



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 06:20 AM UTC

PDB ID : 4PTJ / pdb_00004ptj
Title : Ensemble model for Escherichia coli dihydrofolate reductase at 277K
Authors : Keedy, D.A.; van den Bedem, H.; Sivak, D.A.; Petsko, G.A.; Ringe, D.; Wilson, M.A.; Fraser, J.S.
Deposited on : 2014-03-10
Resolution : 1.05 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

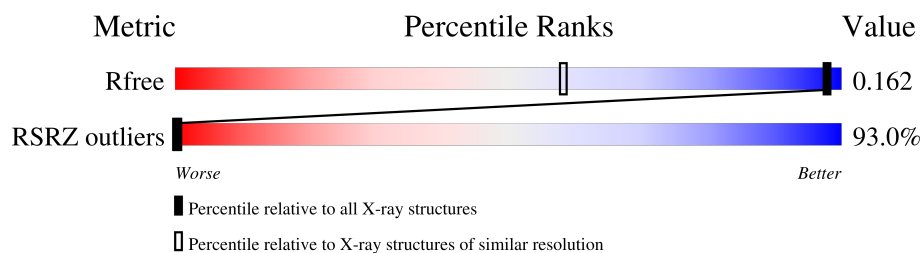
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.05 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	1182 (1.08-1.04)
RSRZ outliers	180081	1181 (1.08-1.04)

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
2	FOL	48-A	201	-	X	-	-

2 Entry composition

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

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

- Molecule 1 is a protein called Dihydrofolate reductase.

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

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

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

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

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

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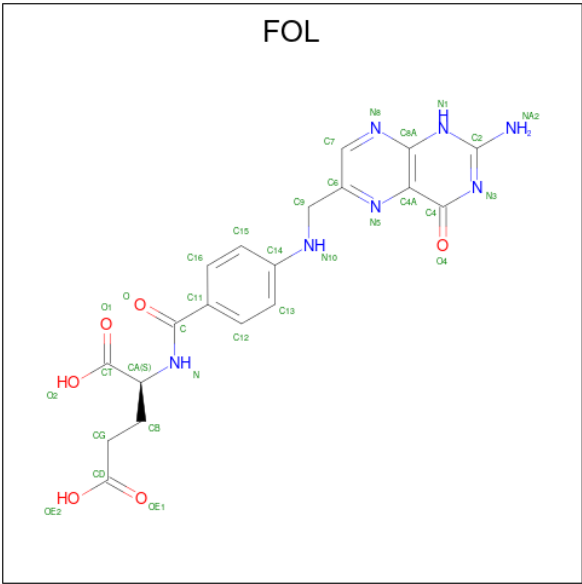
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	101-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	102-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	103-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	104-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241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

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

- Molecule 2 is FOLIC ACID (CCD ID: FOL) (formula: C₁₉H₁₉N₇O₆).



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

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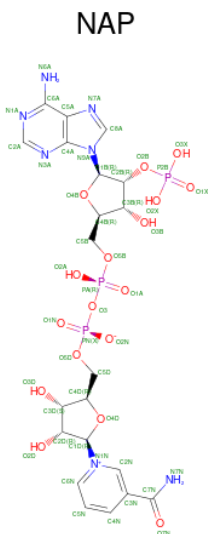
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	92-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	93-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	94-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	95-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	96-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	97-A	1	Total	C	H	N	O	0	0
			49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

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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

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

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

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

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

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

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	2	Total	Mn	0	0
			2	2		
4	2-A	2	Total	Mn	0	0
			2	2		
4	3-A	2	Total	Mn	0	0
			2	2		
4	4-A	2	Total	Mn	0	0
			2	2		
4	5-A	2	Total	Mn	0	0
			2	2		
4	6-A	2	Total	Mn	0	0
			2	2		
4	7-A	2	Total	Mn	0	0
			2	2		
4	8-A	2	Total	Mn	0	0
			2	2		
4	9-A	2	Total	Mn	0	0
			2	2		
4	10-A	2	Total	Mn	0	0
			2	2		
4	11-A	2	Total	Mn	0	0
			2	2		
4	12-A	2	Total	Mn	0	0
			2	2		
4	13-A	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	14-A	2	Total 2	Mn 2	0	0
4	15-A	2	Total 2	Mn 2	0	0
4	16-A	2	Total 2	Mn 2	0	0
4	17-A	2	Total 2	Mn 2	0	0
4	18-A	2	Total 2	Mn 2	0	0
4	19-A	2	Total 2	Mn 2	0	0
4	20-A	2	Total 2	Mn 2	0	0
4	21-A	2	Total 2	Mn 2	0	0
4	22-A	2	Total 2	Mn 2	0	0
4	23-A	2	Total 2	Mn 2	0	0
4	24-A	2	Total 2	Mn 2	0	0
4	25-A	2	Total 2	Mn 2	0	0
4	26-A	2	Total 2	Mn 2	0	0
4	27-A	2	Total 2	Mn 2	0	0
4	28-A	2	Total 2	Mn 2	0	0
4	29-A	2	Total 2	Mn 2	0	0
4	30-A	2	Total 2	Mn 2	0	0
4	31-A	2	Total 2	Mn 2	0	0
4	32-A	2	Total 2	Mn 2	0	0
4	33-A	2	Total 2	Mn 2	0	0
4	34-A	2	Total 2	Mn 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	35-A	2	Total 2	Mn 2	0	0
4	36-A	2	Total 2	Mn 2	0	0
4	37-A	2	Total 2	Mn 2	0	0
4	38-A	2	Total 2	Mn 2	0	0
4	39-A	2	Total 2	Mn 2	0	0
4	40-A	2	Total 2	Mn 2	0	0
4	41-A	2	Total 2	Mn 2	0	0
4	42-A	2	Total 2	Mn 2	0	0
4	43-A	2	Total 2	Mn 2	0	0
4	44-A	2	Total 2	Mn 2	0	0
4	45-A	2	Total 2	Mn 2	0	0
4	46-A	2	Total 2	Mn 2	0	0
4	47-A	2	Total 2	Mn 2	0	0
4	48-A	2	Total 2	Mn 2	0	0
4	49-A	2	Total 2	Mn 2	0	0
4	50-A	2	Total 2	Mn 2	0	0
4	51-A	2	Total 2	Mn 2	0	0
4	52-A	2	Total 2	Mn 2	0	0
4	53-A	2	Total 2	Mn 2	0	0
4	54-A	2	Total 2	Mn 2	0	0
4	55-A	2	Total 2	Mn 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	56-A	2	Total 2	Mn 2	0	0
4	57-A	2	Total 2	Mn 2	0	0
4	58-A	2	Total 2	Mn 2	0	0
4	59-A	2	Total 2	Mn 2	0	0
4	60-A	2	Total 2	Mn 2	0	0
4	61-A	2	Total 2	Mn 2	0	0
4	62-A	2	Total 2	Mn 2	0	0
4	63-A	2	Total 2	Mn 2	0	0
4	64-A	2	Total 2	Mn 2	0	0
4	65-A	2	Total 2	Mn 2	0	0
4	66-A	2	Total 2	Mn 2	0	0
4	67-A	2	Total 2	Mn 2	0	0
4	68-A	2	Total 2	Mn 2	0	0
4	69-A	2	Total 2	Mn 2	0	0
4	70-A	2	Total 2	Mn 2	0	0
4	71-A	2	Total 2	Mn 2	0	0
4	72-A	2	Total 2	Mn 2	0	0
4	73-A	2	Total 2	Mn 2	0	0
4	74-A	2	Total 2	Mn 2	0	0
4	75-A	2	Total 2	Mn 2	0	0
4	76-A	2	Total 2	Mn 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	77-A	2	Total 2	Mn 2	0	0
4	78-A	2	Total 2	Mn 2	0	0
4	79-A	2	Total 2	Mn 2	0	0
4	80-A	2	Total 2	Mn 2	0	0
4	81-A	2	Total 2	Mn 2	0	0
4	82-A	2	Total 2	Mn 2	0	0
4	83-A	2	Total 2	Mn 2	0	0
4	84-A	2	Total 2	Mn 2	0	0
4	85-A	2	Total 2	Mn 2	0	0
4	86-A	2	Total 2	Mn 2	0	0
4	87-A	2	Total 2	Mn 2	0	0
4	88-A	2	Total 2	Mn 2	0	0
4	89-A	2	Total 2	Mn 2	0	0
4	90-A	2	Total 2	Mn 2	0	0
4	91-A	2	Total 2	Mn 2	0	0
4	92-A	2	Total 2	Mn 2	0	0
4	93-A	2	Total 2	Mn 2	0	0
4	94-A	2	Total 2	Mn 2	0	0
4	95-A	2	Total 2	Mn 2	0	0
4	96-A	2	Total 2	Mn 2	0	0
4	97-A	2	Total 2	Mn 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	98-A	2	Total 2	Mn 2	0	0
4	99-A	2	Total 2	Mn 2	0	0
4	100-A	2	Total 2	Mn 2	0	0
4	101-A	2	Total 2	Mn 2	0	0
4	102-A	2	Total 2	Mn 2	0	0
4	103-A	2	Total 2	Mn 2	0	0
4	104-A	2	Total 2	Mn 2	0	0
4	105-A	2	Total 2	Mn 2	0	0
4	106-A	2	Total 2	Mn 2	0	0
4	107-A	2	Total 2	Mn 2	0	0
4	108-A	2	Total 2	Mn 2	0	0
4	109-A	2	Total 2	Mn 2	0	0
4	110-A	2	Total 2	Mn 2	0	0
4	111-A	2	Total 2	Mn 2	0	0
4	112-A	2	Total 2	Mn 2	0	0
4	113-A	2	Total 2	Mn 2	0	0
4	114-A	2	Total 2	Mn 2	0	0
4	115-A	2	Total 2	Mn 2	0	0
4	116-A	2	Total 2	Mn 2	0	0
4	117-A	2	Total 2	Mn 2	0	0
4	118-A	2	Total 2	Mn 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	119-A	2	Total 2	Mn 2	0	0
4	120-A	2	Total 2	Mn 2	0	0
4	121-A	2	Total 2	Mn 2	0	0
4	122-A	2	Total 2	Mn 2	0	0
4	123-A	2	Total 2	Mn 2	0	0
4	124-A	2	Total 2	Mn 2	0	0
4	125-A	2	Total 2	Mn 2	0	0

- Molecule 5 is water.

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

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

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

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

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

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

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

MolProbity 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	34.30Å 45.52Å 98.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 1.05 49.35 – 1.05	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.40-1.05) 96.1 (49.35-1.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 1.05Å)	Xtriage
Refinement program	PHENIX 1.8.4-1496	Depositor
R, R_{free}	0.136 , 0.166 0.143 , 0.162	Depositor DCC
R_{free} test set	3666 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	10.4	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.00 , 23.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	339833	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.36% 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](#)

125 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	CSD	99-A	152	1	4,7,8	3.67	1 (25%)	1,8,10	8.24	1 (100%)
1	CSD	124-A	152	1	4,7,8	2.44	1 (25%)	1,8,10	2.73	1 (100%)
1	CSD	114-A	152	1	4,7,8	1.95	1 (25%)	1,8,10	1.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	38-A	152	1	4,7,8	2.87	1 (25%)	1,8,10	4.47	1 (100%)
1	CSD	67-A	152	1	4,7,8	2.97	1 (25%)	1,8,10	1.33	0
1	CSD	87-A	152	1	4,7,8	4.20	1 (25%)	1,8,10	0.65	0
1	CSD	106-A	152	1	4,7,8	3.86	1 (25%)	1,8,10	0.98	0
1	CSD	20-A	152	1	4,7,8	1.78	1 (25%)	1,8,10	5.85	1 (100%)
1	CSD	94-A	152	1	4,7,8	4.90	1 (25%)	1,8,10	5.35	1 (100%)
1	CSD	113-A	152	1	4,7,8	9.57	3 (75%)	1,8,10	1.81	0
1	CSD	45-A	152	1	4,7,8	6.07	1 (25%)	1,8,10	3.86	1 (100%)
1	CSD	57-A	152	1	4,7,8	4.27	1 (25%)	1,8,10	6.75	1 (100%)
1	CSD	100-A	152	1	4,7,8	8.02	1 (25%)	1,8,10	0.75	0
1	CSD	74-A	152	1	4,7,8	4.17	1 (25%)	1,8,10	3.69	1 (100%)
1	CSD	33-A	152	1	4,7,8	2.90	1 (25%)	1,8,10	4.24	1 (100%)
1	CSD	79-A	152	1	4,7,8	3.01	1 (25%)	1,8,10	1.16	0
1	CSD	78-A	152	1	4,7,8	6.41	1 (25%)	1,8,10	1.39	0
1	CSD	21-A	152	1	4,7,8	2.03	1 (25%)	1,8,10	2.98	1 (100%)
1	CSD	51-A	152	1	4,7,8	5.28	1 (25%)	1,8,10	5.40	1 (100%)
1	CSD	25-A	152	1	4,7,8	1.38	0	1,8,10	6.36	1 (100%)
1	CSD	66-A	152	1	4,7,8	3.03	1 (25%)	1,8,10	2.16	1 (100%)
1	CSD	55-A	152	1	4,7,8	6.23	1 (25%)	1,8,10	9.29	1 (100%)
1	CSD	58-A	152	1	4,7,8	3.83	1 (25%)	1,8,10	0.99	0
1	CSD	85-A	152	1	4,7,8	5.56	1 (25%)	1,8,10	2.16	1 (100%)
1	CSD	68-A	152	1	4,7,8	1.95	1 (25%)	1,8,10	4.05	1 (100%)
1	CSD	39-A	152	1	4,7,8	2.81	1 (25%)	1,8,10	4.78	1 (100%)
1	CSD	92-A	152	1	4,7,8	5.47	1 (25%)	1,8,10	7.31	1 (100%)
1	CSD	110-A	152	1	4,7,8	1.54	1 (25%)	1,8,10	3.28	1 (100%)
1	CSD	47-A	152	1	4,7,8	4.46	1 (25%)	1,8,10	3.25	1 (100%)
1	CSD	5-A	152	1	4,7,8	3.50	1 (25%)	1,8,10	1.51	0
1	CSD	26-A	152	1	4,7,8	8.12	1 (25%)	1,8,10	3.88	1 (100%)
1	CSD	31-A	152	1	4,7,8	3.07	1 (25%)	1,8,10	4.39	1 (100%)
1	CSD	46-A	152	1	4,7,8	2.06	1 (25%)	1,8,10	4.93	1 (100%)
1	CSD	104-A	152	1	4,7,8	4.00	1 (25%)	1,8,10	2.85	1 (100%)
1	CSD	16-A	152	1	4,7,8	11.69	2 (50%)	1,8,10	1.97	0
1	CSD	44-A	152	1	4,7,8	5.88	3 (75%)	1,8,10	2.35	1 (100%)
1	CSD	107-A	152	1	4,7,8	2.31	2 (50%)	1,8,10	12.84	1 (100%)
1	CSD	48-A	152	1	4,7,8	2.47	1 (25%)	1,8,10	2.78	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	84-A	152	1	4,7,8	7.36	1 (25%)	1,8,10	5.89	1 (100%)
1	CSD	111-A	152	1	4,7,8	6.39	1 (25%)	1,8,10	1.17	0
1	CSD	71-A	152	1	4,7,8	3.42	1 (25%)	1,8,10	10.27	1 (100%)
1	CSD	42-A	152	1	4,7,8	5.14	1 (25%)	1,8,10	2.63	1 (100%)
1	CSD	120-A	152	1	4,7,8	6.78	1 (25%)	1,8,10	0.43	0
1	CSD	77-A	152	1	4,7,8	2.02	1 (25%)	1,8,10	6.36	1 (100%)
1	CSD	36-A	152	1	4,7,8	6.91	1 (25%)	1,8,10	0.81	0
1	CSD	63-A	152	1	4,7,8	3.33	1 (25%)	1,8,10	15.14	1 (100%)
1	CSD	80-A	152	1	4,7,8	3.73	2 (50%)	1,8,10	0.83	0
1	CSD	83-A	152	1	4,7,8	4.46	1 (25%)	1,8,10	3.66	1 (100%)
1	CSD	41-A	152	1	4,7,8	2.46	1 (25%)	1,8,10	1.32	0
1	CSD	109-A	152	1	4,7,8	1.99	1 (25%)	1,8,10	1.97	0
1	CSD	115-A	152	1	4,7,8	5.32	1 (25%)	1,8,10	2.71	1 (100%)
1	CSD	18-A	152	1	4,7,8	7.38	1 (25%)	1,8,10	3.74	1 (100%)
1	CSD	19-A	152	1	4,7,8	8.49	2 (50%)	1,8,10	4.32	1 (100%)
1	CSD	103-A	152	1	4,7,8	1.89	1 (25%)	1,8,10	1.19	0
1	CSD	108-A	152	1	4,7,8	4.46	1 (25%)	1,8,10	1.76	0
1	CSD	69-A	152	1	4,7,8	2.25	1 (25%)	1,8,10	5.14	1 (100%)
1	CSD	61-A	152	1	4,7,8	6.19	1 (25%)	1,8,10	6.60	1 (100%)
1	CSD	32-A	152	1	4,7,8	5.65	1 (25%)	1,8,10	5.71	1 (100%)
1	CSD	12-A	152	1	4,7,8	3.19	1 (25%)	1,8,10	2.33	1 (100%)
1	CSD	3-A	152	1	4,7,8	6.30	2 (50%)	1,8,10	7.88	1 (100%)
1	CSD	56-A	152	1	4,7,8	4.01	1 (25%)	1,8,10	17.49	1 (100%)
1	CSD	2-A	152	1	4,7,8	3.60	2 (50%)	1,8,10	6.39	1 (100%)
1	CSD	15-A	152	1	4,7,8	5.24	1 (25%)	1,8,10	1.33	0
1	CSD	11-A	152	1	4,7,8	1.21	0	1,8,10	3.94	1 (100%)
1	CSD	112-A	152	1	4,7,8	6.90	2 (50%)	1,8,10	0.72	0
1	CSD	34-A	152	1	4,7,8	3.27	1 (25%)	1,8,10	7.36	1 (100%)
1	CSD	70-A	152	1	4,7,8	4.03	1 (25%)	1,8,10	0.12	0
1	CSD	91-A	152	1	4,7,8	2.43	1 (25%)	1,8,10	3.93	1 (100%)
1	CSD	65-A	152	1	4,7,8	3.91	1 (25%)	1,8,10	1.65	0
1	CSD	81-A	152	1	4,7,8	6.56	2 (50%)	1,8,10	4.48	1 (100%)
1	CSD	7-A	152	1	4,7,8	4.37	2 (50%)	1,8,10	10.79	1 (100%)
1	CSD	125-A	152	1	4,7,8	9.05	1 (25%)	1,8,10	8.37	1 (100%)
1	CSD	121-A	152	1	4,7,8	3.47	1 (25%)	1,8,10	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	89-A	152	1	4,7,8	2.66	1 (25%)	1,8,10	6.81	1 (100%)
1	CSD	101-A	152	1	4,7,8	3.23	1 (25%)	1,8,10	3.55	1 (100%)
1	CSD	52-A	152	1	4,7,8	3.64	1 (25%)	1,8,10	0.47	0
1	CSD	29-A	152	1	4,7,8	1.87	1 (25%)	1,8,10	4.22	1 (100%)
1	CSD	90-A	152	1	4,7,8	1.41	0	1,8,10	0.15	0
1	CSD	102-A	152	1	4,7,8	4.46	2 (50%)	1,8,10	6.32	1 (100%)
1	CSD	49-A	152	1	4,7,8	1.67	1 (25%)	1,8,10	5.76	1 (100%)
1	CSD	96-A	152	1	4,7,8	4.01	1 (25%)	1,8,10	4.97	1 (100%)
1	CSD	23-A	152	1	4,7,8	2.47	1 (25%)	1,8,10	6.69	1 (100%)
1	CSD	60-A	152	1	4,7,8	7.51	1 (25%)	1,8,10	4.64	1 (100%)
1	CSD	62-A	152	1	4,7,8	4.12	1 (25%)	1,8,10	3.49	1 (100%)
1	CSD	59-A	152	1	4,7,8	3.59	1 (25%)	1,8,10	3.32	1 (100%)
1	CSD	119-A	152	1	4,7,8	2.19	1 (25%)	1,8,10	12.80	1 (100%)
1	CSD	9-A	152	1	4,7,8	5.44	1 (25%)	1,8,10	0.65	0
1	CSD	116-A	152	1	4,7,8	9.19	2 (50%)	1,8,10	2.60	1 (100%)
1	CSD	40-A	152	1	4,7,8	1.22	0	1,8,10	0.19	0
1	CSD	122-A	152	1	4,7,8	2.44	1 (25%)	1,8,10	8.17	1 (100%)
1	CSD	73-A	152	1	4,7,8	3.32	1 (25%)	1,8,10	10.60	1 (100%)
1	CSD	93-A	152	1	4,7,8	4.27	1 (25%)	1,8,10	10.74	1 (100%)
1	CSD	22-A	152	1	4,7,8	7.96	1 (25%)	1,8,10	5.34	1 (100%)
1	CSD	105-A	152	1	4,7,8	2.93	1 (25%)	1,8,10	4.18	1 (100%)
1	CSD	10-A	152	1	4,7,8	4.04	1 (25%)	1,8,10	1.75	0
1	CSD	4-A	152	1	4,7,8	4.40	2 (50%)	1,8,10	9.54	1 (100%)
1	CSD	95-A	152	1	4,7,8	3.88	1 (25%)	1,8,10	6.32	1 (100%)
1	CSD	6-A	152	1	4,7,8	4.46	1 (25%)	1,8,10	10.64	1 (100%)
1	CSD	50-A	152	1	4,7,8	5.92	1 (25%)	1,8,10	1.30	0
1	CSD	72-A	152	1	4,7,8	5.81	1 (25%)	1,8,10	3.77	1 (100%)
1	CSD	118-A	152	1	4,7,8	2.30	1 (25%)	1,8,10	1.44	0
1	CSD	86-A	152	1	4,7,8	2.42	1 (25%)	1,8,10	0.96	0
1	CSD	75-A	152	1	4,7,8	3.58	1 (25%)	1,8,10	4.03	1 (100%)
1	CSD	35-A	152	1	4,7,8	5.46	1 (25%)	1,8,10	2.60	1 (100%)
1	CSD	27-A	152	1	4,7,8	3.33	1 (25%)	1,8,10	3.92	1 (100%)
1	CSD	54-A	152	1	4,7,8	4.40	1 (25%)	1,8,10	0.44	0
1	CSD	1-A	152	1	4,7,8	4.42	1 (25%)	1,8,10	5.01	1 (100%)
1	CSD	28-A	152	1	4,7,8	6.51	1 (25%)	1,8,10	10.78	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	97-A	152	1	4,7,8	5.39	1 (25%)	1,8,10	4.25	1 (100%)
1	CSD	123-A	152	1	4,7,8	1.99	1 (25%)	1,8,10	3.39	1 (100%)
1	CSD	88-A	152	1	4,7,8	5.45	1 (25%)	1,8,10	9.32	1 (100%)
1	CSD	14-A	152	1	4,7,8	1.83	1 (25%)	1,8,10	4.46	1 (100%)
1	CSD	37-A	152	1	4,7,8	4.37	1 (25%)	1,8,10	7.93	1 (100%)
1	CSD	53-A	152	1	4,7,8	3.64	1 (25%)	1,8,10	2.74	1 (100%)
1	CSD	30-A	152	1	4,7,8	1.57	1 (25%)	1,8,10	2.72	1 (100%)
1	CSD	24-A	152	1	4,7,8	2.09	1 (25%)	1,8,10	3.91	1 (100%)
1	CSD	117-A	152	1	4,7,8	4.55	1 (25%)	1,8,10	2.33	1 (100%)
1	CSD	17-A	152	1	4,7,8	3.33	1 (25%)	1,8,10	3.54	1 (100%)
1	CSD	76-A	152	1	4,7,8	1.56	1 (25%)	1,8,10	0.44	0
1	CSD	43-A	152	1	4,7,8	2.17	1 (25%)	1,8,10	1.81	0
1	CSD	13-A	152	1	4,7,8	1.14	0	1,8,10	2.51	1 (100%)
1	CSD	98-A	152	1	4,7,8	5.13	1 (25%)	1,8,10	5.89	1 (100%)
1	CSD	82-A	152	1	4,7,8	4.20	1 (25%)	1,8,10	0.45	0
1	CSD	64-A	152	1	4,7,8	4.04	1 (25%)	1,8,10	0.10	0
1	CSD	8-A	152	1	4,7,8	5.38	1 (25%)	1,8,10	2.97	1 (100%)

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
1	CSD	99-A	152	1	-	1/2/6/8	-
1	CSD	124-A	152	1	-	2/2/6/8	-
1	CSD	114-A	152	1	-	2/2/6/8	-
1	CSD	38-A	152	1	-	1/2/6/8	-
1	CSD	67-A	152	1	-	1/2/6/8	-
1	CSD	87-A	152	1	-	2/2/6/8	-
1	CSD	106-A	152	1	-	1/2/6/8	-
1	CSD	20-A	152	1	-	2/2/6/8	-
1	CSD	94-A	152	1	-	1/2/6/8	-
1	CSD	113-A	152	1	-	2/2/6/8	-
1	CSD	45-A	152	1	-	0/2/6/8	-
1	CSD	57-A	152	1	-	2/2/6/8	-
1	CSD	100-A	152	1	-	1/2/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	74-A	152	1	-	2/2/6/8	-
1	CSD	33-A	152	1	-	2/2/6/8	-
1	CSD	79-A	152	1	-	1/2/6/8	-
1	CSD	78-A	152	1	-	0/2/6/8	-
1	CSD	21-A	152	1	-	1/2/6/8	-
1	CSD	51-A	152	1	-	1/2/6/8	-
1	CSD	25-A	152	1	-	2/2/6/8	-
1	CSD	66-A	152	1	-	1/2/6/8	-
1	CSD	55-A	152	1	-	0/2/6/8	-
1	CSD	58-A	152	1	-	0/2/6/8	-
1	CSD	85-A	152	1	-	0/2/6/8	-
1	CSD	68-A	152	1	-	2/2/6/8	-
1	CSD	39-A	152	1	-	1/2/6/8	-
1	CSD	92-A	152	1	-	0/2/6/8	-
1	CSD	110-A	152	1	-	2/2/6/8	-
1	CSD	47-A	152	1	-	1/2/6/8	-
1	CSD	5-A	152	1	-	1/2/6/8	-
1	CSD	26-A	152	1	-	0/2/6/8	-
1	CSD	31-A	152	1	-	2/2/6/8	-
1	CSD	46-A	152	1	-	1/2/6/8	-
1	CSD	104-A	152	1	-	1/2/6/8	-
1	CSD	16-A	152	1	-	0/2/6/8	-
1	CSD	44-A	152	1	-	2/2/6/8	-
1	CSD	107-A	152	1	-	1/2/6/8	-
1	CSD	48-A	152	1	-	2/2/6/8	-
1	CSD	84-A	152	1	-	0/2/6/8	-
1	CSD	111-A	152	1	-	0/2/6/8	-
1	CSD	71-A	152	1	-	1/2/6/8	-
1	CSD	42-A	152	1	-	1/2/6/8	-
1	CSD	120-A	152	1	-	1/2/6/8	-
1	CSD	77-A	152	1	-	2/2/6/8	-
1	CSD	36-A	152	1	-	0/2/6/8	-
1	CSD	63-A	152	1	-	0/2/6/8	-
1	CSD	80-A	152	1	-	2/2/6/8	-
1	CSD	83-A	152	1	-	1/2/6/8	-
1	CSD	41-A	152	1	-	2/2/6/8	-
1	CSD	109-A	152	1	-	1/2/6/8	-
1	CSD	115-A	152	1	-	1/2/6/8	-
1	CSD	18-A	152	1	-	2/2/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	19-A	152	1	-	1/2/6/8	-
1	CSD	103-A	152	1	-	1/2/6/8	-
1	CSD	108-A	152	1	-	1/2/6/8	-
1	CSD	69-A	152	1	-	2/2/6/8	-
1	CSD	61-A	152	1	-	0/2/6/8	-
1	CSD	32-A	152	1	-	1/2/6/8	-
1	CSD	12-A	152	1	-	1/2/6/8	-
1	CSD	3-A	152	1	-	0/2/6/8	-
1	CSD	56-A	152	1	-	0/2/6/8	-
1	CSD	2-A	152	1	-	1/2/6/8	-
1	CSD	15-A	152	1	-	1/2/6/8	-
1	CSD	11-A	152	1	-	2/2/6/8	-
1	CSD	112-A	152	1	-	1/2/6/8	-
1	CSD	34-A	152	1	-	2/2/6/8	-
1	CSD	70-A	152	1	-	1/2/6/8	-
1	CSD	91-A	152	1	-	1/2/6/8	-
1	CSD	65-A	152	1	-	1/2/6/8	-
1	CSD	81-A	152	1	-	0/2/6/8	-
1	CSD	7-A	152	1	-	0/2/6/8	-
1	CSD	125-A	152	1	-	2/2/6/8	-
1	CSD	121-A	152	1	-	1/2/6/8	-
1	CSD	89-A	152	1	-	1/2/6/8	-
1	CSD	101-A	152	1	-	2/2/6/8	-
1	CSD	52-A	152	1	-	2/2/6/8	-
1	CSD	29-A	152	1	-	2/2/6/8	-
1	CSD	90-A	152	1	-	1/2/6/8	-
1	CSD	102-A	152	1	-	2/2/6/8	-
1	CSD	49-A	152	1	-	1/2/6/8	-
1	CSD	96-A	152	1	-	2/2/6/8	-
1	CSD	23-A	152	1	-	1/2/6/8	-
1	CSD	60-A	152	1	-	1/2/6/8	-
1	CSD	62-A	152	1	-	2/2/6/8	-
1	CSD	59-A	152	1	-	1/2/6/8	-
1	CSD	119-A	152	1	-	1/2/6/8	-
1	CSD	9-A	152	1	-	0/2/6/8	-
1	CSD	116-A	152	1	-	1/2/6/8	-
1	CSD	40-A	152	1	-	2/2/6/8	-
1	CSD	122-A	152	1	-	1/2/6/8	-
1	CSD	73-A	152	1	-	1/2/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	93-A	152	1	-	2/2/6/8	-
1	CSD	22-A	152	1	-	1/2/6/8	-
1	CSD	105-A	152	1	-	1/2/6/8	-
1	CSD	10-A	152	1	-	2/2/6/8	-
1	CSD	4-A	152	1	-	1/2/6/8	-
1	CSD	95-A	152	1	-	2/2/6/8	-
1	CSD	6-A	152	1	-	1/2/6/8	-
1	CSD	50-A	152	1	-	1/2/6/8	-
1	CSD	72-A	152	1	-	0/2/6/8	-
1	CSD	118-A	152	1	-	1/2/6/8	-
1	CSD	86-A	152	1	-	1/2/6/8	-
1	CSD	75-A	152	1	-	2/2/6/8	-
1	CSD	35-A	152	1	-	1/2/6/8	-
1	CSD	27-A	152	1	-	1/2/6/8	-
1	CSD	54-A	152	1	-	1/2/6/8	-
1	CSD	1-A	152	1	-	2/2/6/8	-
1	CSD	28-A	152	1	-	1/2/6/8	-
1	CSD	97-A	152	1	-	2/2/6/8	-
1	CSD	123-A	152	1	-	2/2/6/8	-
1	CSD	88-A	152	1	-	1/2/6/8	-
1	CSD	14-A	152	1	-	2/2/6/8	-
1	CSD	37-A	152	1	-	1/2/6/8	-
1	CSD	53-A	152	1	-	1/2/6/8	-
1	CSD	30-A	152	1	-	1/2/6/8	-
1	CSD	24-A	152	1	-	2/2/6/8	-
1	CSD	117-A	152	1	-	1/2/6/8	-
1	CSD	17-A	152	1	-	0/2/6/8	-
1	CSD	76-A	152	1	-	2/2/6/8	-
1	CSD	43-A	152	1	-	1/2/6/8	-
1	CSD	13-A	152	1	-	1/2/6/8	-
1	CSD	98-A	152	1	-	0/2/6/8	-
1	CSD	82-A	152	1	-	1/2/6/8	-
1	CSD	64-A	152	1	-	0/2/6/8	-
1	CSD	8-A	152	1	-	0/2/6/8	-

The worst 5 of 136 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16-A	152	CSD	OD1-SG	-23.23	1.26	1.47
1	113-A	152	CSD	OD1-SG	-18.55	1.30	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	116-A	152	CSD	OD1-SG	-18.17	1.31	1.47
1	125-A	152	CSD	OD1-SG	-17.93	1.31	1.47
1	19-A	152	CSD	OD1-SG	-16.68	1.32	1.47

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	56-A	152	CSD	OD1-SG-CB	17.49	137.82	105.60
1	63-A	152	CSD	OD1-SG-CB	15.14	133.49	105.60
1	107-A	152	CSD	OD1-SG-CB	-12.84	81.95	105.60
1	119-A	152	CSD	OD1-SG-CB	12.80	129.18	105.60
1	7-A	152	CSD	OD1-SG-CB	10.79	125.48	105.60

There are no chirality outliers.

5 of 141 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1-A	152	CSD	N-CA-CB-SG
1	1-A	152	CSD	CA-CB-SG-OD1
1	2-A	152	CSD	CA-CB-SG-OD1
1	4-A	152	CSD	CA-CB-SG-OD1
1	5-A	152	CSD	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 500 ligands modelled in this entry, 250 are monoatomic - leaving 250 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	115-A	201	-	34,34,34	1.22	4 (11%)	43,47,47	2.58	14 (32%)
3	NAP	92-A	202	-	50,52,52	2.24	10 (20%)	71,80,80	1.36	10 (14%)
3	NAP	47-A	202	-	50,52,52	2.18	9 (18%)	71,80,80	1.31	8 (11%)
2	FOL	35-A	201	-	34,34,34	1.54	6 (17%)	43,47,47	2.05	15 (34%)
2	FOL	76-A	201	-	34,34,34	1.33	5 (14%)	43,47,47	1.94	16 (37%)
2	FOL	104-A	201	-	34,34,34	1.51	4 (11%)	43,47,47	2.20	18 (41%)
3	NAP	57-A	202	-	50,52,52	2.16	9 (18%)	71,80,80	1.34	10 (14%)
3	NAP	28-A	202	-	50,52,52	2.28	9 (18%)	71,80,80	1.28	6 (8%)
2	FOL	74-A	201	-	34,34,34	1.40	3 (8%)	43,47,47	1.86	11 (25%)
2	FOL	60-A	201	-	34,34,34	2.00	8 (23%)	43,47,47	3.25	17 (39%)
3	NAP	18-A	202	-	50,52,52	2.20	11 (22%)	71,80,80	1.42	10 (14%)
2	FOL	113-A	201	-	34,34,34	1.25	3 (8%)	43,47,47	2.11	6 (13%)
2	FOL	49-A	201	-	34,34,34	2.06	11 (32%)	43,47,47	2.66	20 (46%)
3	NAP	53-A	202	-	50,52,52	2.20	8 (16%)	71,80,80	1.29	10 (14%)
2	FOL	96-A	201	-	34,34,34	1.34	5 (14%)	43,47,47	1.94	8 (18%)
3	NAP	64-A	202	-	50,52,52	2.17	9 (18%)	71,80,80	1.34	9 (12%)
3	NAP	108-A	202	-	50,52,52	2.26	10 (20%)	71,80,80	1.26	7 (9%)
2	FOL	57-A	201	-	34,34,34	1.30	3 (8%)	43,47,47	1.56	9 (20%)
2	FOL	124-A	201	-	34,34,34	1.31	3 (8%)	43,47,47	1.67	10 (23%)
3	NAP	34-A	202	-	50,52,52	2.20	10 (20%)	71,80,80	1.30	8 (11%)
2	FOL	28-A	201	-	34,34,34	1.43	4 (11%)	43,47,47	2.07	14 (32%)
2	FOL	42-A	201	-	34,34,34	1.20	4 (11%)	43,47,47	2.19	11 (25%)
3	NAP	61-A	202	-	50,52,52	2.21	9 (18%)	71,80,80	1.24	6 (8%)
3	NAP	113-A	202	-	50,52,52	2.21	10 (20%)	71,80,80	1.32	6 (8%)
3	NAP	11-A	202	-	50,52,52	2.19	9 (18%)	71,80,80	1.31	8 (11%)
3	NAP	40-A	202	-	50,52,52	2.18	9 (18%)	71,80,80	1.31	8 (11%)
2	FOL	89-A	201	-	34,34,34	1.56	4 (11%)	43,47,47	1.81	9 (20%)
3	NAP	22-A	202	-	50,52,52	2.20	9 (18%)	71,80,80	1.24	6 (8%)
3	NAP	65-A	202	-	50,52,52	2.21	10 (20%)	71,80,80	1.33	9 (12%)
3	NAP	78-A	202	-	50,52,52	2.17	9 (18%)	71,80,80	1.26	7 (9%)
2	FOL	21-A	201	-	34,34,34	1.26	0	43,47,47	2.60	15 (34%)
2	FOL	45-A	201	-	34,34,34	1.78	6 (17%)	43,47,47	2.93	18 (41%)
2	FOL	61-A	201	-	34,34,34	2.30	8 (23%)	43,47,47	4.51	21 (48%)
2	FOL	80-A	201	-	34,34,34	1.72	6 (17%)	43,47,47	2.06	16 (37%)
2	FOL	86-A	201	-	34,34,34	1.59	6 (17%)	43,47,47	2.76	15 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	94-A	201	-	34,34,34	1.49	3 (8%)	43,47,47	1.64	11 (25%)
3	NAP	114-A	202	-	50,52,52	2.22	9 (18%)	71,80,80	1.33	7 (9%)
2	FOL	114-A	201	-	34,34,34	1.46	3 (8%)	43,47,47	1.75	12 (27%)
2	FOL	117-A	201	-	34,34,34	1.46	4 (11%)	43,47,47	1.64	8 (18%)
3	NAP	55-A	202	-	50,52,52	2.21	9 (18%)	71,80,80	1.30	8 (11%)
2	FOL	112-A	201	-	34,34,34	1.33	3 (8%)	43,47,47	1.46	9 (20%)
3	NAP	116-A	202	-	50,52,52	2.24	11 (22%)	71,80,80	1.44	10 (14%)
2	FOL	43-A	201	-	34,34,34	1.91	7 (20%)	43,47,47	2.98	19 (44%)
2	FOL	103-A	201	-	34,34,34	1.40	4 (11%)	43,47,47	1.34	6 (13%)
3	NAP	38-A	202	-	50,52,52	2.18	10 (20%)	71,80,80	1.46	13 (18%)
2	FOL	18-A	201	-	34,34,34	1.39	6 (17%)	43,47,47	1.84	11 (25%)
3	NAP	4-A	202	-	50,52,52	2.23	9 (18%)	71,80,80	1.29	9 (12%)
2	FOL	98-A	201	-	34,34,34	1.17	2 (5%)	43,47,47	2.06	12 (27%)
3	NAP	69-A	202	-	50,52,52	2.17	8 (16%)	71,80,80	1.33	9 (12%)
2	FOL	77-A	201	-	34,34,34	1.50	3 (8%)	43,47,47	1.70	12 (27%)
3	NAP	29-A	202	-	50,52,52	2.19	9 (18%)	71,80,80	1.24	7 (9%)
3	NAP	24-A	202	-	50,52,52	2.19	9 (18%)	71,80,80	1.23	6 (8%)
2	FOL	78-A	201	-	34,34,34	1.15	1 (2%)	43,47,47	1.69	11 (25%)
3	NAP	67-A	202	-	50,52,52	2.19	9 (18%)	71,80,80	1.26	8 (11%)
3	NAP	106-A	202	-	50,52,52	2.23	11 (22%)	71,80,80	1.23	6 (8%)
2	FOL	65-A	201	-	34,34,34	1.87	8 (23%)	43,47,47	2.39	16 (37%)
3	NAP	90-A	202	-	50,52,52	2.19	9 (18%)	71,80,80	1.29	8 (11%)
2	FOL	34-A	201	-	34,34,34	1.46	4 (11%)	43,47,47	2.76	21 (48%)
2	FOL	51-A	201	-	34,34,34	1.44	5 (14%)	43,47,47	2.49	19 (44%)
2	FOL	55-A	201	-	34,34,34	1.46	4 (11%)	43,47,47	2.16	11 (25%)
2	FOL	79-A	201	-	34,34,34	1.14	1 (2%)	43,47,47	1.53	10 (23%)
2	FOL	50-A	201	-	34,34,34	1.67	10 (29%)	43,47,47	2.78	15 (34%)
2	FOL	119-A	201	-	34,34,34	1.38	3 (8%)	43,47,47	1.70	10 (23%)
2	FOL	58-A	201	-	34,34,34	2.24	10 (29%)	43,47,47	3.78	19 (44%)
2	FOL	38-A	201	-	34,34,34	1.31	3 (8%)	43,47,47	1.94	11 (25%)
2	FOL	123-A	201	-	34,34,34	1.56	4 (11%)	43,47,47	1.64	9 (20%)
3	NAP	36-A	202	-	50,52,52	2.13	8 (16%)	71,80,80	1.33	10 (14%)
3	NAP	72-A	202	-	50,52,52	2.15	9 (18%)	71,80,80	1.39	12 (16%)
2	FOL	101-A	201	-	34,34,34	1.98	6 (17%)	43,47,47	3.27	20 (46%)
3	NAP	94-A	202	-	50,52,52	2.26	9 (18%)	71,80,80	1.37	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	100-A	202	-	50,52,52	2.12	9 (18%)	71,80,80	1.35	7 (9%)
3	NAP	102-A	202	-	50,52,52	2.14	10 (20%)	71,80,80	1.32	8 (11%)
3	NAP	122-A	202	-	50,52,52	2.19	10 (20%)	71,80,80	1.40	11 (15%)
2	FOL	90-A	201	-	34,34,34	1.46	3 (8%)	43,47,47	1.79	8 (18%)
2	FOL	19-A	201	-	34,34,34	1.32	3 (8%)	43,47,47	1.90	9 (20%)
3	NAP	23-A	202	-	50,52,52	2.19	9 (18%)	71,80,80	1.32	8 (11%)
2	FOL	73-A	201	-	34,34,34	1.37	4 (11%)	43,47,47	1.33	7 (16%)
3	NAP	10-A	202	-	50,52,52	2.20	9 (18%)	71,80,80	1.31	8 (11%)
2	FOL	105-A	201	-	34,34,34	1.51	3 (8%)	43,47,47	1.63	9 (20%)
2	FOL	4-A	201	-	34,34,34	1.56	6 (17%)	43,47,47	2.22	13 (30%)
2	FOL	121-A	201	-	34,34,34	1.25	4 (11%)	43,47,47	1.90	13 (30%)
2	FOL	100-A	201	-	34,34,34	1.22	3 (8%)	43,47,47	2.14	12 (27%)
3	NAP	97-A	202	-	50,52,52	2.18	9 (18%)	71,80,80	1.30	9 (12%)
2	FOL	11-A	201	-	34,34,34	1.67	6 (17%)	43,47,47	2.52	17 (39%)
3	NAP	7-A	202	-	50,52,52	2.14	9 (18%)	71,80,80	1.28	8 (11%)
2	FOL	12-A	201	-	34,34,34	1.62	3 (8%)	43,47,47	1.99	16 (37%)
3	NAP	30-A	202	-	50,52,52	2.15	9 (18%)	71,80,80	1.34	11 (15%)
3	NAP	37-A	202	-	50,52,52	2.16	7 (14%)	71,80,80	1.23	6 (8%)
3	NAP	81-A	202	-	50,52,52	2.24	8 (16%)	71,80,80	1.26	7 (9%)
2	FOL	47-A	201	-	34,34,34	1.42	6 (17%)	43,47,47	2.53	16 (37%)
3	NAP	86-A	202	-	50,52,52	2.21	9 (18%)	71,80,80	1.39	11 (15%)
2	FOL	26-A	201	-	34,34,34	1.15	2 (5%)	43,47,47	1.51	7 (16%)
2	FOL	75-A	201	-	34,34,34	1.49	4 (11%)	43,47,47	1.85	10 (23%)
3	NAP	54-A	202	-	50,52,52	2.19	9 (18%)	71,80,80	1.30	8 (11%)
2	FOL	111-A	201	-	34,34,34	1.38	4 (11%)	43,47,47	1.80	10 (23%)
3	NAP	118-A	202	-	50,52,52	2.24	9 (18%)	71,80,80	1.32	10 (14%)
2	FOL	27-A	201	-	34,34,34	1.18	4 (11%)	43,47,47	2.12	9 (20%)
2	FOL	46-A	201	-	34,34,34	1.61	6 (17%)	43,47,47	2.48	17 (39%)
3	NAP	88-A	202	-	50,52,52	2.17	9 (18%)	71,80,80	1.28	8 (11%)
3	NAP	49-A	202	-	50,52,52	2.21	9 (18%)	71,80,80	1.33	8 (11%)
2	FOL	15-A	201	-	34,34,34	1.39	3 (8%)	43,47,47	1.19	4 (9%)
2	FOL	32-A	201	-	34,34,34	1.17	2 (5%)	43,47,47	1.90	12 (27%)
3	NAP	17-A	202	-	50,52,52	2.27	9 (18%)	71,80,80	1.27	8 (11%)
3	NAP	43-A	202	-	50,52,52	2.16	9 (18%)	71,80,80	1.31	8 (11%)
3	NAP	109-A	202	-	50,52,52	2.22	10 (20%)	71,80,80	1.19	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	124-A	202	-	50,52,52	2.22	9 (18%)	71,80,80	1.41	10 (14%)
3	NAP	101-A	202	-	50,52,52	2.15	8 (16%)	71,80,80	1.24	6 (8%)
2	FOL	31-A	201	-	34,34,34	1.15	4 (11%)	43,47,47	1.67	10 (23%)
2	FOL	53-A	201	-	34,34,34	1.95	4 (11%)	43,47,47	2.49	20 (46%)
2	FOL	70-A	201	-	34,34,34	1.12	1 (2%)	43,47,47	2.45	15 (34%)
2	FOL	91-A	201	-	34,34,34	1.20	2 (5%)	43,47,47	1.65	7 (16%)
3	NAP	26-A	202	-	50,52,52	2.14	9 (18%)	71,80,80	1.28	5 (7%)
3	NAP	75-A	202	-	50,52,52	2.11	8 (16%)	71,80,80	1.31	5 (7%)
2	FOL	107-A	201	-	34,34,34	1.51	7 (20%)	43,47,47	1.77	14 (32%)
3	NAP	84-A	202	-	50,52,52	2.22	10 (20%)	71,80,80	1.31	6 (8%)
3	NAP	70-A	202	-	50,52,52	2.21	9 (18%)	71,80,80	1.39	13 (18%)
3	NAP	20-A	202	-	50,52,52	2.18	10 (20%)	71,80,80	1.33	9 (12%)
2	FOL	17-A	201	-	34,34,34	1.49	5 (14%)	43,47,47	1.91	11 (25%)
3	NAP	2-A	202	-	50,52,52	2.23	9 (18%)	71,80,80	1.37	9 (12%)
3	NAP	71-A	202	-	50,52,52	2.18	9 (18%)	71,80,80	1.35	10 (14%)
3	NAP	111-A	202	-	50,52,52	2.22	10 (20%)	71,80,80	1.30	8 (11%)
2	FOL	5-A	201	-	34,34,34	1.40	3 (8%)	43,47,47	1.65	7 (16%)
2	FOL	30-A	201	-	34,34,34	1.42	5 (14%)	43,47,47	1.83	12 (27%)
3	NAP	1-A	202	-	50,52,52	2.24	9 (18%)	71,80,80	1.36	10 (14%)
2	FOL	63-A	201	-	34,34,34	1.41	6 (17%)	43,47,47	1.98	11 (25%)
2	FOL	22-A	201	-	34,34,34	1.33	3 (8%)	43,47,47	1.99	13 (30%)
2	FOL	54-A	201	-	34,34,34	1.43	5 (14%)	43,47,47	2.34	15 (34%)
2	FOL	40-A	201	-	34,34,34	1.05	0	43,47,47	2.49	14 (32%)
2	FOL	9-A	201	-	34,34,34	1.03	1 (2%)	43,47,47	2.60	17 (39%)
3	NAP	98-A	202	-	50,52,52	2.14	9 (18%)	71,80,80	1.31	5 (7%)
2	FOL	84-A	201	-	34,34,34	1.80	7 (20%)	43,47,47	2.86	19 (44%)
2	FOL	44-A	201	-	34,34,34	1.42	8 (23%)	43,47,47	2.44	14 (32%)
3	NAP	33-A	202	-	50,52,52	2.22	10 (20%)	71,80,80	1.32	9 (12%)
3	NAP	79-A	202	-	50,52,52	2.19	9 (18%)	71,80,80	1.25	6 (8%)
3	NAP	51-A	202	-	50,52,52	2.23	9 (18%)	71,80,80	1.27	5 (7%)
2	FOL	95-A	201	-	34,34,34	1.33	6 (17%)	43,47,47	1.44	7 (16%)
2	FOL	116-A	201	-	34,34,34	1.13	4 (11%)	43,47,47	1.77	11 (25%)
3	NAP	119-A	202	-	50,52,52	2.17	9 (18%)	71,80,80	1.35	9 (12%)
2	FOL	59-A	201	-	34,34,34	2.09	11 (32%)	43,47,47	4.27	20 (46%)
3	NAP	85-A	202	-	50,52,52	2.19	9 (18%)	71,80,80	1.28	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	3-A	201	-	34,34,34	1.10	2 (5%)	43,47,47	1.71	10 (23%)
3	NAP	62-A	202	-	50,52,52	2.15	9 (18%)	71,80,80	1.33	9 (12%)
3	NAP	13-A	202	-	50,52,52	2.18	9 (18%)	71,80,80	1.37	10 (14%)
3	NAP	39-A	202	-	50,52,52	2.18	9 (18%)	71,80,80	1.24	7 (9%)
3	NAP	59-A	202	-	50,52,52	2.23	9 (18%)	71,80,80	1.36	11 (15%)
3	NAP	105-A	202	-	50,52,52	2.22	10 (20%)	71,80,80	1.34	9 (12%)
3	NAP	120-A	202	-	50,52,52	2.16	8 (16%)	71,80,80	1.32	6 (8%)
3	NAP	32-A	202	-	50,52,52	2.14	9 (18%)	71,80,80	1.32	8 (11%)
3	NAP	95-A	202	-	50,52,52	2.22	10 (20%)	71,80,80	1.34	7 (9%)
2	FOL	41-A	201	-	34,34,34	1.27	3 (8%)	43,47,47	1.70	8 (18%)
2	FOL	23-A	201	-	34,34,34	1.32	3 (8%)	43,47,47	1.39	6 (13%)
2	FOL	13-A	201	-	34,34,34	1.13	3 (8%)	43,47,47	2.26	11 (25%)
3	NAP	110-A	202	-	50,52,52	2.22	10 (20%)	71,80,80	1.28	8 (11%)
3	NAP	12-A	202	-	50,52,52	2.16	9 (18%)	71,80,80	1.30	8 (11%)
3	NAP	117-A	202	-	50,52,52	2.22	9 (18%)	71,80,80	1.30	8 (11%)
3	NAP	52-A	202	-	50,52,52	2.23	9 (18%)	71,80,80	1.32	9 (12%)
2	FOL	81-A	201	-	34,34,34	1.26	2 (5%)	43,47,47	2.52	16 (37%)
3	NAP	27-A	202	-	50,52,52	2.17	9 (18%)	71,80,80	1.23	6 (8%)
2	FOL	25-A	201	-	34,34,34	1.06	2 (5%)	43,47,47	1.64	11 (25%)
2	FOL	7-A	201	-	34,34,34	1.27	4 (11%)	43,47,47	1.45	7 (16%)
2	FOL	16-A	201	-	34,34,34	1.73	5 (14%)	43,47,47	1.75	9 (20%)
3	NAP	44-A	202	-	50,52,52	2.22	9 (18%)	71,80,80	1.32	9 (12%)
3	NAP	46-A	202	-	50,52,52	2.22	9 (18%)	71,80,80	1.30	7 (9%)
3	NAP	48-A	202	-	50,52,52	2.20	9 (18%)	71,80,80	1.32	8 (11%)
2	FOL	67-A	201	-	34,34,34	1.49	5 (14%)	43,47,47	2.59	17 (39%)
3	NAP	58-A	202	-	50,52,52	2.24	9 (18%)	71,80,80	1.31	10 (14%)
3	NAP	123-A	202	-	50,52,52	2.22	9 (18%)	71,80,80	1.21	7 (9%)
2	FOL	20-A	201	-	34,34,34	1.24	3 (8%)	43,47,47	1.69	12 (27%)
2	FOL	29-A	201	-	34,34,34	1.27	3 (8%)	43,47,47	1.67	11 (25%)
2	FOL	102-A	201	-	34,34,34	1.40	3 (8%)	43,47,47	2.06	8 (18%)
2	FOL	33-A	201	-	34,34,34	1.45	3 (8%)	43,47,47	2.23	12 (27%)
2	FOL	39-A	201	-	34,34,34	1.12	1 (2%)	43,47,47	1.69	10 (23%)
3	NAP	107-A	202	-	50,52,52	2.18	10 (20%)	71,80,80	1.30	8 (11%)
3	NAP	82-A	202	-	50,52,52	2.17	9 (18%)	71,80,80	1.28	6 (8%)
3	NAP	125-A	202	-	50,52,52	2.16	9 (18%)	71,80,80	1.24	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	6-A	201	-	34,34,34	1.34	4 (11%)	43,47,47	1.34	8 (18%)
2	FOL	99-A	201	-	34,34,34	1.05	3 (8%)	43,47,47	1.81	9 (20%)
2	FOL	48-A	201	-	34,34,34	2.08	12 (35%)	43,47,47	5.11	28 (65%)
2	FOL	64-A	201	-	34,34,34	1.27	5 (14%)	43,47,47	2.89	14 (32%)
2	FOL	8-A	201	-	34,34,34	1.16	3 (8%)	43,47,47	1.66	10 (23%)
2	FOL	110-A	201	-	34,34,34	1.35	4 (11%)	43,47,47	1.92	12 (27%)
3	NAP	121-A	202	-	50,52,52	2.13	9 (18%)	71,80,80	1.39	8 (11%)
3	NAP	45-A	202	-	50,52,52	2.24	10 (20%)	71,80,80	1.30	7 (9%)
2	FOL	109-A	201	-	34,34,34	1.27	4 (11%)	43,47,47	2.40	17 (39%)
3	NAP	80-A	202	-	50,52,52	2.19	10 (20%)	71,80,80	1.18	6 (8%)
3	NAP	83-A	202	-	50,52,52	2.16	10 (20%)	71,80,80	1.36	7 (9%)
3	NAP	5-A	202	-	50,52,52	2.21	10 (20%)	71,80,80	1.36	10 (14%)
3	NAP	77-A	202	-	50,52,52	2.14	8 (16%)	71,80,80	1.27	10 (14%)
3	NAP	19-A	202	-	50,52,52	2.16	9 (18%)	71,80,80	1.39	8 (11%)
3	NAP	35-A	202	-	50,52,52	2.17	9 (18%)	71,80,80	1.29	8 (11%)
3	NAP	76-A	202	-	50,52,52	2.13	8 (16%)	71,80,80	1.22	5 (7%)
3	NAP	87-A	202	-	50,52,52	2.11	9 (18%)	71,80,80	1.35	11 (15%)
2	FOL	14-A	201	-	34,34,34	1.13	2 (5%)	43,47,47	1.77	11 (25%)
2	FOL	83-A	201	-	34,34,34	1.32	4 (11%)	43,47,47	2.40	11 (25%)
2	FOL	1-A	201	-	34,34,34	1.19	5 (14%)	43,47,47	1.60	7 (16%)
3	NAP	74-A	202	-	50,52,52	2.15	9 (18%)	71,80,80	1.32	8 (11%)
2	FOL	92-A	201	-	34,34,34	1.30	3 (8%)	43,47,47	1.46	9 (20%)
2	FOL	71-A	201	-	34,34,34	1.75	7 (20%)	43,47,47	2.51	17 (39%)
3	NAP	50-A	202	-	50,52,52	2.24	9 (18%)	71,80,80	1.41	10 (14%)
2	FOL	24-A	201	-	34,34,34	1.18	3 (8%)	43,47,47	1.98	11 (25%)
3	NAP	3-A	202	-	50,52,52	2.25	10 (20%)	71,80,80	1.41	10 (14%)
3	NAP	68-A	202	-	50,52,52	2.18	9 (18%)	71,80,80	1.39	10 (14%)
3	NAP	73-A	202	-	50,52,52	2.21	9 (18%)	71,80,80	1.42	9 (12%)
3	NAP	93-A	202	-	50,52,52	2.19	9 (18%)	71,80,80	1.33	10 (14%)
2	FOL	88-A	201	-	34,34,34	1.08	2 (5%)	43,47,47	1.81	8 (18%)
3	NAP	63-A	202	-	50,52,52	2.21	8 (16%)	71,80,80	1.36	10 (14%)
3	NAP	66-A	202	-	50,52,52	2.16	9 (18%)	71,80,80	1.29	10 (14%)
3	NAP	89-A	202	-	50,52,52	2.20	9 (18%)	71,80,80	1.34	9 (12%)
2	FOL	62-A	201	-	34,34,34	3.17	12 (35%)	43,47,47	5.44	21 (48%)
2	FOL	72-A	201	-	34,34,34	1.33	6 (17%)	43,47,47	2.67	19 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	41-A	202	-	50,52,52	2.19	9 (18%)	71,80,80	1.32	9 (12%)
3	NAP	115-A	202	-	50,52,52	2.20	9 (18%)	71,80,80	1.31	8 (11%)
2	FOL	68-A	201	-	34,34,34	1.54	8 (23%)	43,47,47	3.15	15 (34%)
2	FOL	52-A	201	-	34,34,34	1.63	7 (20%)	43,47,47	1.99	12 (27%)
2	FOL	87-A	201	-	34,34,34	1.33	4 (11%)	43,47,47	1.80	11 (25%)
2	FOL	93-A	201	-	34,34,34	1.46	6 (17%)	43,47,47	1.71	13 (30%)
3	NAP	112-A	202	-	50,52,52	2.24	10 (20%)	71,80,80	1.35	8 (11%)
2	FOL	82-A	201	-	34,34,34	1.57	5 (14%)	43,47,47	1.77	11 (25%)
3	NAP	103-A	202	-	50,52,52	2.22	10 (20%)	71,80,80	1.25	5 (7%)
2	FOL	66-A	201	-	34,34,34	1.63	7 (20%)	43,47,47	2.60	17 (39%)
2	FOL	2-A	201	-	34,34,34	1.44	4 (11%)	43,47,47	1.57	9 (20%)
3	NAP	8-A	202	-	50,52,52	2.21	9 (18%)	71,80,80	1.30	8 (11%)
3	NAP	31-A	202	-	50,52,52	2.11	9 (18%)	71,80,80	1.38	11 (15%)
3	NAP	21-A	202	-	50,52,52	2.21	9 (18%)	71,80,80	1.30	8 (11%)
3	NAP	16-A	202	-	50,52,52	2.21	9 (18%)	71,80,80	1.36	9 (12%)
3	NAP	25-A	202	-	50,52,52	2.16	9 (18%)	71,80,80	1.24	9 (12%)
2	FOL	69-A	201	-	34,34,34	1.64	5 (14%)	43,47,47	2.38	11 (25%)
3	NAP	42-A	202	-	50,52,52	2.17	9 (18%)	71,80,80	1.32	7 (9%)
2	FOL	106-A	201	-	34,34,34	1.52	7 (20%)	43,47,47	1.63	9 (20%)
3	NAP	15-A	202	-	50,52,52	2.21	9 (18%)	71,80,80	1.30	9 (12%)
3	NAP	91-A	202	-	50,52,52	2.19	9 (18%)	71,80,80	1.34	10 (14%)
2	FOL	36-A	201	-	34,34,34	1.32	3 (8%)	43,47,47	1.40	7 (16%)
3	NAP	6-A	202	-	50,52,52	2.17	10 (20%)	71,80,80	1.34	9 (12%)
2	FOL	122-A	201	-	34,34,34	1.28	4 (11%)	43,47,47	1.64	9 (20%)
3	NAP	56-A	202	-	50,52,52	2.29	10 (20%)	71,80,80	1.41	10 (14%)
2	FOL	85-A	201	-	34,34,34	1.28	4 (11%)	43,47,47	2.16	12 (27%)
3	NAP	99-A	202	-	50,52,52	2.19	9 (18%)	71,80,80	1.30	10 (14%)
2	FOL	10-A	201	-	34,34,34	1.34	4 (11%)	43,47,47	1.24	4 (9%)
2	FOL	108-A	201	-	34,34,34	1.53	5 (14%)	43,47,47	1.65	10 (23%)
3	NAP	96-A	202	-	50,52,52	2.18	9 (18%)	71,80,80	1.24	6 (8%)
2	FOL	120-A	201	-	34,34,34	1.35	4 (11%)	43,47,47	1.59	9 (20%)
3	NAP	104-A	202	-	50,52,52	2.20	9 (18%)	71,80,80	1.25	8 (11%)
2	FOL	97-A	201	-	34,34,34	0.94	2 (5%)	43,47,47	1.84	10 (23%)
3	NAP	9-A	202	-	50,52,52	2.28	11 (22%)	71,80,80	1.38	8 (11%)
2	FOL	56-A	201	-	34,34,34	1.46	5 (14%)	43,47,47	1.98	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	14-A	202	-	50,52,52	2.22	11 (22%)	71,80,80	1.42	9 (12%)
3	NAP	60-A	202	-	50,52,52	2.26	9 (18%)	71,80,80	1.34	10 (14%)
2	FOL	37-A	201	-	34,34,34	1.43	3 (8%)	43,47,47	1.72	9 (20%)
2	FOL	125-A	201	-	34,34,34	1.31	3 (8%)	43,47,47	1.82	12 (27%)
2	FOL	118-A	201	-	34,34,34	1.46	3 (8%)	43,47,47	1.82	10 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	115-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	92-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	47-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	35-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	76-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	104-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	57-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	28-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	74-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	60-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	18-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	113-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	49-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	53-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	96-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	64-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	108-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	57-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	124-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	34-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	28-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	42-A	201	-	-	10/22/22/22	0/3/3/3
3	NAP	61-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	113-A	202	-	-	4/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	11-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	40-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	89-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	22-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	65-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	78-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	21-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	45-A	201	-	-	11/22/22/22	0/3/3/3
2	FOL	61-A	201	-	-	9/22/22/22	0/3/3/3
2	FOL	80-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	86-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	94-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	114-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	114-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	117-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	55-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	112-A	201	-	-	9/22/22/22	0/3/3/3
3	NAP	116-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	43-A	201	-	-	12/22/22/22	0/3/3/3
2	FOL	103-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	38-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	18-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	4-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	98-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	69-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	77-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	29-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	24-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	78-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	67-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	106-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	65-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	90-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	34-A	201	-	-	3/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	51-A	201	-	-	10/22/22/22	0/3/3/3
2	FOL	55-A	201	-	-	10/22/22/22	0/3/3/3
2	FOL	79-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	50-A	201	-	-	9/22/22/22	0/3/3/3
2	FOL	119-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	58-A	201	-	-	8/22/22/22	0/3/3/3
2	FOL	38-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	123-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	36-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	72-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	101-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	94-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	100-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	102-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	122-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	90-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	19-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	23-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	73-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	10-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	105-A	201	-	-	9/22/22/22	0/3/3/3
2	FOL	4-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	121-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	100-A	201	-	-	7/22/22/22	0/3/3/3
3	NAP	97-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	11-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	7-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	12-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	30-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	37-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	81-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	47-A	201	-	-	10/22/22/22	0/3/3/3
3	NAP	86-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	26-A	201	-	-	7/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	75-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	54-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	111-A	201	-	-	7/22/22/22	0/3/3/3
3	NAP	118-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	27-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	46-A	201	-	-	10/22/22/22	0/3/3/3
3	NAP	88-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	49-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	15-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	32-A	201	-	-	7/22/22/22	0/3/3/3
3	NAP	17-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	43-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	109-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	124-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	101-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	31-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	53-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	70-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	91-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	26-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	75-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	107-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	84-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	70-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	20-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	17-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	2-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	71-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	111-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	5-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	30-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	1-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	63-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	22-A	201	-	-	2/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	54-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	40-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	9-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	98-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	84-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	44-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	33-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	79-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	51-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	95-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	116-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	119-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	59-A	201	-	-	10/22/22/22	0/3/3/3
3	NAP	85-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	3-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	62-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	13-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	39-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	59-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	105-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	120-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	32-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	95-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	41-A	201	-	-	8/22/22/22	0/3/3/3
2	FOL	23-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	13-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	110-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	12-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	117-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	52-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	81-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	27-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	25-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	7-A	201	-	-	6/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	16-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	44-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	46-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	48-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	67-A	201	-	-	9/22/22/22	0/3/3/3
3	NAP	58-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	123-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	20-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	29-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	102-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	33-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	39-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	107-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	82-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	125-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	6-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	99-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	48-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	64-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	8-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	110-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	121-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	45-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	109-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	80-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	83-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	5-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	77-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	19-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	35-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	76-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	87-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	14-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	83-A	201	-	-	8/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	1-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	74-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	92-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	71-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	50-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	24-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	3-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	68-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	73-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	93-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	88-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	63-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	66-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	89-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	62-A	201	-	-	9/22/22/22	0/3/3/3
2	FOL	72-A	201	-	-	9/22/22/22	0/3/3/3
3	NAP	41-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	115-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	68-A	201	-	-	10/22/22/22	0/3/3/3
2	FOL	52-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	87-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	93-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	112-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	82-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	103-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	66-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	2-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	8-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	31-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	21-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	16-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	25-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	69-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	42-A	202	-	-	3/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	106-A	201	-	-	7/22/22/22	0/3/3/3
3	NAP	15-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	91-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	36-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	6-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	122-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	56-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	85-A	201	-	-	7/22/22/22	0/3/3/3
3	NAP	99-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	10-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	108-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	96-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	120-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	104-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	97-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	9-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	56-A	201	-	-	8/22/22/22	0/3/3/3
3	NAP	14-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	60-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	37-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	125-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	118-A	201	-	-	4/22/22/22	0/3/3/3

The worst 5 of 1698 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	62-A	201	FOL	C9-C6	11.09	1.74	1.50
3	28-A	202	NAP	O4D-C1D	9.90	1.53	1.40
3	63-A	202	NAP	O4D-C1D	9.87	1.53	1.40
3	118-A	202	NAP	O4D-C1D	9.85	1.53	1.40
3	60-A	202	NAP	O4D-C1D	9.85	1.53	1.40

The worst 5 of 2570 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	62-A	201	FOL	C7-C6-N5	-23.30	105.74	120.87
2	48-A	201	FOL	C7-C6-N5	-16.79	109.97	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	61-A	201	FOL	C9-C6-C7	15.91	149.98	121.38
2	62-A	201	FOL	C9-C6-C7	15.79	149.77	121.38
2	61-A	201	FOL	C7-C6-N5	-12.95	112.46	120.87

There are no chirality outliers.

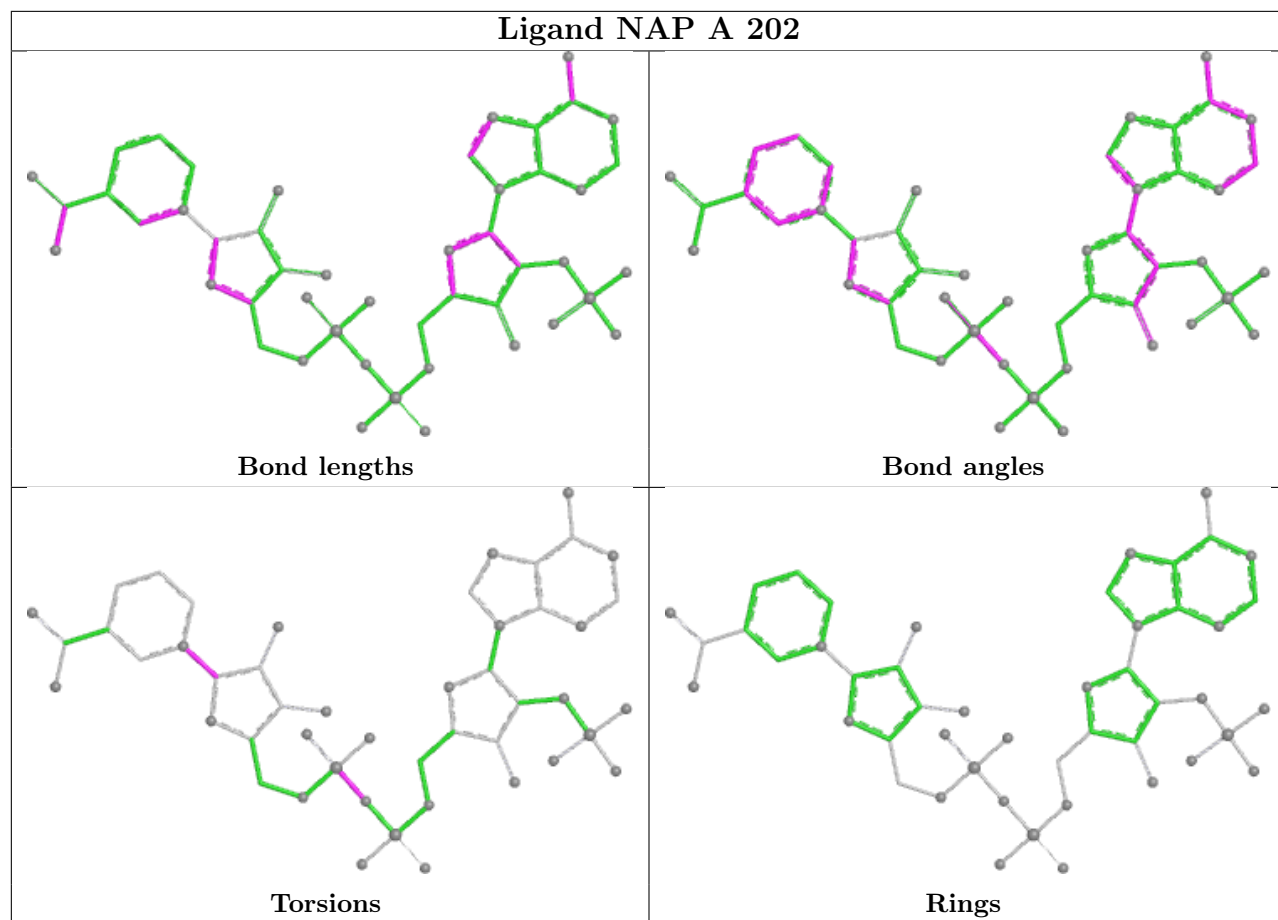
5 of 1054 torsion outliers are listed below:

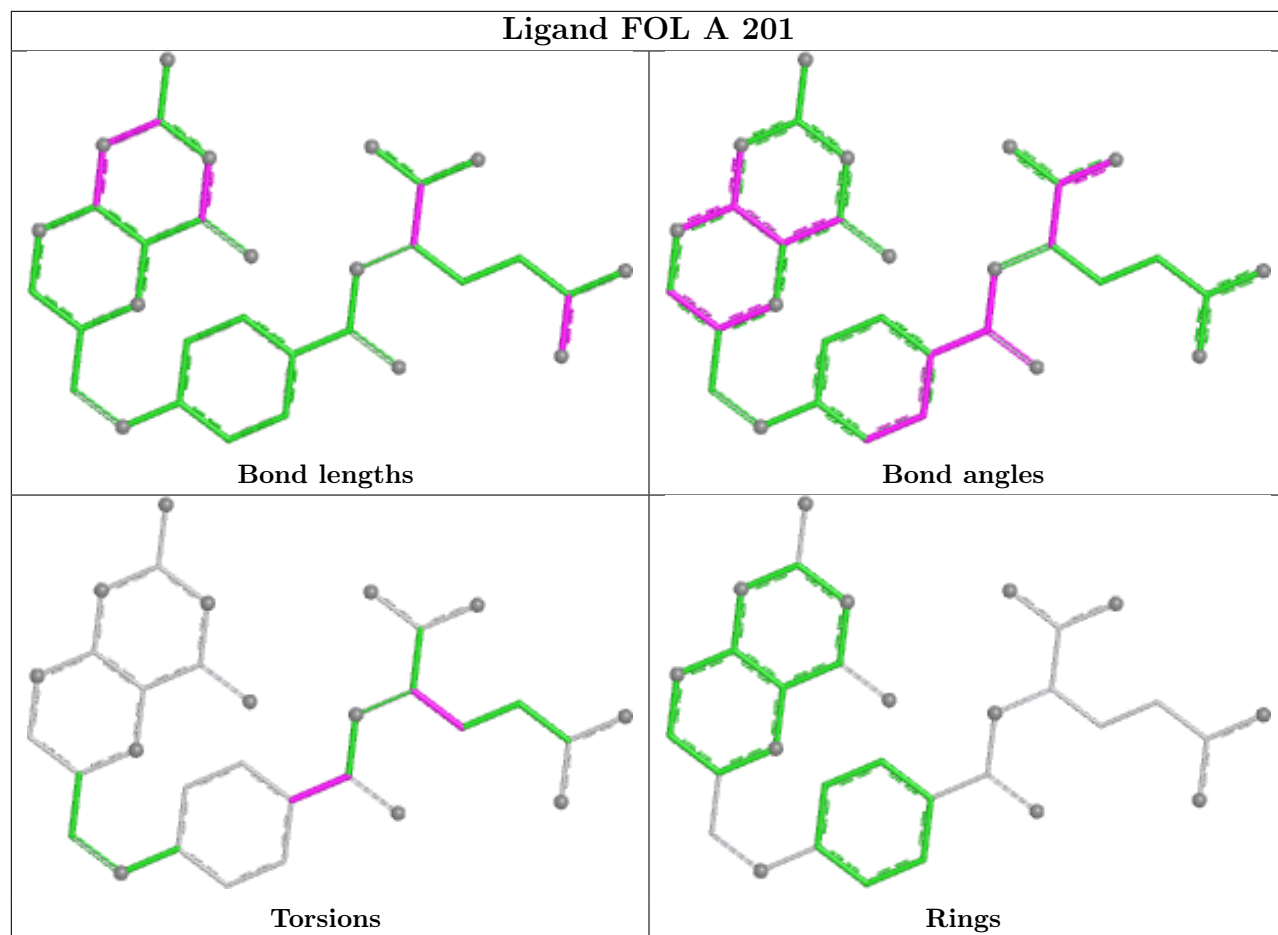
Mol	Chain	Res	Type	Atoms
2	8-A	201	FOL	N-CA-CB-CG
2	19-A	201	FOL	N-CA-CB-CG
2	21-A	201	FOL	C6-C9-N10-C14
2	22-A	201	FOL	N-CA-CB-CG
2	28-A	201	FOL	N-CA-CB-CG

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	158/159 (99%)	4.30	147 (93%) 0 0	0, 0, 0, 0	158 (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	-	-	-	-
All	All	158/19875 (0%)	4.30	147 (93%) 0 0	0, 0, 0, 0	158 (100%)

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	128	TYR	16.5
1	1-A	119	VAL	12.4
1	1-A	140	PHE	10.9
1	1-A	132	ASP	9.7
1	1-A	87	ASP	9.3

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

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
1	CSD	1-A	152	8/9	0.24	0.40	10,11,12,12	11
1	CSD	2-A	152	8/9	-	-	10,11,11,12	11
1	CSD	3-A	152	8/9	-	-	10,11,12,12	11
1	CSD	4-A	152	8/9	-	-	10,11,12,12	11
1	CSD	5-A	152	8/9	-	-	10,11,12,12	11
1	CSD	6-A	152	8/9	-	-	10,11,12,12	11
1	CSD	7-A	152	8/9	-	-	10,11,12,12	11
1	CSD	8-A	152	8/9	-	-	10,11,12,12	11
1	CSD	9-A	152	8/9	-	-	10,11,12,12	11
1	CSD	10-A	152	8/9	-	-	10,11,12,12	11
1	CSD	11-A	152	8/9	-	-	10,11,12,12	11
1	CSD	12-A	152	8/9	-	-	10,11,12,12	11
1	CSD	13-A	152	8/9	-	-	10,11,12,12	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CSD	14-A	152	8/9	-	-	10,11,12,12	11
1	CSD	15-A	152	8/9	-	-	10,11,12,12	11
1	CSD	16-A	152	8/9	-	-	10,11,12,12	11
1	CSD	17-A	152	8/9	-	-	10,11,12,12	11
1	CSD	18-A	152	8/9	-	-	10,11,12,12	11
1	CSD	19-A	152	8/9	-	-	10,11,12,12	11
1	CSD	20-A	152	8/9	-	-	10,11,12,12	11
1	CSD	21-A	152	8/9	-	-	10,11,12,12	11
1	CSD	22-A	152	8/9	-	-	10,11,12,12	11
1	CSD	23-A	152	8/9	-	-	10,11,12,12	11
1	CSD	24-A	152	8/9	-	-	10,11,12,12	11
1	CSD	25-A	152	8/9	-	-	10,11,12,12	11
1	CSD	26-A	152	8/9	-	-	10,11,12,12	11
1	CSD	27-A	152	8/9	-	-	10,11,12,12	11
1	CSD	28-A	152	8/9	-	-	10,11,12,12	11
1	CSD	29-A	152	8/9	-	-	10,11,12,12	11
1	CSD	30-A	152	8/9	-	-	10,11,12,12	11
1	CSD	31-A	152	8/9	-	-	10,11,12,12	11
1	CSD	32-A	152	8/9	-	-	10,11,12,12	11
1	CSD	33-A	152	8/9	-	-	10,11,12,12	11
1	CSD	34-A	152	8/9	-	-	10,11,12,12	11
1	CSD	35-A	152	8/9	-	-	10,11,12,12	11
1	CSD	36-A	152	8/9	-	-	10,11,12,12	11
1	CSD	37-A	152	8/9	-	-	10,11,12,12	11
1	CSD	38-A	152	8/9	-	-	10,11,12,12	11
1	CSD	39-A	152	8/9	-	-	10,11,12,12	11
1	CSD	40-A	152	8/9	-	-	10,11,12,12	11
1	CSD	41-A	152	8/9	-	-	10,11,12,12	11
1	CSD	42-A	152	8/9	-	-	10,11,12,12	11
1	CSD	43-A	152	8/9	-	-	10,11,12,12	11
1	CSD	44-A	152	8/9	-	-	10,11,12,12	11
1	CSD	45-A	152	8/9	-	-	10,11,12,12	11
1	CSD	46-A	152	8/9	-	-	10,11,12,12	11
1	CSD	47-A	152	8/9	-	-	10,11,12,12	11
1	CSD	48-A	152	8/9	-	-	10,11,12,12	11
1	CSD	49-A	152	8/9	-	-	10,11,12,12	11
1	CSD	50-A	152	8/9	-	-	10,11,12,12	11
1	CSD	51-A	152	8/9	-	-	10,11,12,12	11
1	CSD	52-A	152	8/9	-	-	10,11,12,12	11
1	CSD	53-A	152	8/9	-	-	10,11,12,12	11
1	CSD	54-A	152	8/9	-	-	10,11,12,12	11
1	CSD	55-A	152	8/9	-	-	10,11,12,12	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CSD	56-A	152	8/9	-	-	10,11,12,12	11
1	CSD	57-A	152	8/9	-	-	10,11,12,12	11
1	CSD	58-A	152	8/9	-	-	10,11,12,12	11
1	CSD	59-A	152	8/9	-	-	10,11,12,12	11
1	CSD	60-A	152	8/9	-	-	10,11,12,12	11
1	CSD	61-A	152	8/9	-	-	10,11,12,12	11
1	CSD	62-A	152	8/9	-	-	10,11,12,12	11
1	CSD	63-A	152	8/9	-	-	10,11,11,12	11
1	CSD	64-A	152	8/9	-	-	10,11,12,12	11
1	CSD	65-A	152	8/9	-	-	10,11,12,12	11
1	CSD	66-A	152	8/9	-	-	10,11,12,12	11
1	CSD	67-A	152	8/9	-	-	10,11,12,12	11
1	CSD	68-A	152	8/9	-	-	10,11,12,12	11
1	CSD	69-A	152	8/9	-	-	10,11,12,12	11
1	CSD	70-A	152	8/9	-	-	10,11,12,12	11
1	CSD	71-A	152	8/9	-	-	10,11,12,12	11
1	CSD	72-A	152	8/9	-	-	10,11,12,12	11
1	CSD	73-A	152	8/9	-	-	10,11,12,12	11
1	CSD	74-A	152	8/9	-	-	10,11,12,12	11
1	CSD	75-A	152	8/9	-	-	10,11,12,12	11
1	CSD	76-A	152	8/9	-	-	10,11,12,12	11
1	CSD	77-A	152	8/9	-	-	10,11,12,12	11
1	CSD	78-A	152	8/9	-	-	10,11,12,12	11
1	CSD	79-A	152	8/9	-	-	10,11,12,12	11
1	CSD	80-A	152	8/9	-	-	10,11,12,12	11
1	CSD	81-A	152	8/9	-	-	10,11,12,12	11
1	CSD	82-A	152	8/9	-	-	10,11,12,12	11
1	CSD	83-A	152	8/9	-	-	10,11,12,12	11
1	CSD	84-A	152	8/9	-	-	10,11,12,12	11
1	CSD	85-A	152	8/9	-	-	10,11,12,12	11
1	CSD	86-A	152	8/9	-	-	10,11,12,12	11
1	CSD	87-A	152	8/9	-	-	10,11,12,12	11
1	CSD	88-A	152	8/9	-	-	10,11,12,12	11
1	CSD	89-A	152	8/9	-	-	10,11,12,12	11
1	CSD	90-A	152	8/9	-	-	10,11,12,12	11
1	CSD	91-A	152	8/9	-	-	10,11,12,12	11
1	CSD	92-A	152	8/9	-	-	10,11,12,12	11
1	CSD	93-A	152	8/9	-	-	10,11,12,12	11
1	CSD	94-A	152	8/9	-	-	10,11,12,12	11
1	CSD	95-A	152	8/9	-	-	10,11,12,12	11
1	CSD	96-A	152	8/9	-	-	10,11,12,12	11
1	CSD	97-A	152	8/9	-	-	10,11,12,12	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CSD	98-A	152	8/9	-	-	10,11,12,12	11
1	CSD	99-A	152	8/9	-	-	10,11,12,12	11
1	CSD	100-A	152	8/9	-	-	10,11,12,12	11
1	CSD	101-A	152	8/9	-	-	10,11,12,12	11
1	CSD	102-A	152	8/9	-	-	10,11,12,12	11
1	CSD	103-A	152	8/9	-	-	10,11,12,12	11
1	CSD	104-A	152	8/9	-	-	10,11,12,12	11
1	CSD	105-A	152	8/9	-	-	10,11,12,12	11
1	CSD	106-A	152	8/9	-	-	10,11,12,12	11
1	CSD	107-A	152	8/9	-	-	10,11,12,12	11
1	CSD	108-A	152	8/9	-	-	10,11,12,12	11
1	CSD	109-A	152	8/9	-	-	10,11,12,12	11
1	CSD	110-A	152	8/9	-	-	10,11,12,12	11
1	CSD	111-A	152	8/9	-	-	10,11,12,12	11
1	CSD	112-A	152	8/9	-	-	10,11,12,12	11
1	CSD	113-A	152	8/9	-	-	10,11,12,12	11
1	CSD	114-A	152	8/9	-	-	10,11,12,12	11
1	CSD	115-A	152	8/9	-	-	10,11,12,12	11
1	CSD	116-A	152	8/9	-	-	10,11,12,12	11
1	CSD	117-A	152	8/9	-	-	10,11,12,12	11
1	CSD	118-A	152	8/9	-	-	10,11,12,12	11
1	CSD	119-A	152	8/9	-	-	10,11,12,12	11
1	CSD	120-A	152	8/9	-	-	10,11,12,12	11
1	CSD	121-A	152	8/9	-	-	10,11,12,12	11
1	CSD	122-A	152	8/9	-	-	10,11,12,12	11
1	CSD	123-A	152	8/9	-	-	10,11,12,12	11
1	CSD	124-A	152	8/9	-	-	10,11,12,12	11
1	CSD	125-A	152	8/9	-	-	10,11,12,12	11

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(\AA^2)	Q<0.9
2	FOL	1-A	201	32/32	0.65	0.21	9,10,11,12	49
2	FOL	2-A	201	32/32	-	-	9,10,11,12	49
2	FOL	3-A	201	32/32	-	-	9,10,12,12	49
2	FOL	4-A	201	32/32	-	-	9,10,11,12	49
2	FOL	5-A	201	32/32	-	-	9,10,11,11	49
2	FOL	6-A	201	32/32	-	-	9,10,12,12	49
2	FOL	7-A	201	32/32	-	-	9,10,11,12	49
2	FOL	8-A	201	32/32	-	-	9,9,12,12	49
2	FOL	9-A	201	32/32	-	-	9,10,12,12	49
2	FOL	10-A	201	32/32	-	-	9,10,11,12	49
2	FOL	11-A	201	32/32	-	-	9,10,12,12	49
2	FOL	12-A	201	32/32	-	-	9,10,12,12	49
2	FOL	13-A	201	32/32	-	-	9,10,12,13	49
2	FOL	14-A	201	32/32	-	-	9,10,12,12	49
2	FOL	15-A	201	32/32	-	-	9,10,12,12	49
2	FOL	16-A	201	32/32	-	-	9,10,12,12	49
2	FOL	17-A	201	32/32	-	-	9,10,12,13	49
2	FOL	18-A	201	32/32	-	-	9,10,12,12	49
2	FOL	19-A	201	32/32	-	-	9,10,11,12	49
2	FOL	20-A	201	32/32	-	-	9,10,12,12	49
2	FOL	21-A	201	32/32	-	-	9,10,12,12	49
2	FOL	22-A	201	32/32	-	-	9,10,12,13	49
2	FOL	23-A	201	32/32	-	-	9,10,12,13	49
2	FOL	24-A	201	32/32	-	-	9,10,12,13	49
2	FOL	25-A	201	32/32	-	-	9,10,12,13	49
2	FOL	26-A	201	32/32	-	-	9,10,11,12	49
2	FOL	27-A	201	32/32	-	-	9,10,12,12	49
2	FOL	28-A	201	32/32	-	-	9,10,11,12	49
2	FOL	29-A	201	32/32	-	-	9,10,12,12	49
2	FOL	30-A	201	32/32	-	-	9,10,12,12	49
2	FOL	31-A	201	32/32	-	-	9,10,12,12	49
2	FOL	32-A	201	32/32	-	-	9,10,12,12	49
2	FOL	33-A	201	32/32	-	-	9,10,11,12	49
2	FOL	34-A	201	32/32	-	-	9,10,12,12	49
2	FOL	35-A	201	32/32	-	-	9,10,11,12	49
2	FOL	36-A	201	32/32	-	-	9,10,11,12	49
2	FOL	37-A	201	32/32	-	-	9,10,12,12	49
2	FOL	38-A	201	32/32	-	-	9,10,12,12	49
2	FOL	39-A	201	32/32	-	-	9,10,12,12	49
2	FOL	40-A	201	32/32	-	-	9,10,11,12	49
2	FOL	41-A	201	32/32	-	-	9,10,11,11	49
2	FOL	42-A	201	32/32	-	-	9,10,11,12	49
2	FOL	43-A	201	32/32	-	-	9,9,11,11	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FOL	44-A	201	32/32	-	-	9,10,11,11	49
2	FOL	45-A	201	32/32	-	-	9,10,11,12	49
2	FOL	46-A	201	32/32	-	-	9,10,11,11	49
2	FOL	47-A	201	32/32	-	-	9,10,11,11	49
2	FOL	48-A	201	32/32	-	-	9,10,11,12	49
2	FOL	49-A	201	32/32	-	-	9,10,11,12	49
2	FOL	50-A	201	32/32	-	-	9,10,12,12	49
2	FOL	51-A	201	32/32	-	-	9,10,12,12	49
2	FOL	52-A	201	32/32	-	-	9,10,12,12	49
2	FOL	53-A	201	32/32	-	-	9,10,12,12	49
2	FOL	54-A	201	32/32	-	-	9,10,12,12	49
2	FOL	55-A	201	32/32	-	-	9,10,12,12	49
2	FOL	56-A	201	32/32	-	-	9,10,12,12	49
2	FOL	57-A	201	32/32	-	-	9,10,12,12	49
2	FOL	58-A	201	32/32	-	-	9,10,12,12	49
2	FOL	59-A	201	32/32	-	-	9,10,12,12	49
2	FOL	60-A	201	32/32	-	-	9,10,12,13	49
2	FOL	61-A	201	32/32	-	-	9,10,13,13	49
2	FOL	62-A	201	32/32	-	-	9,10,13,14	49
2	FOL	63-A	201	32/32	-	-	9,10,13,14	49
2	FOL	64-A	201	32/32	-	-	9,10,13,14	49
2	FOL	65-A	201	32/32	-	-	9,10,13,14	49
2	FOL	66-A	201	32/32	-	-	9,10,12,13	49
2	FOL	67-A	201	32/32	-	-	9,10,13,13	49
2	FOL	68-A	201	32/32	-	-	9,10,12,13	49
2	FOL	69-A	201	32/32	-	-	9,10,12,13	49
2	FOL	70-A	201	32/32	-	-	9,10,12,13	49
2	FOL	71-A	201	32/32	-	-	9,10,12,13	49
2	FOL	72-A	201	32/32	-	-	9,10,11,12	49
2	FOL	73-A	201	32/32	-	-	9,10,12,12	49
2	FOL	74-A	201	32/32	-	-	9,10,12,13	49
2	FOL	75-A	201	32/32	-	-	9,10,12,13	49
2	FOL	76-A	201	32/32	-	-	9,10,12,12	49
2	FOL	77-A	201	32/32	-	-	9,10,12,12	49
2	FOL	78-A	201	32/32	-	-	9,10,12,12	49
2	FOL	79-A	201	32/32	-	-	9,10,12,13	49
2	FOL	80-A	201	32/32	-	-	9,10,12,13	49
2	FOL	81-A	201	32/32	-	-	9,10,12,12	49
2	FOL	82-A	201	32/32	-	-	9,10,12,12	49
2	FOL	83-A	201	32/32	-	-	9,10,11,12	49
2	FOL	84-A	201	32/32	-	-	9,10,12,12	49
2	FOL	85-A	201	32/32	-	-	9,10,12,12	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FOL	86-A	201	32/32	-	-	9,10,12,12	49
2	FOL	87-A	201	32/32	-	-	9,10,11,12	49
2	FOL	88-A	201	32/32	-	-	9,10,12,12	49
2	FOL	89-A	201	32/32	-	-	9,10,12,12	49
2	FOL	90-A	201	32/32	-	-	9,10,12,12	49
2	FOL	91-A	201	32/32	-	-	9,10,12,12	49
2	FOL	92-A	201	32/32	-	-	9,10,12,12	49
2	FOL	93-A	201	32/32	-	-	9,10,11,12	49
2	FOL	94-A	201	32/32	-	-	9,10,12,12	49
2	FOL	95-A	201	32/32	-	-	9,10,12,12	49
2	FOL	96-A	201	32/32	-	-	9,10,12,12	49
2	FOL	97-A	201	32/32	-	-	9,10,11,13	49
2	FOL	98-A	201	32/32	-	-	9,10,12,12	49
2	FOL	99-A	201	32/32	-	-	9,10,11,12	49
2	FOL	100-A	201	32/32	-	-	9,10,12,13	49
2	FOL	101-A	201	32/32	-	-	9,9,11,12	49
2	FOL	102-A	201	32/32	-	-	9,10,11,12	49
2	FOL	103-A	201	32/32	-	-	9,10,12,12	49
2	FOL	104-A	201	32/32	-	-	9,10,12,13	49
2	FOL	105-A	201	32/32	-	-	9,10,12,12	49
2	FOL	106-A	201	32/32	-	-	9,10,12,12	49
2	FOL	107-A	201	32/32	-	-	9,10,12,13	49
2	FOL	108-A	201	32/32	-	-	9,10,12,12	49
2	FOL	109-A	201	32/32	-	-	9,10,12,13	49
2	FOL	110-A	201	32/32	-	-	9,10,12,13	49
2	FOL	111-A	201	32/32	-	-	9,10,12,12	49
2	FOL	112-A	201	32/32	-	-	9,10,12,13	49
2	FOL	113-A	201	32/32	-	-	9,10,12,13	49
2	FOL	114-A	201	32/32	-	-	9,10,12,12	49
2	FOL	115-A	201	32/32	-	-	9,10,11,12	49
2	FOL	116-A	201	32/32	-	-	9,10,12,12	49
2	FOL	117-A	201	32/32	-	-	9,10,12,12	49
2	FOL	118-A	201	32/32	-	-	9,10,12,13	49
2	FOL	119-A	201	32/32	-	-	9,10,12,12	49
2	FOL	120-A	201	32/32	-	-	9,10,12,12	49
2	FOL	121-A	201	32/32	-	-	9,10,11,12	49
2	FOL	122-A	201	32/32	-	-	9,10,12,12	49
2	FOL	123-A	201	32/32	-	-	9,10,12,12	49
2	FOL	124-A	201	32/32	-	-	9,10,11,12	49
2	FOL	125-A	201	32/32	-	-	9,9,12,13	49
4	MN	1-A	204	1/1	0.91	0.60	10,10,10,10	1
3	NAP	2-A	202	48/48	-	-	9,10,12,13	73

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAP	3-A	202	48/48	-	-	9,10,12,13	73
3	NAP	4-A	202	48/48	-	-	9,10,12,13	73
3	NAP	5-A	202	48/48	-	-	9,10,12,13	73
3	NAP	6-A	202	48/48	-	-	9,10,12,13	73
3	NAP	7-A	202	48/48	-	-	9,10,12,12	73
3	NAP	8-A	202	48/48	-	-	9,10,12,13	73
3	NAP	9-A	202	48/48	-	-	9,10,12,12	73
3	NAP	10-A	202	48/48	-	-	9,10,12,12	73
3	NAP	11-A	202	48/48	-	-	9,10,12,12	73
3	NAP	12-A	202	48/48	-	-	9,10,12,12	73
3	NAP	13-A	202	48/48	-	-	9,10,12,13	73
3	NAP	14-A	202	48/48	-	-	9,10,12,12	73
3	NAP	15-A	202	48/48	-	-	9,10,12,13	73
3	NAP	16-A	202	48/48	-	-	9,10,12,13	73
3	NAP	17-A	202	48/48	-	-	9,10,12,13	73
3	NAP	18-A	202	48/48	-	-	9,10,12,12	73
3	NAP	19-A	202	48/48	-	-	9,10,12,13	73
3	NAP	20-A	202	48/48	-	-	9,10,12,13	73
3	NAP	21-A	202	48/48	-	-	9,10,12,13	73
3	NAP	22-A	202	48/48	-	-	9,10,12,13	73
3	NAP	23-A	202	48/48	-	-	9,10,12,13	73
3	NAP	24-A	202	48/48	-	-	9,10,12,13	73
3	NAP	25-A	202	48/48	-	-	9,10,12,13	73
3	NAP	26-A	202	48/48	-	-	9,10,12,12	73
3	NAP	27-A	202	48/48	-	-	9,10,12,13	73
3	NAP	28-A	202	48/48	-	-	9,10,12,13	73
3	NAP	29-A	202	48/48	-	-	9,10,12,12	73
3	NAP	30-A	202	48/48	-	-	9,10,12,12	73
3	NAP	31-A	202	48/48	-	-	9,10,12,12	73
3	NAP	32-A	202	48/48	-	-	9,10,12,13	73
3	NAP	33-A	202	48/48	-	-	9,10,12,13	73
3	NAP	34-A	202	48/48	-	-	9,10,12,13	73
3	NAP	35-A	202	48/48	-	-	9,10,12,13	73
3	NAP	36-A	202	48/48	-	-	9,10,12,13	73
3	NAP	37-A	202	48/48	-	-	9,10,12,13	73
3	NAP	38-A	202	48/48	-	-	9,10,12,13	73
3	NAP	39-A	202	48/48	-	-	9,10,12,13	73
3	NAP	40-A	202	48/48	-	-	9,10,12,13	73
3	NAP	41-A	202	48/48	-	-	9,10,12,13	73
3	NAP	42-A	202	48/48	-	-	9,10,12,13	73
3	NAP	43-A	202	48/48	-	-	9,10,12,13	73
3	NAP	44-A	202	48/48	-	-	9,10,12,13	73

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAP	45-A	202	48/48	-	-	9,10,12,12	73
3	NAP	46-A	202	48/48	-	-	9,10,12,12	73
3	NAP	47-A	202	48/48	-	-	9,10,12,13	73
3	NAP	48-A	202	48/48	-	-	9,10,12,13	73
3	NAP	49-A	202	48/48	-	-	9,10,12,13	73
3	NAP	50-A	202	48/48	-	-	9,10,12,13	73
3	NAP	51-A	202	48/48	-	-	9,10,12,13	73
3	NAP	52-A	202	48/48	-	-	9,10,12,13	73
3	NAP	53-A	202	48/48	-	-	9,10,12,13	73
3	NAP	54-A	202	48/48	-	-	9,10,12,13	73
3	NAP	55-A	202	48/48	-	-	9,10,12,13	73
3	NAP	56-A	202	48/48	-	-	9,10,12,13	73
3	NAP	57-A	202	48/48	-	-	9,10,12,12	73
3	NAP	58-A	202	48/48	-	-	9,10,12,13	73
3	NAP	59-A	202	48/48	-	-	9,10,12,13	73
3	NAP	60-A	202	48/48	-	-	9,10,12,12	73
3	NAP	61-A	202	48/48	-	-	9,10,12,13	73
3	NAP	62-A	202	48/48	-	-	9,10,12,13	73
3	NAP	63-A	202	48/48	-	-	9,10,12,13	73
3	NAP	64-A	202	48/48	-	-	9,10,12,13	73
3	NAP	65-A	202	48/48	-	-	9,10,12,13	73
3	NAP	66-A	202	48/48	-	-	9,10,12,13	73
3	NAP	67-A	202	48/48	-	-	9,10,12,12	73
3	NAP	68-A	202	48/48	-	-	9,10,12,12	73
3	NAP	69-A	202	48/48	-	-	9,10,12,13	73
3	NAP	70-A	202	48/48	-	-	9,10,12,13	73
3	NAP	71-A	202	48/48	-	-	9,10,12,13	73
3	NAP	72-A	202	48/48	-	-	9,10,12,12	73
3	NAP	73-A	202	48/48	-	-	9,10,12,12	73
3	NAP	74-A	202	48/48	-	-	9,10,12,13	73
3	NAP	75-A	202	48/48	-	-	9,10,12,13	73
3	NAP	76-A	202	48/48	-	-	9,10,12,13	73
3	NAP	77-A	202	48/48	-	-	9,10,12,12	73
3	NAP	78-A	202	48/48	-	-	9,10,12,13	73
3	NAP	79-A	202	48/48	-	-	9,10,12,13	73
3	NAP	80-A	202	48/48	-	-	9,10,12,13	73
3	NAP	81-A	202	48/48	-	-	9,10,12,12	73
3	NAP	82-A	202	48/48	-	-	9,10,12,13	73
3	NAP	83-A	202	48/48	-	-	9,10,12,13	73
3	NAP	84-A	202	48/48	-	-	9,10,12,13	73
3	NAP	85-A	202	48/48	-	-	9,10,12,13	73
3	NAP	86-A	202	48/48	-	-	9,10,12,13	73

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAP	87-A	202	48/48	-	-	9,10,12,13	73
3	NAP	88-A	202	48/48	-	-	9,10,12,13	73
3	NAP	89-A	202	48/48	-	-	9,10,12,12	73
3	NAP	90-A	202	48/48	-	-	9,10,12,12	73
3	NAP	91-A	202	48/48	-	-	9,10,12,13	73
3	NAP	92-A	202	48/48	-	-	9,10,12,13	73
3	NAP	93-A	202	48/48	-	-	9,10,12,12	73
3	NAP	94-A	202	48/48	-	-	9,10,12,13	73
3	NAP	95-A	202	48/48	-	-	9,10,12,13	73
3	NAP	96-A	202	48/48	-	-	9,10,12,13	73
3	NAP	97-A	202	48/48	-	-	9,10,12,12	73
3	NAP	98-A	202	48/48	-	-	9,10,12,13	73
3	NAP	99-A	202	48/48	-	-	9,10,12,13	73
3	NAP	100-A	202	48/48	-	-	9,10,12,13	73
3	NAP	101-A	202	48/48	-	-	9,10,12,13	73
3	NAP	102-A	202	48/48	-	-	9,10,12,13	73
3	NAP	103-A	202	48/48	-	-	9,10,12,13	73
3	NAP	104-A	202	48/48	-	-	9,10,12,12	73
3	NAP	105-A	202	48/48	-	-	9,10,12,12	73
3	NAP	106-A	202	48/48	-	-	9,10,12,13	73
3	NAP	107-A	202	48/48	-	-	9,10,12,12	73
3	NAP	108-A	202	48/48	-	-	9,10,12,13	73
3	NAP	109-A	202	48/48	-	-	9,10,12,13	73
3	NAP	110-A	202	48/48	-	-	9,10,12,13	73
3	NAP	111-A	202	48/48	-	-	9,10,12,13	73
3	NAP	112-A	202	48/48	-	-	9,10,12,13	73
3	NAP	113-A	202	48/48	-	-	9,10,12,13	73
3	NAP	114-A	202	48/48	-	-	9,10,12,13	73
3	NAP	115-A	202	48/48	-	-	9,10,12,12	73
3	NAP	116-A	202	48/48	-	-	9,10,12,12	73
3	NAP	117-A	202	48/48	-	-	9,10,12,12	73
3	NAP	118-A	202	48/48	-	-	9,10,12,13	73
3	NAP	119-A	202	48/48	-	-	9,10,12,13	73
3	NAP	120-A	202	48/48	-	-	9,10,12,13	73
3	NAP	121-A	202	48/48	-	-	9,10,12,12	73
3	NAP	122-A	202	48/48	-	-	9,10,12,12	73
3	NAP	123-A	202	48/48	-	-	9,10,12,13	73
3	NAP	124-A	202	48/48	-	-	9,10,12,13	73
3	NAP	125-A	202	48/48	-	-	9,10,12,13	73
3	NAP	1-A	202	48/48	0.93	0.11	9,10,12,12	73
4	MN	2-A	203	1/1	-	-	13,13,13,13	1
4	MN	3-A	203	1/1	-	-	13,13,13,13	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MN	4-A	203	1/1	-	-	13,13,13,13	1
4	MN	5-A	203	1/1	-	-	14,14,14,14	1
4	MN	6-A	203	1/1	-	-	13,13,13,13	1
4	MN	7-A	203	1/1	-	-	13,13,13,13	1
4	MN	8-A	203	1/1	-	-	14,14,14,14	1
4	MN	9-A	203	1/1	-	-	13,13,13,13	1
4	MN	10-A	203	1/1	-	-	13,13,13,13	1
4	MN	11-A	203	1/1	-	-	13,13,13,13	1
4	MN	12-A	203	1/1	-	-	13,13,13,13	1
4	MN	13-A	203	1/1	-	-	14,14,14,14	1
4	MN	14-A	203	1/1	-	-	14,14,14,14	1
4	MN	15-A	203	1/1	-	-	14,14,14,14	1
4	MN	16-A	203	1/1	-	-	14,14,14,14	1
4	MN	17-A	203	1/1	-	-	14,14,14,14	1
4	MN	18-A	203	1/1	-	-	13,13,13,13	1
4	MN	19-A	203	1/1	-	-	14,14,14,14	1
4	MN	20-A	203	1/1	-	-	14,14,14,14	1
4	MN	21-A	203	1/1	-	-	13,13,13,13	1
4	MN	22-A	203	1/1	-	-	14,14,14,14	1
4	MN	23-A	203	1/1	-	-	14,14,14,14	1
4	MN	24-A	203	1/1	-	-	13,13,13,13	1
4	MN	25-A	203	1/1	-	-	13,13,13,13	1
4	MN	26-A	203	1/1	-	-	13,13,13,13	1
4	MN	27-A	203	1/1	-	-	13,13,13,13	1
4	MN	28-A	203	1/1	-	-	13,13,13,13	1
4	MN	29-A	203	1/1	-	-	13,13,13,13	1
4	MN	30-A	203	1/1	-	-	13,13,13,13	1
4	MN	31-A	203	1/1	-	-	13,13,13,13	1
4	MN	32-A	203	1/1	-	-	13,13,13,13	1
4	MN	33-A	203	1/1	-	-	14,14,14,14	1
4	MN	34-A	203	1/1	-	-	13,13,13,13	1
4	MN	35-A	203	1/1	-	-	13,13,13,13	1
4	MN	36-A	203	1/1	-	-	14,14,14,14	1
4	MN	37-A	203	1/1	-	-	13,13,13,13	1
4	MN	38-A	203	1/1	-	-	14,14,14,14	1
4	MN	39-A	203	1/1	-	-	14,14,14,14	1
4	MN	40-A	203	1/1	-	-	14,14,14,14	1
4	MN	41-A	203	1/1	-	-	13,13,13,13	1
4	MN	42-A	203	1/1	-	-	14,14,14,14	1
4	MN	43-A	203	1/1	-	-	13,13,13,13	1
4	MN	44-A	203	1/1	-	-	13,13,13,13	1
4	MN	45-A	203	1/1	-	-	14,14,14,14	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MN	46-A	203	1/1	-	-	13,13,13,13	1
4	MN	47-A	203	1/1	-	-	13,13,13,13	1
4	MN	48-A	203	1/1	-	-	13,13,13,13	1
4	MN	49-A	203	1/1	-	-	13,13,13,13	1
4	MN	50-A	203	1/1	-	-	14,14,14,14	1
4	MN	51-A	203	1/1	-	-	14,14,14,14	1
4	MN	52-A	203	1/1	-	-	14,14,14,14	1
4	MN	53-A	203	1/1	-	-	14,14,14,14	1
4	MN	54-A	203	1/1	-	-	13,13,13,13	1
4	MN	55-A	203	1/1	-	-	13,13,13,13	1
4	MN	56-A	203	1/1	-	-	13,13,13,13	1
4	MN	57-A	203	1/1	-	-	13,13,13,13	1
4	MN	58-A	203	1/1	-	-	13,13,13,13	1
4	MN	59-A	203	1/1	-	-	14,14,14,14	1
4	MN	60-A	203	1/1	-	-	14,14,14,14	1
4	MN	61-A	203	1/1	-	-	13,13,13,13	1
4	MN	62-A	203	1/1	-	-	14,14,14,14	1
4	MN	63-A	203	1/1	-	-	13,13,13,13	1
4	MN	64-A	203	1/1	-	-	13,13,13,13	1
4	MN	65-A	203	1/1	-	-	13,13,13,13	1
4	MN	66-A	203	1/1	-	-	14,14,14,14	1
4	MN	67-A	203	1/1	-	-	14,14,14,14	1
4	MN	68-A	203	1/1	-	-	14,14,14,14	1
4	MN	69-A	203	1/1	-	-	13,13,13,13	1
4	MN	70-A	203	1/1	-	-	13,13,13,13	1
4	MN	71-A	203	1/1	-	-	13,13,13,13	1
4	MN	72-A	203	1/1	-	-	13,13,13,13	1
4	MN	73-A	203	1/1	-	-	13,13,13,13	1
4	MN	74-A	203	1/1	-	-	13,13,13,13	1
4	MN	75-A	203	1/1	-	-	13,13,13,13	1
4	MN	76-A	203	1/1	-	-	13,13,13,13	1
4	MN	77-A	203	1/1	-	-	14,14,14,14	1
4	MN	78-A	203	1/1	-	-	14,14,14,14	1
4	MN	79-A	203	1/1	-	-	14,14,14,14	1
4	MN	80-A	203	1/1	-	-	14,14,14,14	1
4	MN	81-A	203	1/1	-	-	14,14,14,14	1
4	MN	82-A	203	1/1	-	-	13,13,13,13	1
4	MN	83-A	203	1/1	-	-	14,14,14,14	1
4	MN	84-A	203	1/1	-	-	13,13,13,13	1
4	MN	85-A	203	1/1	-	-	13,13,13,13	1
4	MN	86-A	203	1/1	-	-	13,13,13,13	1
4	MN	87-A	203	1/1	-	-	13,13,13,13	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MN	88-A	203	1/1	-	-	13,13,13,13	1
4	MN	89-A	203	1/1	-	-	13,13,13,13	1
4	MN	90-A	203	1/1	-	-	13,13,13,13	1
4	MN	91-A	203	1/1	-	-	13,13,13,13	1
4	MN	92-A	203	1/1	-	-	13,13,13,13	1
4	MN	93-A	203	1/1	-	-	13,13,13,13	1
4	MN	94-A	203	1/1	-	-	13,13,13,13	1
4	MN	95-A	203	1/1	-	-	14,14,14,14	1
4	MN	96-A	203	1/1	-	-	13,13,13,13	1
4	MN	97-A	203	1/1	-	-	13,13,13,13	1
4	MN	98-A	203	1/1	-	-	13,13,13,13	1
4	MN	99-A	203	1/1	-	-	13,13,13,13	1
4	MN	100-A	203	1/1	-	-	14,14,14,14	1
4	MN	101-A	203	1/1	-	-	14,14,14,14	1
4	MN	102-A	203	1/1	-	-	13,13,13,13	1
4	MN	103-A	203	1/1	-	-	13,13,13,13	1
4	MN	104-A	203	1/1	-	-	13,13,13,13	1
4	MN	105-A	203	1/1	-	-	13,13,13,13	1
4	MN	106-A	203	1/1	-	-	13,13,13,13	1
4	MN	107-A	203	1/1	-	-	13,13,13,13	1
4	MN	108-A	203	1/1	-	-	13,13,13,13	1
4	MN	109-A	203	1/1	-	-	14,14,14,14	1
4	MN	110-A	203	1/1	-	-	14,14,14,14	1
4	MN	111-A	203	1/1	-	-	13,13,13,13	1
4	MN	112-A	203	1/1	-	-	14,14,14,14	1
4	MN	113-A	203	1/1	-	-	13,13,13,13	1
4	MN	114-A	203	1/1	-	-	13,13,13,13	1
4	MN	115-A	203	1/1	-	-	13,13,13,13	1
4	MN	116-A	203	1/1	-	-	14,14,14,14	1
4	MN	117-A	203	1/1	-	-	13,13,13,13	1
4	MN	118-A	203	1/1	-	-	13,13,13,13	1
4	MN	119-A	203	1/1	-	-	13,13,13,13	1
4	MN	120-A	203	1/1	-	-	13,13,13,13	1
4	MN	121-A	203	1/1	-	-	13,13,13,13	1
4	MN	122-A	203	1/1	-	-	14,14,14,14	1
4	MN	123-A	203	1/1	-	-	13,13,13,13	1
4	MN	124-A	203	1/1	-	-	13,13,13,13	1
4	MN	125-A	203	1/1	-	-	14,14,14,14	1
4	MN	1-A	203	1/1	0.99	0.07	14,14,14,14	1
4	MN	2-A	204	1/1	-	-	10,10,10,10	1
4	MN	3-A	204	1/1	-	-	9,9,9,9	1
4	MN	4-A	204	1/1	-	-	9,9,9,9	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MN	5-A	204	1/1	-	-	9,9,9,9	1
4	MN	6-A	204	1/1	-	-	9,9,9,9	1
4	MN	7-A	204	1/1	-	-	10,10,10,10	1
4	MN	8-A	204	1/1	-	-	10,10,10,10	1
4	MN	9-A	204	1/1	-	-	9,9,9,9	1
4	MN	10-A	204	1/1	-	-	10,10,10,10	1
4	MN	11-A	204	1/1	-	-	10,10,10,10	1
4	MN	12-A	204	1/1	-	-	9,9,9,9	1
4	MN	13-A	204	1/1	-	-	10,10,10,10	1
4	MN	14-A	204	1/1	-	-	10,10,10,10	1
4	MN	15-A	204	1/1	-	-	11,11,11,11	1
4	MN	16-A	204	1/1	-	-	10,10,10,10	1
4	MN	17-A	204	1/1	-	-	10,10,10,10	1
4	MN	18-A	204	1/1	-	-	10,10,10,10	1
4	MN	19-A	204	1/1	-	-	10,10,10,10	1
4	MN	20-A	204	1/1	-	-	10,10,10,10	1
4	MN	21-A	204	1/1	-	-	10,10,10,10	1
4	MN	22-A	204	1/1	-	-	10,10,10,10	1
4	MN	23-A	204	1/1	-	-	10,10,10,10	1
4	MN	24-A	204	1/1	-	-	11,11,11,11	1
4	MN	25-A	204	1/1	-	-	10,10,10,10	1
4	MN	26-A	204	1/1	-	-	10,10,10,10	1
4	MN	27-A	204	1/1	-	-	10,10,10,10	1
4	MN	28-A	204	1/1	-	-	10,10,10,10	1
4	MN	29-A	204	1/1	-	-	10,10,10,10	1
4	MN	30-A	204	1/1	-	-	9,9,9,9	1
4	MN	31-A	204	1/1	-	-	10,10,10,10	1
4	MN	32-A	204	1/1	-	-	10,10,10,10	1
4	MN	33-A	204	1/1	-	-	10,10,10,10	1
4	MN	34-A	204	1/1	-	-	10,10,10,10	1
4	MN	35-A	204	1/1	-	-	10,10,10,10	1
4	MN	36-A	204	1/1	-	-	11,11,11,11	1
4	MN	37-A	204	1/1	-	-	11,11,11,11	1
4	MN	38-A	204	1/1	-	-	12,12,12,12	1
4	MN	39-A	204	1/1	-	-	11,11,11,11	1
4	MN	40-A	204	1/1	-	-	10,10,10,10	1
4	MN	41-A	204	1/1	-	-	10,10,10,10	1
4	MN	42-A	204	1/1	-	-	11,11,11,11	1
4	MN	43-A	204	1/1	-	-	9,9,9,9	1
4	MN	44-A	204	1/1	-	-	10,10,10,10	1
4	MN	45-A	204	1/1	-	-	10,10,10,10	1
4	MN	46-A	204	1/1	-	-	10,10,10,10	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MN	47-A	204	1/1	-	-	10,10,10,10	1
4	MN	48-A	204	1/1	-	-	10,10,10,10	1
4	MN	49-A	204	1/1	-	-	10,10,10,10	1
4	MN	50-A	204	1/1	-	-	11,11,11,11	1
4	MN	51-A	204	1/1	-	-	11,11,11,11	1
4	MN	52-A	204	1/1	-	-	11,11,11,11	1
4	MN	53-A	204	1/1	-	-	11,11,11,11	1
4	MN	54-A	204	1/1	-	-	11,11,11,11	1
4	MN	55-A	204	1/1	-	-	12,12,12,12	1
4	MN	56-A	204	1/1	-	-	11,11,11,11	1
4	MN	57-A	204	1/1	-	-	11,11,11,11	1
4	MN	58-A	204	1/1	-	-	11,11,11,11	1
4	MN	59-A	204	1/1	-	-	12,12,12,12	1
4	MN	60-A	204	1/1	-	-	12,12,12,12	1
4	MN	61-A	204	1/1	-	-	12,12,12,12	1
4	MN	62-A	204	1/1	-	-	13,13,13,13	1
4	MN	63-A	204	1/1	-	-	12,12,12,12	1
4	MN	64-A	204	1/1	-	-	13,13,13,13	1
4	MN	65-A	204	1/1	-	-	13,13,13,13	1
4	MN	66-A	204	1/1	-	-	13,13,13,13	1
4	MN	67-A	204	1/1	-	-	13,13,13,13	1
4	MN	68-A	204	1/1	-	-	11,11,11,11	1
4	MN	69-A	204	1/1	-	-	11,11,11,11	1
4	MN	70-A	204	1/1	-	-	11,11,11,11	1
4	MN	71-A	204	1/1	-	-	11,11,11,11	1
4	MN	72-A	204	1/1	-	-	11,11,11,11	1
4	MN	73-A	204	1/1	-	-	11,11,11,11	1
4	MN	74-A	204	1/1	-	-	11,11,11,11	1
4	MN	75-A	204	1/1	-	-	11,11,11,11	1
4	MN	76-A	204	1/1	-	-	10,10,10,10	1
4	MN	77-A	204	1/1	-	-	11,11,11,11	1
4	MN	78-A	204	1/1	-	-	11,11,11,11	1
4	MN	79-A	204	1/1	-	-	12,12,12,12	1
4	MN	80-A	204	1/1	-	-	12,12,12,12	1
4	MN	81-A	204	1/1	-	-	12,12,12,12	1
4	MN	82-A	204	1/1	-	-	12,12,12,12	1
4	MN	83-A	204	1/1	-	-	12,12,12,12	1
4	MN	84-A	204	1/1	-	-	12,12,12,12	1
4	MN	85-A	204	1/1	-	-	12,12,12,12	1
4	MN	86-A	204	1/1	-	-	11,11,11,11	1
4	MN	87-A	204	1/1	-	-	11,11,11,11	1
4	MN	88-A	204	1/1	-	-	12,12,12,12	1

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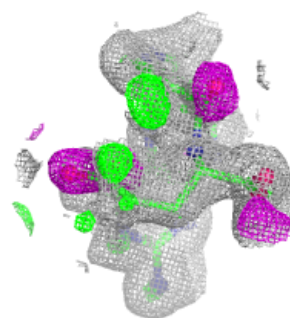
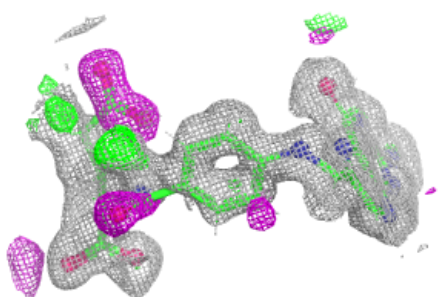
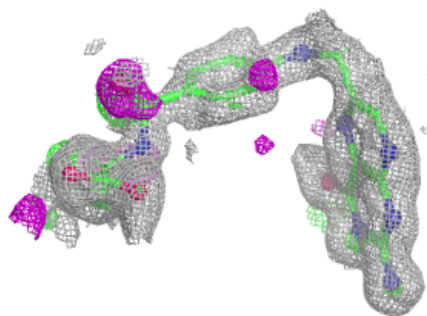
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MN	89-A	204	1/1	-	-	12,12,12,12	1
4	MN	90-A	204	1/1	-	-	12,12,12,12	1
4	MN	91-A	204	1/1	-	-	12,12,12,12	1
4	MN	92-A	204	1/1	-	-	11,11,11,11	1
4	MN	93-A	204	1/1	-	-	10,10,10,10	1
4	MN	94-A	204	1/1	-	-	11,11,11,11	1
4	MN	95-A	204	1/1	-	-	11,11,11,11	1
4	MN	96-A	204	1/1	-	-	11,11,11,11	1
4	MN	97-A	204	1/1	-	-	11,11,11,11	1
4	MN	98-A	204	1/1	-	-	11,11,11,11	1
4	MN	99-A	204	1/1	-	-	12,12,12,12	1
4	MN	100-A	204	1/1	-	-	11,11,11,11	1
4	MN	101-A	204	1/1	-	-	11,11,11,11	1
4	MN	102-A	204	1/1	-	-	11,11,11,11	1
4	MN	103-A	204	1/1	-	-	11,11,11,11	1
4	MN	104-A	204	1/1	-	-	11,11,11,11	1
4	MN	105-A	204	1/1	-	-	11,11,11,11	1
4	MN	106-A	204	1/1	-	-	11,11,11,11	1
4	MN	107-A	204	1/1	-	-	11,11,11,11	1
4	MN	108-A	204	1/1	-	-	11,11,11,11	1
4	MN	109-A	204	1/1	-	-	11,11,11,11	1
4	MN	110-A	204	1/1	-	-	11,11,11,11	1
4	MN	111-A	204	1/1	-	-	11,11,11,11	1
4	MN	112-A	204	1/1	-	-	12,12,12,12	1
4	MN	113-A	204	1/1	-	-	12,12,12,12	1
4	MN	114-A	204	1/1	-	-	12,12,12,12	1
4	MN	115-A	204	1/1	-	-	12,12,12,12	1
4	MN	116-A	204	1/1	-	-	11,11,11,11	1
4	MN	117-A	204	1/1	-	-	11,11,11,11	1
4	MN	118-A	204	1/1	-	-	12,12,12,12	1
4	MN	119-A	204	1/1	-	-	13,13,13,13	1
4	MN	120-A	204	1/1	-	-	12,12,12,12	1
4	MN	121-A	204	1/1	-	-	12,12,12,12	1
4	MN	122-A	204	1/1	-	-	13,13,13,13	1
4	MN	123-A	204	1/1	-	-	12,12,12,12	1
4	MN	124-A	204	1/1	-	-	12,12,12,12	1
4	MN	125-A	204	1/1	-	-	11,11,11,11	1

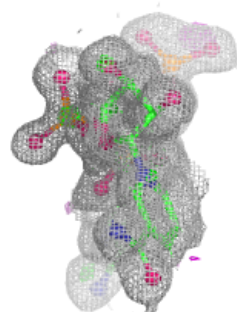
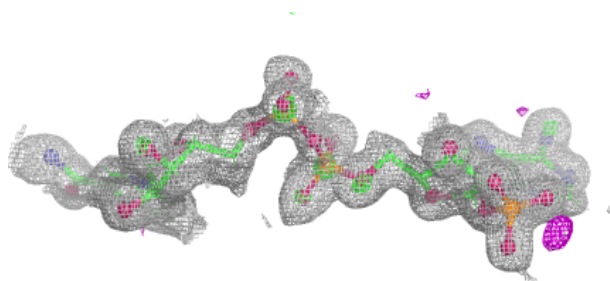
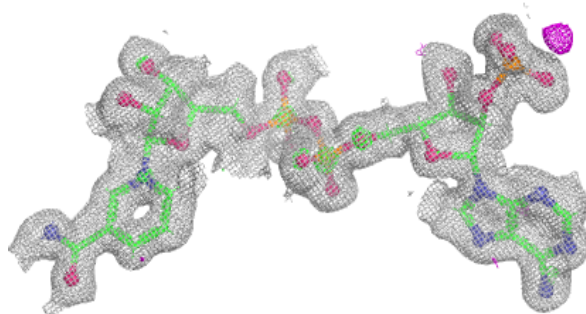
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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 202:**

$2mF_o-DF_c$ (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.