1
3	CA	95-A	203	1/1	-	-	10,10,10,10	1
3	CA	96-A	203	1/1	-	-	10,10,10,10	1
3	CA	97-A	203	1/1	-	-	10,10,10,10	1
3	CA	98-A	203	1/1	-	-	11,11,11,11	1
3	CA	99-A	203	1/1	-	-	11,11,11,11	1
3	CA	100-A	203	1/1	-	-	10,10,10,10	1
3	CA	101-A	203	1/1	-	-	10,10,10,10	1
3	CA	102-A	203	1/1	-	-	10,10,10,10	1
3	CA	103-A	203	1/1	-	-	9,9,9,9	1
3	CA	104-A	203	1/1	-	-	10,10,10,10	1
3	CA	105-A	203	1/1	-	-	10,10,10,10	1
3	CA	106-A	203	1/1	-	-	9,9,9,9	1
3	CA	107-A	203	1/1	-	-	9,9,9,9	1
3	CA	108-A	203	1/1	-	-	9,9,9,9	1
3	CA	109-A	203	1/1	-	-	9,9,9,9	1
3	CA	110-A	203	1/1	-	-	9,9,9,9	1
3	CA	111-A	203	1/1	-	-	10,10,10,10	1
3	CA	112-A	203	1/1	-	-	9,9,9,9	1
3	CA	113-A	203	1/1	-	-	10,10,10,10	1
3	CA	114-A	203	1/1	-	-	10,10,10,10	1
3	CA	115-A	203	1/1	-	-	10,10,10,10	1
3	CA	116-A	203	1/1	-	-	9,9,9,9	1
3	CA	117-A	203	1/1	-	-	9,9,9,9	1
3	CA	118-A	203	1/1	-	-	9,9,9,9	1
3	CA	119-A	203	1/1	-	-	10,10,10,10	1
3	CA	120-A	203	1/1	-	-	9,9,9,9	1
3	CA	121-A	203	1/1	-	-	10,10,10,10	1
3	CA	122-A	203	1/1	-	-	9,9,9,9	1
3	CA	123-A	203	1/1	-	-	9,9,9,9	1
3	CA	124-A	203	1/1	-	-	9,9,9,9	1
3	CA	125-A	203	1/1	-	-	10,10,10,10	1
3	CA	126-A	203	1/1	-	-	10,10,10,10	1
3	CA	127-A	203	1/1	-	-	10,10,10,10	1
3	CA	128-A	203	1/1	-	-	10,10,10,10	1
3	CA	129-A	203	1/1	-	-	10,10,10,10	1
3	CA	130-A	203	1/1	-	-	10,10,10,10	1
3	CA	131-A	203	1/1	-	-	10,10,10,10	1
3	CA	132-A	203	1/1	-	-	11,11,11,11	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	133-A	203	1/1	-	-	10,10,10,10	1
3	CA	134-A	203	1/1	-	-	9,9,9,9	1
3	CA	135-A	203	1/1	-	-	9,9,9,9	1
3	CA	136-A	203	1/1	-	-	9,9,9,9	1
3	CA	137-A	203	1/1	-	-	9,9,9,9	1
3	CA	138-A	203	1/1	-	-	9,9,9,9	1
3	CA	139-A	203	1/1	-	-	9,9,9,9	1
3	CA	140-A	203	1/1	-	-	10,10,10,10	1
3	CA	141-A	203	1/1	-	-	10,10,10,10	1
3	CA	142-A	203	1/1	-	-	10,10,10,10	1
3	CA	143-A	203	1/1	-	-	9,9,9,9	1
3	CA	144-A	203	1/1	-	-	10,10,10,10	1
3	CA	145-A	203	1/1	-	-	9,9,9,9	1
3	CA	146-A	203	1/1	-	-	9,9,9,9	1
3	CA	147-A	203	1/1	-	-	9,9,9,9	1
3	CA	148-A	203	1/1	-	-	9,9,9,9	1
3	CA	149-A	203	1/1	-	-	9,9,9,9	1
3	CA	150-A	203	1/1	-	-	9,9,9,9	1
3	CA	151-A	203	1/1	-	-	9,9,9,9	1
3	CA	152-A	203	1/1	-	-	10,10,10,10	1
3	CA	153-A	203	1/1	-	-	10,10,10,10	1
3	CA	154-A	203	1/1	-	-	9,9,9,9	1
3	CA	155-A	203	1/1	-	-	10,10,10,10	1
3	CA	156-A	203	1/1	-	-	10,10,10,10	1
3	CA	157-A	203	1/1	-	-	10,10,10,10	1
3	CA	158-A	203	1/1	-	-	10,10,10,10	1
3	CA	159-A	203	1/1	-	-	10,10,10,10	1
3	CA	160-A	203	1/1	-	-	10,10,10,10	1
3	CA	161-A	203	1/1	-	-	10,10,10,10	1
3	CA	162-A	203	1/1	-	-	10,10,10,10	1
3	CA	163-A	203	1/1	-	-	10,10,10,10	1
3	CA	164-A	203	1/1	-	-	10,10,10,10	1
3	CA	165-A	203	1/1	-	-	10,10,10,10	1
3	CA	166-A	203	1/1	-	-	11,11,11,11	1
3	CA	167-A	203	1/1	-	-	10,10,10,10	1
4	NAP	1-A	204	48/48	0.92	0.09	7,8,9,10	72
4	NAP	2-A	204	48/48	-	-	7,8,9,10	72
4	NAP	3-A	204	48/48	-	-	7,8,9,10	72
4	NAP	4-A	204	48/48	-	-	7,8,9,10	72
4	NAP	5-A	204	48/48	-	-	7,8,9,10	72
4	NAP	6-A	204	48/48	-	-	7,8,9,10	72
4	NAP	7-A	204	48/48	-	-	7,8,9,10	72

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAP	8-A	204	48/48	-	-	7,8,9,10	72
4	NAP	9-A	204	48/48	-	-	7,8,9,10	72
4	NAP	10-A	204	48/48	-	-	7,8,9,10	72
4	NAP	11-A	204	48/48	-	-	7,8,9,10	72
4	NAP	12-A	204	48/48	-	-	7,8,9,10	72
4	NAP	13-A	204	48/48	-	-	7,8,9,10	72
4	NAP	14-A	204	48/48	-	-	7,8,9,10	72
4	NAP	15-A	204	48/48	-	-	7,8,9,10	72
4	NAP	16-A	204	48/48	-	-	7,8,9,10	72
4	NAP	17-A	204	48/48	-	-	7,8,9,10	72
4	NAP	18-A	204	48/48	-	-	7,8,9,10	72
4	NAP	19-A	204	48/48	-	-	7,8,9,10	72
4	NAP	20-A	204	48/48	-	-	7,8,9,10	72
4	NAP	21-A	204	48/48	-	-	7,8,9,10	72
4	NAP	22-A	204	48/48	-	-	7,8,9,10	72
4	NAP	23-A	204	48/48	-	-	7,8,9,10	72
4	NAP	24-A	204	48/48	-	-	7,8,9,10	72
4	NAP	25-A	204	48/48	-	-	7,8,9,10	72
4	NAP	26-A	204	48/48	-	-	7,8,9,10	72
4	NAP	27-A	204	48/48	-	-	7,8,9,10	72
4	NAP	28-A	204	48/48	-	-	7,8,9,10	72
4	NAP	29-A	204	48/48	-	-	7,8,9,10	72
4	NAP	30-A	204	48/48	-	-	7,8,9,10	72
4	NAP	31-A	204	48/48	-	-	7,8,9,10	72
4	NAP	32-A	204	48/48	-	-	7,8,9,10	72
4	NAP	33-A	204	48/48	-	-	7,8,9,10	72
4	NAP	34-A	204	48/48	-	-	7,8,9,10	72
4	NAP	35-A	204	48/48	-	-	7,8,9,10	72
4	NAP	36-A	204	48/48	-	-	7,8,9,10	72
4	NAP	37-A	204	48/48	-	-	7,8,9,10	72
4	NAP	38-A	204	48/48	-	-	7,8,9,10	72
4	NAP	39-A	204	48/48	-	-	7,8,9,10	72
4	NAP	40-A	204	48/48	-	-	7,8,9,10	72
4	NAP	41-A	204	48/48	-	-	7,8,9,10	72
4	NAP	42-A	204	48/48	-	-	7,8,9,10	72
4	NAP	43-A	204	48/48	-	-	7,8,9,10	72
4	NAP	44-A	204	48/48	-	-	7,8,9,10	72
4	NAP	45-A	204	48/48	-	-	7,8,9,10	72
4	NAP	46-A	204	48/48	-	-	7,8,9,10	72
4	NAP	47-A	204	48/48	-	-	7,8,9,10	72
4	NAP	48-A	204	48/48	-	-	7,8,9,10	72
4	NAP	49-A	204	48/48	-	-	7,8,9,10	72

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAP	50-A	204	48/48	-	-	7,8,9,10	72
4	NAP	51-A	204	48/48	-	-	7,8,9,10	72
4	NAP	52-A	204	48/48	-	-	7,8,9,10	72
4	NAP	53-A	204	48/48	-	-	7,8,9,10	72
4	NAP	54-A	204	48/48	-	-	7,8,9,10	72
4	NAP	55-A	204	48/48	-	-	7,8,9,10	72
4	NAP	56-A	204	48/48	-	-	7,8,9,10	72
4	NAP	57-A	204	48/48	-	-	7,8,9,10	72
4	NAP	58-A	204	48/48	-	-	7,8,9,10	72
4	NAP	59-A	204	48/48	-	-	7,8,9,10	72
4	NAP	60-A	204	48/48	-	-	7,8,9,10	72
4	NAP	61-A	204	48/48	-	-	7,8,9,10	72
4	NAP	62-A	204	48/48	-	-	7,8,9,10	72
4	NAP	63-A	204	48/48	-	-	7,8,9,10	72
4	NAP	64-A	204	48/48	-	-	7,8,9,10	72
4	NAP	65-A	204	48/48	-	-	7,8,9,10	72
4	NAP	66-A	204	48/48	-	-	7,8,9,10	72
4	NAP	67-A	204	48/48	-	-	7,8,9,10	72
4	NAP	68-A	204	48/48	-	-	7,8,9,10	72
4	NAP	69-A	204	48/48	-	-	7,8,9,10	72
4	NAP	70-A	204	48/48	-	-	7,8,9,10	72
4	NAP	71-A	204	48/48	-	-	7,8,9,10	72
4	NAP	72-A	204	48/48	-	-	7,8,9,10	72
4	NAP	73-A	204	48/48	-	-	7,8,9,10	72
4	NAP	74-A	204	48/48	-	-	7,8,9,10	72
4	NAP	75-A	204	48/48	-	-	7,8,9,10	72
4	NAP	76-A	204	48/48	-	-	7,8,9,10	72
4	NAP	77-A	204	48/48	-	-	7,8,9,10	72
4	NAP	78-A	204	48/48	-	-	7,8,9,10	72
4	NAP	79-A	204	48/48	-	-	7,8,9,10	72
4	NAP	80-A	204	48/48	-	-	7,8,9,10	72
4	NAP	81-A	204	48/48	-	-	7,8,9,10	72
4	NAP	82-A	204	48/48	-	-	7,8,9,10	72
4	NAP	83-A	204	48/48	-	-	7,8,9,10	72
4	NAP	84-A	204	48/48	-	-	7,8,9,10	72
4	NAP	85-A	204	48/48	-	-	7,8,9,10	72
4	NAP	86-A	204	48/48	-	-	7,8,9,10	72
4	NAP	87-A	204	48/48	-	-	7,8,9,10	72
4	NAP	88-A	204	48/48	-	-	7,8,9,10	72
4	NAP	89-A	204	48/48	-	-	7,8,9,10	72
4	NAP	90-A	204	48/48	-	-	7,8,9,10	72
4	NAP	91-A	204	48/48	-	-	7,8,9,10	72

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAP	92-A	204	48/48	-	-	7,8,9,10	72
4	NAP	93-A	204	48/48	-	-	7,8,9,10	72
4	NAP	94-A	204	48/48	-	-	7,8,9,10	72
4	NAP	95-A	204	48/48	-	-	7,8,9,10	72
4	NAP	96-A	204	48/48	-	-	7,8,9,10	72
4	NAP	97-A	204	48/48	-	-	7,8,9,10	72
4	NAP	98-A	204	48/48	-	-	7,8,9,10	72
4	NAP	99-A	204	48/48	-	-	7,8,9,10	72
4	NAP	100-A	204	48/48	-	-	7,8,9,10	72
4	NAP	101-A	204	48/48	-	-	7,8,9,10	72
4	NAP	102-A	204	48/48	-	-	7,8,9,10	72
4	NAP	103-A	204	48/48	-	-	7,8,9,10	72
4	NAP	104-A	204	48/48	-	-	7,8,9,10	72
4	NAP	105-A	204	48/48	-	-	7,8,9,10	72
4	NAP	106-A	204	48/48	-	-	7,8,9,10	72
4	NAP	107-A	204	48/48	-	-	7,8,9,10	72
4	NAP	108-A	204	48/48	-	-	7,8,9,10	72
4	NAP	109-A	204	48/48	-	-	7,8,9,10	72
4	NAP	110-A	204	48/48	-	-	7,8,9,10	72
4	NAP	111-A	204	48/48	-	-	7,8,9,10	72
4	NAP	112-A	204	48/48	-	-	7,8,9,10	72
4	NAP	113-A	204	48/48	-	-	7,8,9,10	72
4	NAP	114-A	204	48/48	-	-	7,8,9,10	72
4	NAP	115-A	204	48/48	-	-	7,8,9,10	72
4	NAP	116-A	204	48/48	-	-	7,8,9,10	72
4	NAP	117-A	204	48/48	-	-	7,8,9,10	72
4	NAP	118-A	204	48/48	-	-	7,8,9,10	72
4	NAP	119-A	204	48/48	-	-	7,8,9,10	72
4	NAP	120-A	204	48/48	-	-	7,8,9,10	72
4	NAP	121-A	204	48/48	-	-	7,8,9,10	72
4	NAP	122-A	204	48/48	-	-	7,8,9,10	72
4	NAP	123-A	204	48/48	-	-	7,8,9,10	72
4	NAP	124-A	204	48/48	-	-	7,8,9,10	72
4	NAP	125-A	204	48/48	-	-	7,8,9,10	72
4	NAP	126-A	204	48/48	-	-	7,8,9,10	72
4	NAP	127-A	204	48/48	-	-	7,8,9,10	72
4	NAP	128-A	204	48/48	-	-	7,8,9,10	72
4	NAP	129-A	204	48/48	-	-	7,8,9,10	72
4	NAP	130-A	204	48/48	-	-	7,8,9,10	72
4	NAP	131-A	204	48/48	-	-	7,8,9,10	72
4	NAP	132-A	204	48/48	-	-	7,8,9,10	72
4	NAP	133-A	204	48/48	-	-	7,8,9,10	72

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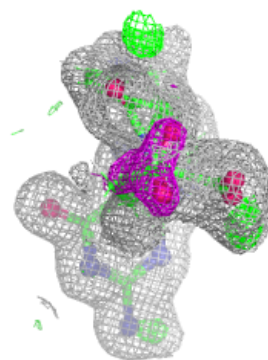
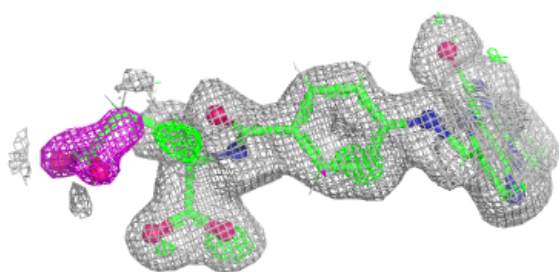
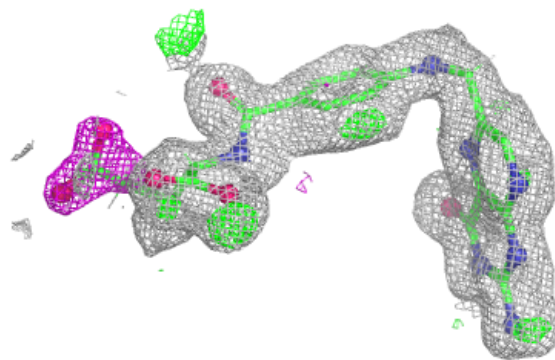
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAP	134-A	204	48/48	-	-	7,8,9,10	72
4	NAP	135-A	204	48/48	-	-	7,8,9,10	72
4	NAP	136-A	204	48/48	-	-	7,8,9,10	72
4	NAP	137-A	204	48/48	-	-	7,8,9,10	72
4	NAP	138-A	204	48/48	-	-	7,8,9,10	72
4	NAP	139-A	204	48/48	-	-	7,8,9,10	72
4	NAP	140-A	204	48/48	-	-	7,8,9,10	72
4	NAP	141-A	204	48/48	-	-	7,8,9,10	72
4	NAP	142-A	204	48/48	-	-	7,8,9,10	72
4	NAP	143-A	204	48/48	-	-	7,8,9,10	72
4	NAP	144-A	204	48/48	-	-	7,8,9,10	72
4	NAP	145-A	204	48/48	-	-	7,8,9,10	72
4	NAP	146-A	204	48/48	-	-	7,8,9,10	72
4	NAP	147-A	204	48/48	-	-	7,8,9,10	72
4	NAP	148-A	204	48/48	-	-	7,8,9,10	72
4	NAP	149-A	204	48/48	-	-	7,8,9,10	72
4	NAP	150-A	204	48/48	-	-	7,8,9,10	72
4	NAP	151-A	204	48/48	-	-	7,8,9,10	72
4	NAP	152-A	204	48/48	-	-	7,8,9,10	72
4	NAP	153-A	204	48/48	-	-	7,8,9,10	72
4	NAP	154-A	204	48/48	-	-	7,8,9,10	72
4	NAP	155-A	204	48/48	-	-	7,8,9,10	72
4	NAP	156-A	204	48/48	-	-	7,8,9,10	72
4	NAP	157-A	204	48/48	-	-	7,8,9,10	72
4	NAP	158-A	204	48/48	-	-	7,8,9,10	72
4	NAP	159-A	204	48/48	-	-	7,8,9,10	72
4	NAP	160-A	204	48/48	-	-	7,8,9,10	72
4	NAP	161-A	204	48/48	-	-	7,8,9,10	72
4	NAP	162-A	204	48/48	-	-	7,8,9,10	72
4	NAP	163-A	204	48/48	-	-	7,8,9,10	72
4	NAP	164-A	204	48/48	-	-	7,8,9,10	72
4	NAP	165-A	204	48/48	-	-	7,8,9,10	72
4	NAP	166-A	204	48/48	-	-	7,8,9,10	72
4	NAP	167-A	204	48/48	-	-	7,8,9,10	72

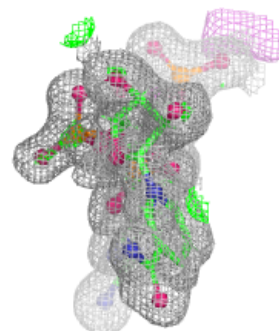
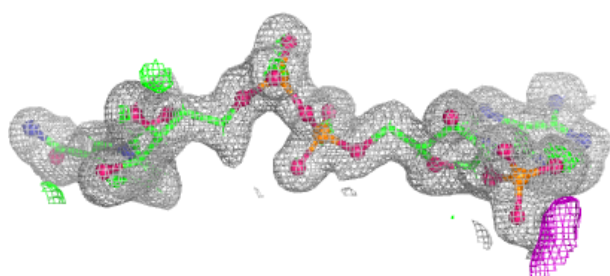
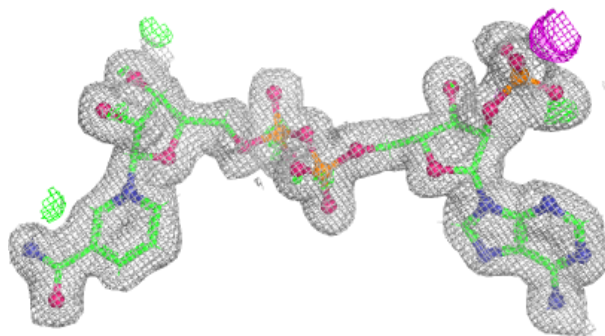
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FOL A 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAP A 204:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



5.5 Other polymers [i](#)

There are no such residues in this entry.