



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 12:32 PM UTC

PDB ID : 4P3R / pdb_00004p3r
Title : Cryogenic WT DHFR, time-averaged ensemble
Authors : Keedy, D.A.; van den Bedem, H.; Fraser, J.S.
Deposited on : 2014-03-10
Resolution : 1.15 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

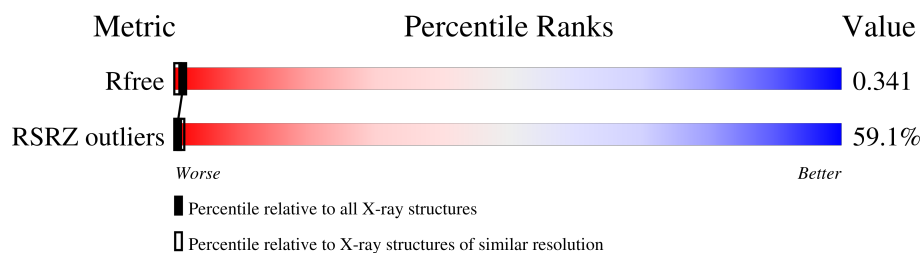
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.15 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	1380 (1.16-1.12)
RSRZ outliers	180081	1379 (1.16-1.12)

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 699653 atoms, of which 315500 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
			2492	805	1224	217	239	7			
1	2-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	3-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	4-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	5-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	6-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	7-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	8-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	9-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	10-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	11-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	12-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	13-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	14-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	15-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	16-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	18-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	19-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	20-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	21-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	22-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	23-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	24-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	25-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	26-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	27-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	28-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	29-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	30-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	31-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	32-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	33-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	34-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	35-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	36-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	37-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	39-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	40-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	41-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	42-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	43-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	44-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	45-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	46-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	47-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	48-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	49-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	50-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	51-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	52-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	53-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	54-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	55-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	56-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	57-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	58-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	59-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	60-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	61-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	62-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	63-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	64-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	65-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	66-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	67-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	68-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	69-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	70-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	71-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	72-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	73-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	74-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	75-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	76-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	77-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	78-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	79-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	80-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	81-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	82-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	83-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	84-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	85-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	86-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	87-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	88-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	89-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	90-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	91-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	92-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	93-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	94-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	95-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	96-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	97-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	98-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	99-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	100-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	101-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	102-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	103-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	104-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	105-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	106-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	107-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	108-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	109-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	110-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	111-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	112-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	113-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	114-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	115-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	116-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	117-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	118-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	119-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	120-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	121-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	122-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	123-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	124-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	125-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	126-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	127-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	128-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	129-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	130-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	131-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	132-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	133-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	134-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	135-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	136-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	137-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	138-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	139-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	140-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	141-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	142-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	143-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	144-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	145-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	146-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	147-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	148-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	149-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	150-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	151-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	152-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	153-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	154-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	155-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	156-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	157-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	158-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	159-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	160-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	161-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	162-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	163-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	164-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	165-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	166-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	167-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	168-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	169-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	170-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	171-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	172-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	173-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	174-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	175-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	176-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	177-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	178-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	179-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	180-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	181-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	182-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	183-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	184-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	185-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	186-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	187-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	188-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	189-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	190-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	191-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	192-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	193-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	194-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	195-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	196-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	197-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	198-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	199-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	200-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	201-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	202-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	203-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	204-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	205-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	206-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	207-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	208-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	209-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	210-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	211-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	212-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	213-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	214-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	215-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	216-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	217-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	218-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	219-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	220-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	221-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	222-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	223-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	224-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	225-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	226-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			

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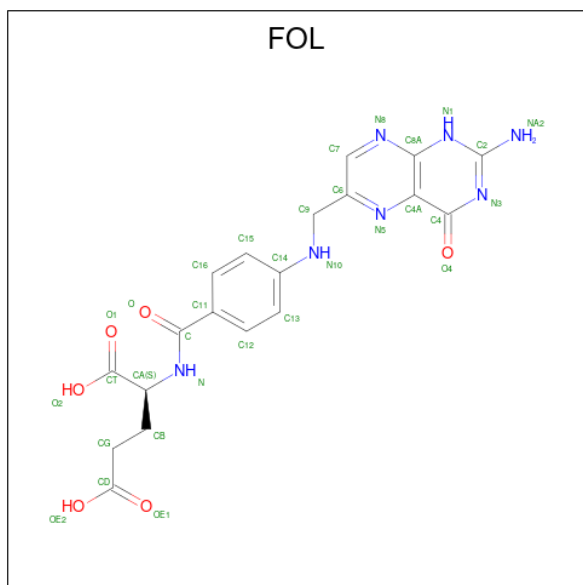
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	227-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	228-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	229-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	230-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	231-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	232-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	233-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	234-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	235-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	236-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	237-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	238-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	239-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	240-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	241-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	242-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	243-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	244-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	245-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	246-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	247-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	248-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	249-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	250-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			

- 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		
2	8-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	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
2	29-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	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
2	50-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	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
2	71-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	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
2	92-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	93-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	94-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	95-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	96-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	97-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	98-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	99-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	100-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	101-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	102-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	103-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	104-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	105-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	106-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	107-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	108-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	109-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	110-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	111-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	112-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	113-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	114-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	115-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	116-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	117-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	118-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	119-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	120-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	121-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	122-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	123-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	124-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	125-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	126-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	127-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	128-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	129-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	130-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	131-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	132-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	133-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	134-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	135-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	136-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	137-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	138-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	139-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	140-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	141-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	142-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	143-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	144-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	145-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	146-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	147-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	148-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	149-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	150-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	151-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	152-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	153-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	154-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	155-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	156-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	157-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	158-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	159-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	160-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	161-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	162-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	163-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	164-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	165-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	166-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	167-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	168-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	169-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	170-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	171-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	172-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	173-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	174-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	175-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	176-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

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

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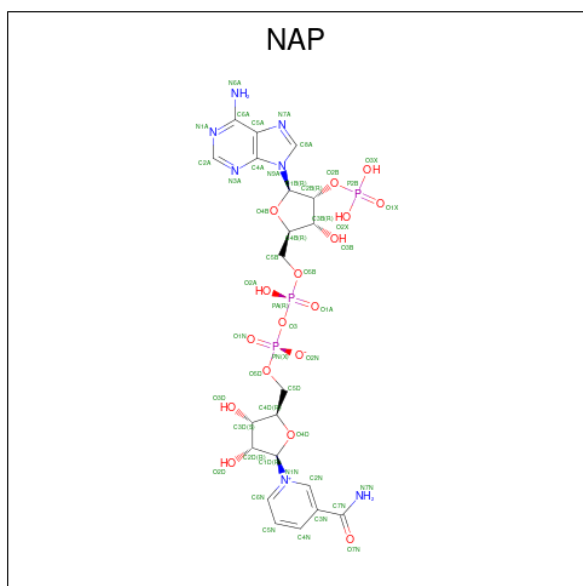
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	219-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	220-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	221-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	222-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	223-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	224-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	225-A	1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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $\text{C}_{21}\text{H}_{28}\text{N}_7\text{O}_{17}\text{P}_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	1-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	2-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	3-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	4-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	5-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	6-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	7-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	8-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	9-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	10-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	11-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	12-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	13-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	14-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	15-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	16-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	17-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	18-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	19-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	20-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	21-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		
3	22-A	1	Total	C	H	N	O	P	0	0
			69	21	21	7	17	3		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	23-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	24-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	25-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	26-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	27-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	28-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	29-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	30-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	31-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	32-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	33-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	34-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	35-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	36-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	37-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	38-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	39-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	40-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	41-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	42-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	43-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	44-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	45-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	46-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	47-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	48-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	49-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	50-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	51-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	52-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	53-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	54-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	55-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	56-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	57-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	58-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	59-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	60-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	61-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	62-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	63-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	64-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	65-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	66-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	67-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	68-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	69-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	70-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	71-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	72-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	73-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	74-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	75-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	76-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	77-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	78-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	79-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	80-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	81-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	82-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	83-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	84-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	85-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	86-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	87-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	88-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	89-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	90-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	91-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	92-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	93-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	94-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	95-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	96-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	97-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	98-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	99-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	100-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	101-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	102-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	103-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	104-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	105-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	106-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	107-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	108-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	109-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	110-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	111-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	112-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	113-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	114-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	115-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	116-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	117-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	118-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	119-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	120-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	121-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	122-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	123-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	124-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	125-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	126-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	127-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	128-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	129-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	130-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	131-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	132-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	133-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	134-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	135-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	136-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	137-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	138-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	139-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	140-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	141-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	142-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	143-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	144-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	145-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	146-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	147-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	148-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	149-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	150-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	151-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	152-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	153-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	154-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	155-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	156-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	157-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	158-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	159-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	160-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	161-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	162-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	163-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	164-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	165-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	166-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	167-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	168-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	169-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	170-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	171-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	172-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	173-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	174-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	175-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	176-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	177-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	178-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	179-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	180-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	181-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	182-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	183-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	184-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	185-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	186-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	187-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	188-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	189-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	190-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	191-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	192-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	193-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	194-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	195-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	196-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	197-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	198-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	199-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	200-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	201-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	202-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	203-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	204-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	205-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	206-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	207-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	208-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	209-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	210-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	211-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	212-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	213-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	214-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	215-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	216-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	217-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	218-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	219-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	220-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	221-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	222-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	223-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	224-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	225-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	226-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	227-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	228-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	229-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	230-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	231-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	232-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	233-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	234-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	235-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	236-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	237-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	238-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	239-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	240-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	241-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	242-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	243-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	244-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	245-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	246-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	247-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	248-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	249-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0
3	250-A	1	Total 69	C 21	H 21	N 7	O 17	P 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	200	Total	O	0	0
			200	200		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	2-A	206	Total 206	O 206	0	0
4	3-A	185	Total 185	O 185	0	0
4	4-A	175	Total 175	O 175	0	0
4	5-A	186	Total 186	O 186	0	0
4	6-A	185	Total 185	O 185	0	0
4	7-A	202	Total 202	O 202	0	0
4	8-A	200	Total 200	O 200	0	0
4	9-A	201	Total 201	O 201	0	0
4	10-A	204	Total 204	O 204	0	0
4	11-A	205	Total 205	O 205	0	0
4	12-A	197	Total 197	O 197	0	0
4	13-A	192	Total 192	O 192	0	0
4	14-A	189	Total 189	O 189	0	0
4	15-A	173	Total 173	O 173	0	0
4	16-A	176	Total 176	O 176	0	0
4	17-A	188	Total 188	O 188	0	0
4	18-A	195	Total 195	O 195	0	0
4	19-A	196	Total 196	O 196	0	0
4	20-A	211	Total 211	O 211	0	0
4	21-A	189	Total 189	O 189	0	0
4	22-A	191	Total 191	O 191	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	23-A	173	Total 173	O 173	0	0
4	24-A	183	Total 183	O 183	0	0
4	25-A	174	Total 174	O 174	0	0
4	26-A	195	Total 195	O 195	0	0
4	27-A	188	Total 188	O 188	0	0
4	28-A	181	Total 181	O 181	0	0
4	29-A	183	Total 183	O 183	0	0
4	30-A	186	Total 186	O 186	0	0
4	31-A	191	Total 191	O 191	0	0
4	32-A	187	Total 187	O 187	0	0
4	33-A	190	Total 190	O 190	0	0
4	34-A	194	Total 194	O 194	0	0
4	35-A	201	Total 201	O 201	0	0
4	36-A	197	Total 197	O 197	0	0
4	37-A	196	Total 196	O 196	0	0
4	38-A	203	Total 203	O 203	0	0
4	39-A	181	Total 181	O 181	0	0
4	40-A	171	Total 171	O 171	0	0
4	41-A	179	Total 179	O 179	0	0
4	42-A	176	Total 176	O 176	0	0
4	43-A	176	Total 176	O 176	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	44-A	183	Total 183	O 183	0	0
4	45-A	187	Total 187	O 187	0	0
4	46-A	197	Total 197	O 197	0	0
4	47-A	191	Total 191	O 191	0	0
4	48-A	184	Total 184	O 184	0	0
4	49-A	195	Total 195	O 195	0	0
4	50-A	189	Total 189	O 189	0	0
4	51-A	198	Total 198	O 198	0	0
4	52-A	190	Total 190	O 190	0	0
4	53-A	182	Total 182	O 182	0	0
4	54-A	180	Total 180	O 180	0	0
4	55-A	185	Total 185	O 185	0	0
4	56-A	184	Total 184	O 184	0	0
4	57-A	191	Total 191	O 191	0	0
4	58-A	187	Total 187	O 187	0	0
4	59-A	192	Total 192	O 192	0	0
4	60-A	173	Total 173	O 173	0	0
4	61-A	186	Total 186	O 186	0	0
4	62-A	201	Total 201	O 201	0	0
4	63-A	201	Total 201	O 201	0	0
4	64-A	188	Total 188	O 188	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	65-A	187	Total 187	O 187	0	0
4	66-A	174	Total 174	O 174	0	0
4	67-A	184	Total 184	O 184	0	0
4	68-A	178	Total 178	O 178	0	0
4	69-A	173	Total 173	O 173	0	0
4	70-A	171	Total 171	O 171	0	0
4	71-A	171	Total 171	O 171	0	0
4	72-A	196	Total 196	O 196	0	0
4	73-A	207	Total 207	O 207	0	0
4	74-A	191	Total 191	O 191	0	0
4	75-A	193	Total 193	O 193	0	0
4	76-A	182	Total 182	O 182	0	0
4	77-A	176	Total 176	O 176	0	0
4	78-A	184	Total 184	O 184	0	0
4	79-A	193	Total 193	O 193	0	0
4	80-A	201	Total 201	O 201	0	0
4	81-A	187	Total 187	O 187	0	0
4	82-A	175	Total 175	O 175	0	0
4	83-A	175	Total 175	O 175	0	0
4	84-A	172	Total 172	O 172	0	0
4	85-A	186	Total 186	O 186	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	86-A	199	Total 199	O 199	0	0
4	87-A	200	Total 200	O 200	0	0
4	88-A	191	Total 191	O 191	0	0
4	89-A	189	Total 189	O 189	0	0
4	90-A	180	Total 180	O 180	0	0
4	91-A	190	Total 190	O 190	0	0
4	92-A	181	Total 181	O 181	0	0
4	93-A	177	Total 177	O 177	0	0
4	94-A	189	Total 189	O 189	0	0
4	95-A	173	Total 173	O 173	0	0
4	96-A	182	Total 182	O 182	0	0
4	97-A	188	Total 188	O 188	0	0
4	98-A	191	Total 191	O 191	0	0
4	99-A	198	Total 198	O 198	0	0
4	100-A	200	Total 200	O 200	0	0
4	101-A	204	Total 204	O 204	0	0
4	102-A	189	Total 189	O 189	0	0
4	103-A	211	Total 211	O 211	0	0
4	104-A	202	Total 202	O 202	0	0
4	105-A	196	Total 196	O 196	0	0
4	106-A	189	Total 189	O 189	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	107-A	179	Total 179	O 179	0	0
4	108-A	185	Total 185	O 185	0	0
4	109-A	186	Total 186	O 186	0	0
4	110-A	186	Total 186	O 186	0	0
4	111-A	181	Total 181	O 181	0	0
4	112-A	175	Total 175	O 175	0	0
4	113-A	183	Total 183	O 183	0	0
4	114-A	189	Total 189	O 189	0	0
4	115-A	183	Total 183	O 183	0	0
4	116-A	194	Total 194	O 194	0	0
4	117-A	190	Total 190	O 190	0	0
4	118-A	194	Total 194	O 194	0	0
4	119-A	194	Total 194	O 194	0	0
4	120-A	204	Total 204	O 204	0	0
4	121-A	191	Total 191	O 191	0	0
4	122-A	192	Total 192	O 192	0	0
4	123-A	195	Total 195	O 195	0	0
4	124-A	186	Total 186	O 186	0	0
4	125-A	185	Total 185	O 185	0	0
4	126-A	178	Total 178	O 178	0	0
4	127-A	185	Total 185	O 185	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	128-A	175	Total 175	O 175	0	0
4	129-A	180	Total 180	O 180	0	0
4	130-A	186	Total 186	O 186	0	0
4	131-A	201	Total 201	O 201	0	0
4	132-A	205	Total 205	O 205	0	0
4	133-A	205	Total 205	O 205	0	0
4	134-A	209	Total 209	O 209	0	0
4	135-A	195	Total 195	O 195	0	0
4	136-A	205	Total 205	O 205	0	0
4	137-A	190	Total 190	O 190	0	0
4	138-A	174	Total 174	O 174	0	0
4	139-A	186	Total 186	O 186	0	0
4	140-A	186	Total 186	O 186	0	0
4	141-A	196	Total 196	O 196	0	0
4	142-A	203	Total 203	O 203	0	0
4	143-A	192	Total 192	O 192	0	0
4	144-A	187	Total 187	O 187	0	0
4	145-A	176	Total 176	O 176	0	0
4	146-A	176	Total 176	O 176	0	0
4	147-A	162	Total 162	O 162	0	0
4	148-A	163	Total 163	O 163	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	149-A	178	Total 178	O 178	0	0
4	150-A	190	Total 190	O 190	0	0
4	151-A	204	Total 204	O 204	0	0
4	152-A	187	Total 187	O 187	0	0
4	153-A	191	Total 191	O 191	0	0
4	154-A	190	Total 190	O 190	0	0
4	155-A	187	Total 187	O 187	0	0
4	156-A	190	Total 190	O 190	0	0
4	157-A	193	Total 193	O 193	0	0
4	158-A	181	Total 181	O 181	0	0
4	159-A	176	Total 176	O 176	0	0
4	160-A	185	Total 185	O 185	0	0
4	161-A	187	Total 187	O 187	0	0
4	162-A	196	Total 196	O 196	0	0
4	163-A	204	Total 204	O 204	0	0
4	164-A	198	Total 198	O 198	0	0
4	165-A	215	Total 215	O 215	0	0
4	166-A	194	Total 194	O 194	0	0
4	167-A	175	Total 175	O 175	0	0
4	168-A	176	Total 176	O 176	0	0
4	169-A	184	Total 184	O 184	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	170-A	190	Total 190	O 190	0	0
4	171-A	187	Total 187	O 187	0	0
4	172-A	187	Total 187	O 187	0	0
4	173-A	191	Total 191	O 191	0	0
4	174-A	199	Total 199	O 199	0	0
4	175-A	196	Total 196	O 196	0	0
4	176-A	194	Total 194	O 194	0	0
4	177-A	203	Total 203	O 203	0	0
4	178-A	188	Total 188	O 188	0	0
4	179-A	175	Total 175	O 175	0	0
4	180-A	169	Total 169	O 169	0	0
4	181-A	192	Total 192	O 192	0	0
4	182-A	187	Total 187	O 187	0	0
4	183-A	185	Total 185	O 185	0	0
4	184-A	179	Total 179	O 179	0	0
4	185-A	197	Total 197	O 197	0	0
4	186-A	187	Total 187	O 187	0	0
4	187-A	191	Total 191	O 191	0	0
4	188-A	203	Total 203	O 203	0	0
4	189-A	209	Total 209	O 209	0	0
4	190-A	197	Total 197	O 197	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	191-A	179	Total 179	O 179	0	0
4	192-A	185	Total 185	O 185	0	0
4	193-A	183	Total 183	O 183	0	0
4	194-A	182	Total 182	O 182	0	0
4	195-A	173	Total 173	O 173	0	0
4	196-A	184	Total 184	O 184	0	0
4	197-A	181	Total 181	O 181	0	0
4	198-A	181	Total 181	O 181	0	0
4	199-A	184	Total 184	O 184	0	0
4	200-A	192	Total 192	O 192	0	0
4	201-A	207	Total 207	O 207	0	0
4	202-A	194	Total 194	O 194	0	0
4	203-A	184	Total 184	O 184	0	0
4	204-A	182	Total 182	O 182	0	0
4	205-A	193	Total 193	O 193	0	0
4	206-A	190	Total 190	O 190	0	0
4	207-A	180	Total 180	O 180	0	0
4	208-A	178	Total 178	O 178	0	0
4	209-A	185	Total 185	O 185	0	0
4	210-A	184	Total 184	O 184	0	0
4	211-A	184	Total 184	O 184	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	212-A	191	Total 191	O 191	0	0
4	213-A	202	Total 202	O 202	0	0
4	214-A	190	Total 190	O 190	0	0
4	215-A	193	Total 193	O 193	0	0
4	216-A	195	Total 195	O 195	0	0
4	217-A	197	Total 197	O 197	0	0
4	218-A	197	Total 197	O 197	0	0
4	219-A	192	Total 192	O 192	0	0
4	220-A	177	Total 177	O 177	0	0
4	221-A	183	Total 183	O 183	0	0
4	222-A	182	Total 182	O 182	0	0
4	223-A	181	Total 181	O 181	0	0
4	224-A	203	Total 203	O 203	0	0
4	225-A	205	Total 205	O 205	0	0
4	226-A	202	Total 202	O 202	0	0
4	227-A	189	Total 189	O 189	0	0
4	228-A	162	Total 162	O 162	0	0
4	229-A	180	Total 180	O 180	0	0
4	230-A	174	Total 174	O 174	0	0
4	231-A	206	Total 206	O 206	0	0
4	232-A	211	Total 211	O 211	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	233-A	195	Total 195	O 195	0	0
4	234-A	184	Total 184	O 184	0	0
4	235-A	167	Total 167	O 167	0	0
4	236-A	172	Total 172	O 172	0	0
4	237-A	184	Total 184	O 184	0	0
4	238-A	198	Total 198	O 198	0	0
4	239-A	194	Total 194	O 194	0	0
4	240-A	206	Total 206	O 206	0	0
4	241-A	208	Total 208	O 208	0	0
4	242-A	179	Total 179	O 179	0	0
4	243-A	184	Total 184	O 184	0	0
4	244-A	181	Total 181	O 181	0	0
4	245-A	178	Total 178	O 178	0	0
4	246-A	197	Total 197	O 197	0	0
4	247-A	186	Total 186	O 186	0	0
4	248-A	182	Total 182	O 182	0	0
4	249-A	195	Total 195	O 195	0	0
4	250-A	202	Total 202	O 202	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	34.04Å 44.82Å 98.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.77 – 1.15 40.77 – 1.15	Depositor EDS
% Data completeness (in resolution range)	94.4 (40.77-1.15) 92.9 (40.77-1.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.99 (at 1.15Å)	Xtrriage
Refinement program	PHENIX (phenix.ensemble_refinement: 1.8.4_1496)	Depositor
R, R_{free}	0.109 , 0.136 (Not available) , 0.341	Depositor DCC
R_{free} test set	2598 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	6.9	Xtrriage
Anisotropy	0.279	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.00 , 19.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	699653	wwPDB-VP
Average B, all atoms (Å ²)	5.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

4.2 Too-close contacts [i](#)

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

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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

4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

500 ligands 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
2	FOL	187-A	201	-	34,34,34	1.29	2 (5%)	43,47,47	1.50	7 (16%)
3	NAP	17-A	202	-	50,52,52	1.90	9 (18%)	71,80,80	1.69	13 (18%)
2	FOL	24-A	201	-	34,34,34	1.05	1 (2%)	43,47,47	1.35	6 (13%)
2	FOL	119-A	201	-	34,34,34	1.22	3 (8%)	43,47,47	1.21	5 (11%)
2	FOL	180-A	201	-	34,34,34	1.37	4 (11%)	43,47,47	1.90	12 (27%)
2	FOL	222-A	201	-	34,34,34	1.46	5 (14%)	43,47,47	2.83	15 (34%)
3	NAP	122-A	202	-	50,52,52	1.80	9 (18%)	71,80,80	1.58	11 (15%)
2	FOL	247-A	201	-	34,34,34	0.96	0	43,47,47	1.53	10 (23%)
3	NAP	29-A	202	-	50,52,52	1.91	7 (14%)	71,80,80	2.04	16 (22%)
3	NAP	218-A	202	-	50,52,52	1.71	8 (16%)	71,80,80	1.67	11 (15%)
3	NAP	43-A	202	-	50,52,52	1.73	10 (20%)	71,80,80	1.68	13 (18%)
3	NAP	159-A	202	-	50,52,52	2.11	10 (20%)	71,80,80	2.96	21 (29%)
2	FOL	189-A	201	-	34,34,34	1.20	2 (5%)	43,47,47	1.37	6 (13%)
3	NAP	181-A	202	-	50,52,52	1.76	10 (20%)	71,80,80	1.68	14 (19%)
2	FOL	185-A	201	-	34,34,34	1.13	1 (2%)	43,47,47	1.61	6 (13%)
2	FOL	117-A	201	-	34,34,34	1.06	0	43,47,47	1.56	8 (18%)
3	NAP	10-A	202	-	50,52,52	1.76	11 (22%)	71,80,80	1.64	15 (21%)
2	FOL	90-A	201	-	34,34,34	1.01	2 (5%)	43,47,47	1.46	8 (18%)
2	FOL	244-A	201	-	34,34,34	1.01	1 (2%)	43,47,47	1.55	6 (13%)
3	NAP	229-A	202	-	50,52,52	1.72	9 (18%)	71,80,80	1.64	13 (18%)
2	FOL	83-A	201	-	34,34,34	1.34	3 (8%)	43,47,47	1.63	10 (23%)
2	FOL	78-A	201	-	34,34,34	1.15	2 (5%)	43,47,47	1.61	9 (20%)
2	FOL	177-A	201	-	34,34,34	1.35	3 (8%)	43,47,47	2.27	12 (27%)
3	NAP	234-A	202	-	50,52,52	1.77	10 (20%)	71,80,80	1.59	16 (22%)
3	NAP	169-A	202	-	50,52,52	1.73	11 (22%)	71,80,80	1.78	15 (21%)
3	NAP	23-A	202	-	50,52,52	1.75	8 (16%)	71,80,80	1.50	11 (15%)
3	NAP	125-A	202	-	50,52,52	1.72	8 (16%)	71,80,80	1.60	9 (12%)
2	FOL	139-A	201	-	34,34,34	1.09	2 (5%)	43,47,47	1.59	11 (25%)
2	FOL	68-A	201	-	34,34,34	1.07	1 (2%)	43,47,47	1.77	3 (6%)
3	NAP	87-A	202	-	50,52,52	1.71	8 (16%)	71,80,80	1.71	12 (16%)
2	FOL	36-A	201	-	34,34,34	0.95	0	43,47,47	1.48	8 (18%)
3	NAP	197-A	202	-	50,52,52	1.74	8 (16%)	71,80,80	1.57	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	103-A	201	-	34,34,34	1.07	2 (5%)	43,47,47	2.06	14 (32%)
2	FOL	129-A	201	-	34,34,34	1.02	2 (5%)	43,47,47	1.47	6 (13%)
3	NAP	115-A	202	-	50,52,52	1.82	13 (26%)	71,80,80	1.75	15 (21%)
2	FOL	162-A	201	-	34,34,34	0.92	1 (2%)	43,47,47	1.27	4 (9%)
2	FOL	94-A	201	-	34,34,34	1.19	2 (5%)	43,47,47	1.37	8 (18%)
2	FOL	147-A	201	-	34,34,34	1.19	4 (11%)	43,47,47	1.63	9 (20%)
3	NAP	138-A	202	-	50,52,52	1.73	10 (20%)	71,80,80	1.64	12 (16%)
3	NAP	200-A	202	-	50,52,52	1.73	9 (18%)	71,80,80	1.68	13 (18%)
2	FOL	204-A	201	-	34,34,34	1.12	3 (8%)	43,47,47	1.49	6 (13%)
3	NAP	103-A	202	-	50,52,52	1.91	9 (18%)	71,80,80	1.63	8 (11%)
2	FOL	61-A	201	-	34,34,34	1.20	2 (5%)	43,47,47	2.04	14 (32%)
3	NAP	71-A	202	-	50,52,52	1.73	8 (16%)	71,80,80	1.72	14 (19%)
2	FOL	80-A	201	-	34,34,34	1.05	2 (5%)	43,47,47	1.71	7 (16%)
2	FOL	114-A	201	-	34,34,34	1.10	3 (8%)	43,47,47	1.32	6 (13%)
3	NAP	183-A	202	-	50,52,52	1.70	9 (18%)	71,80,80	1.57	11 (15%)
2	FOL	99-A	201	-	34,34,34	1.08	1 (2%)	43,47,47	1.69	9 (20%)
3	NAP	220-A	202	-	50,52,52	1.68	7 (14%)	71,80,80	1.65	13 (18%)
2	FOL	93-A	201	-	34,34,34	1.18	3 (8%)	43,47,47	1.50	6 (13%)
2	FOL	47-A	201	-	34,34,34	1.04	2 (5%)	43,47,47	1.55	8 (18%)
3	NAP	16-A	202	-	50,52,52	1.74	8 (16%)	71,80,80	1.58	12 (16%)
3	NAP	38-A	202	-	50,52,52	1.70	9 (18%)	71,80,80	1.67	13 (18%)
2	FOL	23-A	201	-	34,34,34	1.41	5 (14%)	43,47,47	1.68	11 (25%)
3	NAP	177-A	202	-	50,52,52	1.73	8 (16%)	71,80,80	1.60	13 (18%)
2	FOL	115-A	201	-	34,34,34	1.06	0	43,47,47	1.58	7 (16%)
2	FOL	246-A	201	-	34,34,34	0.88	0	43,47,47	1.33	5 (11%)
3	NAP	57-A	202	-	50,52,52	1.71	8 (16%)	71,80,80	1.66	14 (19%)
2	FOL	96-A	201	-	34,34,34	1.05	2 (5%)	43,47,47	1.35	5 (11%)
2	FOL	104-A	201	-	34,34,34	1.05	2 (5%)	43,47,47	1.63	10 (23%)
2	FOL	46-A	201	-	34,34,34	1.08	0	43,47,47	1.46	6 (13%)
2	FOL	208-A	201	-	34,34,34	1.25	2 (5%)	43,47,47	2.34	10 (23%)
2	FOL	135-A	201	-	34,34,34	1.33	3 (8%)	43,47,47	1.31	4 (9%)
2	FOL	43-A	201	-	34,34,34	1.00	1 (2%)	43,47,47	1.36	6 (13%)
2	FOL	223-A	201	-	34,34,34	1.43	4 (11%)	43,47,47	2.07	8 (18%)
2	FOL	203-A	201	-	34,34,34	1.13	1 (2%)	43,47,47	1.66	12 (27%)
3	NAP	152-A	202	-	50,52,52	1.79	11 (22%)	71,80,80	1.57	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	62-A	201	-	34,34,34	1.21	1 (2%)	43,47,47	1.81	7 (16%)
3	NAP	173-A	202	-	50,52,52	1.70	9 (18%)	71,80,80	1.60	12 (16%)
3	NAP	90-A	202	-	50,52,52	1.73	11 (22%)	71,80,80	1.63	15 (21%)
2	FOL	228-A	201	-	34,34,34	1.13	3 (8%)	43,47,47	1.60	5 (11%)
3	NAP	139-A	202	-	50,52,52	1.73	9 (18%)	71,80,80	1.56	10 (14%)
3	NAP	249-A	202	-	50,52,52	1.74	11 (22%)	71,80,80	1.69	15 (21%)
3	NAP	207-A	202	-	50,52,52	1.76	9 (18%)	71,80,80	1.60	12 (16%)
2	FOL	55-A	201	-	34,34,34	0.96	1 (2%)	43,47,47	1.74	12 (27%)
3	NAP	9-A	202	-	50,52,52	1.77	9 (18%)	71,80,80	1.61	13 (18%)
2	FOL	179-A	201	-	34,34,34	1.16	2 (5%)	43,47,47	1.62	8 (18%)
2	FOL	13-A	201	-	34,34,34	1.09	2 (5%)	43,47,47	1.33	5 (11%)
3	NAP	157-A	202	-	50,52,52	1.79	9 (18%)	71,80,80	1.63	13 (18%)
3	NAP	108-A	202	-	50,52,52	1.81	11 (22%)	71,80,80	1.79	16 (22%)
3	NAP	65-A	202	-	50,52,52	1.81	11 (22%)	71,80,80	1.66	11 (15%)
3	NAP	192-A	202	-	50,52,52	1.89	7 (14%)	71,80,80	1.90	15 (21%)
2	FOL	238-A	201	-	34,34,34	1.14	3 (8%)	43,47,47	1.63	8 (18%)
2	FOL	116-A	201	-	34,34,34	1.08	1 (2%)	43,47,47	1.32	6 (13%)
3	NAP	239-A	202	-	50,52,52	2.00	9 (18%)	71,80,80	2.13	13 (18%)
3	NAP	130-A	202	-	50,52,52	1.72	9 (18%)	71,80,80	1.60	12 (16%)
3	NAP	93-A	202	-	50,52,52	1.73	8 (16%)	71,80,80	1.69	16 (22%)
2	FOL	126-A	201	-	34,34,34	1.10	2 (5%)	43,47,47	1.87	10 (23%)
3	NAP	180-A	202	-	50,52,52	1.78	9 (18%)	71,80,80	1.50	10 (14%)
3	NAP	222-A	202	-	50,52,52	1.80	9 (18%)	71,80,80	1.81	13 (18%)
3	NAP	48-A	202	-	50,52,52	1.76	10 (20%)	71,80,80	1.62	13 (18%)
2	FOL	26-A	201	-	34,34,34	0.89	1 (2%)	43,47,47	1.45	6 (13%)
2	FOL	14-A	201	-	34,34,34	0.99	1 (2%)	43,47,47	1.72	7 (16%)
2	FOL	181-A	201	-	34,34,34	1.13	2 (5%)	43,47,47	1.61	7 (16%)
3	NAP	156-A	202	-	50,52,52	1.76	9 (18%)	71,80,80	1.58	10 (14%)
2	FOL	58-A	201	-	34,34,34	1.22	2 (5%)	43,47,47	1.29	6 (13%)
2	FOL	10-A	201	-	34,34,34	1.05	3 (8%)	43,47,47	1.59	8 (18%)
3	NAP	140-A	202	-	50,52,52	1.75	9 (18%)	71,80,80	1.69	14 (19%)
2	FOL	27-A	201	-	34,34,34	0.94	0	43,47,47	1.49	6 (13%)
3	NAP	133-A	202	-	50,52,52	1.78	10 (20%)	71,80,80	1.90	18 (25%)
2	FOL	217-A	201	-	34,34,34	1.31	2 (5%)	43,47,47	2.58	21 (48%)
3	NAP	117-A	202	-	50,52,52	1.81	10 (20%)	71,80,80	1.67	14 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	72-A	201	-	34,34,34	1.20	2 (5%)	43,47,47	1.38	5 (11%)
2	FOL	151-A	201	-	34,34,34	1.01	1 (2%)	43,47,47	1.60	7 (16%)
3	NAP	147-A	202	-	50,52,52	1.76	8 (16%)	71,80,80	1.57	14 (19%)
3	NAP	242-A	202	-	50,52,52	2.19	12 (24%)	71,80,80	3.53	20 (28%)
2	FOL	97-A	201	-	34,34,34	0.98	1 (2%)	43,47,47	1.16	4 (9%)
2	FOL	233-A	201	-	34,34,34	1.21	2 (5%)	43,47,47	1.61	8 (18%)
3	NAP	244-A	202	-	50,52,52	1.71	10 (20%)	71,80,80	2.36	18 (25%)
3	NAP	196-A	202	-	50,52,52	1.70	8 (16%)	71,80,80	1.63	12 (16%)
2	FOL	86-A	201	-	34,34,34	1.03	3 (8%)	43,47,47	1.42	8 (18%)
3	NAP	203-A	202	-	50,52,52	1.71	9 (18%)	71,80,80	1.53	10 (14%)
2	FOL	236-A	201	-	34,34,34	1.25	2 (5%)	43,47,47	1.42	7 (16%)
2	FOL	2-A	201	-	34,34,34	1.17	2 (5%)	43,47,47	1.42	10 (23%)
2	FOL	167-A	201	-	34,34,34	1.09	2 (5%)	43,47,47	1.48	7 (16%)
2	FOL	178-A	201	-	34,34,34	1.09	2 (5%)	43,47,47	1.30	6 (13%)
3	NAP	77-A	202	-	50,52,52	1.76	7 (14%)	71,80,80	1.69	12 (16%)
2	FOL	12-A	201	-	34,34,34	1.28	3 (8%)	43,47,47	1.81	7 (16%)
3	NAP	208-A	202	-	50,52,52	1.81	10 (20%)	71,80,80	1.68	13 (18%)
3	NAP	166-A	202	-	50,52,52	1.73	8 (16%)	71,80,80	1.66	11 (15%)
3	NAP	111-A	202	-	50,52,52	1.77	10 (20%)	71,80,80	1.71	17 (23%)
3	NAP	104-A	202	-	50,52,52	1.75	9 (18%)	71,80,80	1.67	12 (16%)
2	FOL	75-A	201	-	34,34,34	1.13	2 (5%)	43,47,47	1.45	6 (13%)
3	NAP	202-A	202	-	50,52,52	1.71	11 (22%)	71,80,80	1.71	14 (19%)
2	FOL	211-A	201	-	34,34,34	1.16	1 (2%)	43,47,47	1.47	8 (18%)
3	NAP	178-A	202	-	50,52,52	1.93	8 (16%)	71,80,80	1.69	10 (14%)
3	NAP	198-A	202	-	50,52,52	1.74	10 (20%)	71,80,80	1.66	13 (18%)
2	FOL	142-A	201	-	34,34,34	1.23	3 (8%)	43,47,47	1.39	7 (16%)
2	FOL	191-A	201	-	34,34,34	1.13	1 (2%)	43,47,47	1.62	8 (18%)
2	FOL	163-A	201	-	34,34,34	1.08	1 (2%)	43,47,47	1.41	7 (16%)
2	FOL	196-A	201	-	34,34,34	1.38	4 (11%)	43,47,47	1.42	3 (6%)
3	NAP	20-A	202	-	50,52,52	1.71	7 (14%)	71,80,80	1.68	12 (16%)
2	FOL	39-A	201	-	34,34,34	1.26	4 (11%)	43,47,47	1.96	10 (23%)
2	FOL	85-A	201	-	34,34,34	1.20	1 (2%)	43,47,47	1.50	7 (16%)
2	FOL	206-A	201	-	34,34,34	1.26	2 (5%)	43,47,47	1.61	8 (18%)
2	FOL	224-A	201	-	34,34,34	1.58	5 (14%)	43,47,47	1.51	6 (13%)
2	FOL	249-A	201	-	34,34,34	1.15	3 (8%)	43,47,47	1.56	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	44-A	202	-	50,52,52	1.67	8 (16%)	71,80,80	1.64	13 (18%)
2	FOL	241-A	201	-	34,34,34	0.92	0	43,47,47	1.87	11 (25%)
3	NAP	189-A	202	-	50,52,52	1.69	9 (18%)	71,80,80	1.60	12 (16%)
2	FOL	101-A	201	-	34,34,34	1.09	1 (2%)	43,47,47	1.24	4 (9%)
3	NAP	37-A	202	-	50,52,52	1.74	9 (18%)	71,80,80	1.67	15 (21%)
3	NAP	199-A	202	-	50,52,52	1.71	8 (16%)	71,80,80	1.57	14 (19%)
2	FOL	1-A	201	-	34,34,34	0.94	0	43,47,47	1.51	9 (20%)
2	FOL	35-A	201	-	34,34,34	1.27	3 (8%)	43,47,47	2.59	12 (27%)
2	FOL	19-A	201	-	34,34,34	1.26	3 (8%)	43,47,47	2.03	11 (25%)
3	NAP	185-A	202	-	50,52,52	1.75	9 (18%)	71,80,80	1.61	12 (16%)
2	FOL	184-A	201	-	34,34,34	1.29	4 (11%)	43,47,47	1.78	7 (16%)
2	FOL	197-A	201	-	34,34,34	1.37	3 (8%)	43,47,47	1.14	3 (6%)
3	NAP	88-A	202	-	50,52,52	1.71	8 (16%)	71,80,80	1.57	13 (18%)
3	NAP	187-A	202	-	50,52,52	1.70	8 (16%)	71,80,80	1.64	11 (15%)
2	FOL	226-A	201	-	34,34,34	1.06	3 (8%)	43,47,47	1.18	6 (13%)
2	FOL	159-A	201	-	34,34,34	1.17	3 (8%)	43,47,47	1.33	4 (9%)
3	NAP	83-A	202	-	50,52,52	1.71	8 (16%)	71,80,80	1.58	12 (16%)
2	FOL	41-A	201	-	34,34,34	1.04	1 (2%)	43,47,47	1.44	8 (18%)
2	FOL	190-A	201	-	34,34,34	1.25	3 (8%)	43,47,47	1.48	9 (20%)
2	FOL	102-A	201	-	34,34,34	1.07	1 (2%)	43,47,47	1.35	6 (13%)
2	FOL	48-A	201	-	34,34,34	0.95	1 (2%)	43,47,47	1.40	6 (13%)
3	NAP	241-A	202	-	50,52,52	1.67	8 (16%)	71,80,80	1.64	13 (18%)
3	NAP	160-A	202	-	50,52,52	1.68	8 (16%)	71,80,80	2.84	19 (26%)
3	NAP	42-A	202	-	50,52,52	1.74	9 (18%)	71,80,80	1.51	13 (18%)
2	FOL	53-A	201	-	34,34,34	1.03	2 (5%)	43,47,47	1.57	9 (20%)
2	FOL	81-A	201	-	34,34,34	1.05	1 (2%)	43,47,47	1.34	6 (13%)
3	NAP	58-A	202	-	50,52,52	1.72	9 (18%)	71,80,80	1.72	16 (22%)
3	NAP	128-A	202	-	50,52,52	1.75	11 (22%)	71,80,80	1.54	12 (16%)
2	FOL	7-A	201	-	34,34,34	1.12	3 (8%)	43,47,47	1.29	4 (9%)
2	FOL	193-A	201	-	34,34,34	1.32	3 (8%)	43,47,47	2.14	12 (27%)
3	NAP	219-A	202	-	50,52,52	1.72	9 (18%)	71,80,80	1.58	14 (19%)
2	FOL	106-A	201	-	34,34,34	1.26	2 (5%)	43,47,47	1.83	11 (25%)
3	NAP	113-A	202	-	50,52,52	1.70	11 (22%)	71,80,80	1.66	14 (19%)
2	FOL	133-A	201	-	34,34,34	1.17	4 (11%)	43,47,47	1.59	8 (18%)
2	FOL	121-A	201	-	34,34,34	1.06	2 (5%)	43,47,47	1.15	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	77-A	201	-	34,34,34	1.18	2 (5%)	43,47,47	1.75	11 (25%)
2	FOL	175-A	201	-	34,34,34	1.35	2 (5%)	43,47,47	1.68	8 (18%)
3	NAP	4-A	202	-	50,52,52	1.81	11 (22%)	71,80,80	3.23	15 (21%)
3	NAP	86-A	202	-	50,52,52	1.72	10 (20%)	71,80,80	1.57	13 (18%)
3	NAP	211-A	202	-	50,52,52	1.75	8 (16%)	71,80,80	1.60	12 (16%)
3	NAP	55-A	202	-	50,52,52	2.00	11 (22%)	71,80,80	1.80	14 (19%)
3	NAP	236-A	202	-	50,52,52	1.84	9 (18%)	71,80,80	1.74	11 (15%)
2	FOL	176-A	201	-	34,34,34	1.48	5 (14%)	43,47,47	2.09	10 (23%)
3	NAP	13-A	202	-	50,52,52	1.71	7 (14%)	71,80,80	1.58	12 (16%)
3	NAP	50-A	202	-	50,52,52	1.76	8 (16%)	71,80,80	1.66	15 (21%)
3	NAP	179-A	202	-	50,52,52	2.07	8 (16%)	71,80,80	1.77	15 (21%)
2	FOL	108-A	201	-	34,34,34	1.26	2 (5%)	43,47,47	1.45	7 (16%)
3	NAP	63-A	202	-	50,52,52	2.32	10 (20%)	71,80,80	1.85	13 (18%)
3	NAP	123-A	202	-	50,52,52	1.79	9 (18%)	71,80,80	1.64	12 (16%)
3	NAP	193-A	202	-	50,52,52	1.78	10 (20%)	71,80,80	1.70	15 (21%)
2	FOL	110-A	201	-	34,34,34	1.09	1 (2%)	43,47,47	1.54	8 (18%)
3	NAP	107-A	202	-	50,52,52	1.72	9 (18%)	71,80,80	1.74	13 (18%)
3	NAP	132-A	202	-	50,52,52	2.84	9 (18%)	71,80,80	1.90	17 (23%)
3	NAP	191-A	202	-	50,52,52	2.74	10 (20%)	71,80,80	1.91	15 (21%)
2	FOL	161-A	201	-	34,34,34	0.99	1 (2%)	43,47,47	1.17	4 (9%)
3	NAP	21-A	202	-	50,52,52	1.72	7 (14%)	71,80,80	1.58	12 (16%)
2	FOL	113-A	201	-	34,34,34	1.24	3 (8%)	43,47,47	1.78	11 (25%)
3	NAP	149-A	202	-	50,52,52	1.78	11 (22%)	71,80,80	1.61	11 (15%)
3	NAP	170-A	202	-	50,52,52	1.75	11 (22%)	71,80,80	1.57	13 (18%)
3	NAP	39-A	202	-	50,52,52	1.69	8 (16%)	71,80,80	1.61	11 (15%)
2	FOL	20-A	201	-	34,34,34	0.93	1 (2%)	43,47,47	1.61	8 (18%)
3	NAP	59-A	202	-	50,52,52	1.82	12 (24%)	71,80,80	1.72	14 (19%)
3	NAP	85-A	202	-	50,52,52	1.67	9 (18%)	71,80,80	1.83	11 (15%)
3	NAP	206-A	202	-	50,52,52	1.74	9 (18%)	71,80,80	1.59	12 (16%)
2	FOL	67-A	201	-	34,34,34	1.09	1 (2%)	43,47,47	1.22	6 (13%)
3	NAP	224-A	202	-	50,52,52	1.72	9 (18%)	71,80,80	1.52	12 (16%)
3	NAP	100-A	202	-	50,52,52	1.72	9 (18%)	71,80,80	1.67	12 (16%)
3	NAP	92-A	202	-	50,52,52	1.73	10 (20%)	71,80,80	1.61	13 (18%)
2	FOL	174-A	201	-	34,34,34	1.11	1 (2%)	43,47,47	1.67	11 (25%)
3	NAP	2-A	202	-	50,52,52	1.96	8 (16%)	71,80,80	3.03	15 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	37-A	201	-	34,34,34	1.32	7 (20%)	43,47,47	1.92	9 (20%)
2	FOL	218-A	201	-	34,34,34	1.28	3 (8%)	43,47,47	2.16	11 (25%)
2	FOL	16-A	201	-	34,34,34	1.13	2 (5%)	43,47,47	2.24	13 (30%)
2	FOL	64-A	201	-	34,34,34	1.17	3 (8%)	43,47,47	2.03	13 (30%)
3	NAP	62-A	202	-	50,52,52	1.93	8 (16%)	71,80,80	2.03	14 (19%)
3	NAP	81-A	202	-	50,52,52	1.75	9 (18%)	71,80,80	1.62	13 (18%)
3	NAP	80-A	202	-	50,52,52	1.75	9 (18%)	71,80,80	1.69	13 (18%)
2	FOL	118-A	201	-	34,34,34	0.99	0	43,47,47	1.51	7 (16%)
3	NAP	167-A	202	-	50,52,52	1.72	8 (16%)	71,80,80	1.74	14 (19%)
2	FOL	88-A	201	-	34,34,34	1.27	2 (5%)	43,47,47	1.58	9 (20%)
3	NAP	226-A	202	-	50,52,52	1.76	10 (20%)	71,80,80	1.52	11 (15%)
2	FOL	18-A	201	-	34,34,34	1.18	3 (8%)	43,47,47	2.30	12 (27%)
3	NAP	190-A	202	-	50,52,52	1.71	7 (14%)	71,80,80	1.63	10 (14%)
2	FOL	173-A	201	-	34,34,34	1.06	1 (2%)	43,47,47	1.36	7 (16%)
2	FOL	229-A	201	-	34,34,34	1.30	5 (14%)	43,47,47	2.20	13 (30%)
3	NAP	41-A	202	-	50,52,52	1.72	9 (18%)	71,80,80	1.79	15 (21%)
2	FOL	160-A	201	-	34,34,34	1.02	2 (5%)	43,47,47	1.33	6 (13%)
2	FOL	92-A	201	-	34,34,34	1.02	2 (5%)	43,47,47	1.49	6 (13%)
3	NAP	171-A	202	-	50,52,52	1.71	7 (14%)	71,80,80	1.58	14 (19%)
3	NAP	18-A	202	-	50,52,52	2.04	9 (18%)	71,80,80	1.89	16 (22%)
2	FOL	216-A	201	-	34,34,34	1.05	2 (5%)	43,47,47	1.58	9 (20%)
2	FOL	232-A	201	-	34,34,34	1.34	3 (8%)	43,47,47	1.53	7 (16%)
3	NAP	121-A	202	-	50,52,52	1.85	9 (18%)	71,80,80	1.62	11 (15%)
2	FOL	22-A	201	-	34,34,34	1.17	2 (5%)	43,47,47	1.30	5 (11%)
3	NAP	106-A	202	-	50,52,52	1.70	9 (18%)	71,80,80	1.65	15 (21%)
2	FOL	152-A	201	-	34,34,34	0.99	0	43,47,47	1.43	5 (11%)
2	FOL	33-A	201	-	34,34,34	1.05	1 (2%)	43,47,47	1.62	7 (16%)
2	FOL	182-A	201	-	34,34,34	0.97	1 (2%)	43,47,47	1.32	3 (6%)
2	FOL	4-A	201	-	34,34,34	1.05	2 (5%)	43,47,47	1.39	7 (16%)
2	FOL	11-A	201	-	34,34,34	1.19	2 (5%)	43,47,47	1.60	7 (16%)
3	NAP	14-A	202	-	50,52,52	1.76	13 (26%)	71,80,80	1.64	12 (16%)
3	NAP	119-A	202	-	50,52,52	2.03	11 (22%)	71,80,80	1.90	14 (19%)
2	FOL	65-A	201	-	34,34,34	1.22	2 (5%)	43,47,47	1.85	14 (32%)
2	FOL	214-A	201	-	34,34,34	1.27	2 (5%)	43,47,47	1.42	7 (16%)
2	FOL	200-A	201	-	34,34,34	0.96	2 (5%)	43,47,47	1.87	7 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	63-A	201	-	34,34,34	1.00	1 (2%)	43,47,47	1.46	6 (13%)
2	FOL	245-A	201	-	34,34,34	1.03	2 (5%)	43,47,47	1.76	10 (23%)
3	NAP	8-A	202	-	50,52,52	1.79	8 (16%)	71,80,80	1.66	13 (18%)
2	FOL	144-A	201	-	34,34,34	1.23	3 (8%)	43,47,47	2.06	16 (37%)
3	NAP	233-A	202	-	50,52,52	1.80	10 (20%)	71,80,80	1.64	12 (16%)
2	FOL	168-A	201	-	34,34,34	1.12	2 (5%)	43,47,47	1.30	6 (13%)
3	NAP	60-A	202	-	50,52,52	1.80	10 (20%)	71,80,80	1.64	10 (14%)
2	FOL	109-A	201	-	34,34,34	1.33	3 (8%)	43,47,47	1.83	6 (13%)
2	FOL	199-A	201	-	34,34,34	1.34	4 (11%)	43,47,47	2.00	9 (20%)
3	NAP	15-A	202	-	50,52,52	1.72	8 (16%)	71,80,80	1.59	12 (16%)
3	NAP	78-A	202	-	50,52,52	1.72	7 (14%)	71,80,80	1.60	14 (19%)
3	NAP	102-A	202	-	50,52,52	1.68	8 (16%)	71,80,80	1.67	12 (16%)
2	FOL	183-A	201	-	34,34,34	1.22	3 (8%)	43,47,47	1.29	5 (11%)
2	FOL	70-A	201	-	34,34,34	1.09	2 (5%)	43,47,47	1.50	6 (13%)
3	NAP	175-A	202	-	50,52,52	1.71	10 (20%)	71,80,80	1.64	11 (15%)
3	NAP	7-A	202	-	50,52,52	1.77	11 (22%)	71,80,80	1.55	13 (18%)
3	NAP	124-A	202	-	50,52,52	1.77	8 (16%)	71,80,80	1.56	10 (14%)
2	FOL	198-A	201	-	34,34,34	1.29	3 (8%)	43,47,47	1.41	5 (11%)
2	FOL	240-A	201	-	34,34,34	1.15	2 (5%)	43,47,47	1.26	6 (13%)
3	NAP	64-A	202	-	50,52,52	1.80	10 (20%)	71,80,80	1.63	11 (15%)
2	FOL	45-A	201	-	34,34,34	0.97	2 (5%)	43,47,47	1.63	7 (16%)
2	FOL	207-A	201	-	34,34,34	1.18	3 (8%)	43,47,47	1.76	13 (30%)
3	NAP	165-A	202	-	50,52,52	1.74	10 (20%)	71,80,80	3.24	16 (22%)
2	FOL	60-A	201	-	34,34,34	1.13	2 (5%)	43,47,47	1.41	7 (16%)
2	FOL	131-A	201	-	34,34,34	1.06	2 (5%)	43,47,47	1.61	8 (18%)
3	NAP	40-A	202	-	50,52,52	1.73	10 (20%)	71,80,80	1.72	14 (19%)
3	NAP	134-A	202	-	50,52,52	1.73	8 (16%)	71,80,80	1.56	11 (15%)
2	FOL	219-A	201	-	34,34,34	1.44	3 (8%)	43,47,47	2.72	15 (34%)
3	NAP	105-A	202	-	50,52,52	1.76	10 (20%)	71,80,80	1.73	17 (23%)
3	NAP	68-A	202	-	50,52,52	1.72	10 (20%)	71,80,80	1.73	15 (21%)
2	FOL	15-A	201	-	34,34,34	1.01	2 (5%)	43,47,47	1.73	5 (11%)
2	FOL	130-A	201	-	34,34,34	1.16	2 (5%)	43,47,47	1.71	9 (20%)
3	NAP	162-A	202	-	50,52,52	1.84	8 (16%)	71,80,80	2.59	15 (21%)
3	NAP	22-A	202	-	50,52,52	1.71	7 (14%)	71,80,80	1.63	12 (16%)
3	NAP	51-A	202	-	50,52,52	1.78	11 (22%)	71,80,80	1.84	14 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	250-A	201	-	34,34,34	1.30	2 (5%)	43,47,47	1.70	10 (23%)
3	NAP	204-A	202	-	50,52,52	1.73	8 (16%)	71,80,80	1.60	12 (16%)
2	FOL	54-A	201	-	34,34,34	1.28	2 (5%)	43,47,47	1.31	8 (18%)
3	NAP	19-A	202	-	50,52,52	1.67	9 (18%)	71,80,80	1.66	13 (18%)
3	NAP	216-A	202	-	50,52,52	1.73	9 (18%)	71,80,80	1.70	14 (19%)
2	FOL	107-A	201	-	34,34,34	1.13	2 (5%)	43,47,47	1.45	6 (13%)
2	FOL	212-A	201	-	34,34,34	1.01	0	43,47,47	1.59	5 (11%)
2	FOL	239-A	201	-	34,34,34	1.15	2 (5%)	43,47,47	1.90	7 (16%)
3	NAP	61-A	202	-	50,52,52	1.86	10 (20%)	71,80,80	1.56	8 (11%)
3	NAP	174-A	202	-	50,52,52	1.70	9 (18%)	71,80,80	1.70	14 (19%)
2	FOL	49-A	201	-	34,34,34	1.19	2 (5%)	43,47,47	1.74	7 (16%)
3	NAP	232-A	202	-	50,52,52	1.75	10 (20%)	71,80,80	1.59	14 (19%)
3	NAP	74-A	202	-	50,52,52	2.09	9 (18%)	71,80,80	1.85	16 (22%)
2	FOL	91-A	201	-	34,34,34	1.33	3 (8%)	43,47,47	1.43	8 (18%)
2	FOL	105-A	201	-	34,34,34	1.14	2 (5%)	43,47,47	1.51	8 (18%)
3	NAP	11-A	202	-	50,52,52	1.73	8 (16%)	71,80,80	1.56	11 (15%)
3	NAP	221-A	202	-	50,52,52	1.72	9 (18%)	71,80,80	1.60	11 (15%)
3	NAP	96-A	202	-	50,52,52	1.72	7 (14%)	71,80,80	1.80	12 (16%)
3	NAP	53-A	202	-	50,52,52	1.73	9 (18%)	71,80,80	1.66	16 (22%)
2	FOL	42-A	201	-	34,34,34	1.04	0	43,47,47	1.72	9 (20%)
3	NAP	94-A	202	-	50,52,52	1.73	8 (16%)	71,80,80	1.57	14 (19%)
3	NAP	235-A	202	-	50,52,52	1.93	11 (22%)	71,80,80	1.94	16 (22%)
3	NAP	47-A	202	-	50,52,52	1.71	8 (16%)	71,80,80	1.67	12 (16%)
3	NAP	201-A	202	-	50,52,52	1.82	9 (18%)	71,80,80	1.67	13 (18%)
3	NAP	141-A	202	-	50,52,52	2.13	9 (18%)	71,80,80	1.83	14 (19%)
3	NAP	194-A	202	-	50,52,52	1.78	9 (18%)	71,80,80	1.79	14 (19%)
3	NAP	144-A	202	-	50,52,52	1.87	9 (18%)	71,80,80	1.46	8 (11%)
3	NAP	31-A	202	-	50,52,52	1.75	9 (18%)	71,80,80	1.57	14 (19%)
3	NAP	186-A	202	-	50,52,52	1.74	8 (16%)	71,80,80	1.58	12 (16%)
3	NAP	146-A	202	-	50,52,52	1.81	7 (14%)	71,80,80	1.54	11 (15%)
2	FOL	148-A	201	-	34,34,34	1.16	2 (5%)	43,47,47	1.60	8 (18%)
3	NAP	118-A	202	-	50,52,52	1.93	9 (18%)	71,80,80	1.76	12 (16%)
2	FOL	201-A	201	-	34,34,34	1.10	2 (5%)	43,47,47	1.34	5 (11%)
2	FOL	194-A	201	-	34,34,34	1.40	2 (5%)	43,47,47	1.32	7 (16%)
2	FOL	213-A	201	-	34,34,34	0.94	1 (2%)	43,47,47	1.61	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	87-A	201	-	34,34,34	1.10	2 (5%)	43,47,47	1.18	3 (6%)
3	NAP	195-A	202	-	50,52,52	1.73	8 (16%)	71,80,80	1.60	12 (16%)
2	FOL	100-A	201	-	34,34,34	1.22	3 (8%)	43,47,47	1.44	7 (16%)
2	FOL	186-A	201	-	34,34,34	1.38	2 (5%)	43,47,47	1.42	6 (13%)
2	FOL	3-A	201	-	34,34,34	1.10	1 (2%)	43,47,47	1.46	8 (18%)
3	NAP	135-A	202	-	50,52,52	1.78	10 (20%)	71,80,80	1.74	14 (19%)
2	FOL	124-A	201	-	34,34,34	1.02	0	43,47,47	1.64	5 (11%)
2	FOL	154-A	201	-	34,34,34	1.11	2 (5%)	43,47,47	1.63	7 (16%)
3	NAP	143-A	202	-	50,52,52	2.88	14 (28%)	71,80,80	2.24	18 (25%)
3	NAP	237-A	202	-	50,52,52	2.80	12 (24%)	71,80,80	2.13	16 (22%)
2	FOL	50-A	201	-	34,34,34	1.03	0	43,47,47	1.80	11 (25%)
2	FOL	51-A	201	-	34,34,34	1.21	2 (5%)	43,47,47	1.31	4 (9%)
2	FOL	171-A	201	-	34,34,34	1.05	1 (2%)	43,47,47	1.93	13 (30%)
2	FOL	188-A	201	-	34,34,34	1.37	3 (8%)	43,47,47	1.47	7 (16%)
2	FOL	210-A	201	-	34,34,34	1.12	1 (2%)	43,47,47	1.63	9 (20%)
3	NAP	126-A	202	-	50,52,52	1.72	9 (18%)	71,80,80	1.58	12 (16%)
2	FOL	230-A	201	-	34,34,34	0.95	1 (2%)	43,47,47	1.48	7 (16%)
2	FOL	205-A	201	-	34,34,34	1.13	2 (5%)	43,47,47	1.49	8 (18%)
3	NAP	137-A	202	-	50,52,52	1.74	9 (18%)	71,80,80	1.54	13 (18%)
3	NAP	46-A	202	-	50,52,52	1.79	10 (20%)	71,80,80	1.60	12 (16%)
3	NAP	148-A	202	-	50,52,52	1.79	9 (18%)	71,80,80	1.66	13 (18%)
3	NAP	27-A	202	-	50,52,52	1.73	9 (18%)	71,80,80	1.62	13 (18%)
3	NAP	150-A	202	-	50,52,52	1.78	10 (20%)	71,80,80	1.62	11 (15%)
3	NAP	109-A	202	-	50,52,52	1.92	9 (18%)	71,80,80	1.68	12 (16%)
3	NAP	36-A	202	-	50,52,52	1.71	9 (18%)	71,80,80	1.74	14 (19%)
3	NAP	184-A	202	-	50,52,52	1.72	10 (20%)	71,80,80	1.56	13 (18%)
3	NAP	158-A	202	-	50,52,52	1.73	5 (10%)	71,80,80	1.57	12 (16%)
2	FOL	157-A	201	-	34,34,34	1.25	2 (5%)	43,47,47	1.92	11 (25%)
3	NAP	250-A	202	-	50,52,52	1.68	10 (20%)	71,80,80	1.62	13 (18%)
3	NAP	95-A	202	-	50,52,52	1.79	7 (14%)	71,80,80	1.77	13 (18%)
2	FOL	34-A	201	-	34,34,34	1.33	4 (11%)	43,47,47	1.56	9 (20%)
2	FOL	89-A	201	-	34,34,34	0.98	1 (2%)	43,47,47	1.37	8 (18%)
3	NAP	212-A	202	-	50,52,52	1.86	10 (20%)	71,80,80	1.72	12 (16%)
3	NAP	25-A	202	-	50,52,52	1.77	11 (22%)	71,80,80	1.66	14 (19%)
2	FOL	231-A	201	-	34,34,34	1.08	0	43,47,47	1.67	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	246-A	202	-	50,52,52	1.69	11 (22%)	71,80,80	3.06	14 (19%)
3	NAP	214-A	202	-	50,52,52	1.68	9 (18%)	71,80,80	1.76	12 (16%)
2	FOL	145-A	201	-	34,34,34	1.29	2 (5%)	43,47,47	1.57	8 (18%)
2	FOL	5-A	201	-	34,34,34	1.05	1 (2%)	43,47,47	1.55	11 (25%)
2	FOL	195-A	201	-	34,34,34	1.20	1 (2%)	43,47,47	1.75	9 (20%)
3	NAP	230-A	202	-	50,52,52	1.70	9 (18%)	71,80,80	1.59	13 (18%)
2	FOL	134-A	201	-	34,34,34	1.20	2 (5%)	43,47,47	1.51	6 (13%)
3	NAP	3-A	202	-	50,52,52	2.02	10 (20%)	71,80,80	2.84	20 (28%)
3	NAP	35-A	202	-	50,52,52	1.75	11 (22%)	71,80,80	1.64	14 (19%)
2	FOL	220-A	201	-	34,34,34	1.71	8 (23%)	43,47,47	2.82	16 (37%)
2	FOL	123-A	201	-	34,34,34	0.98	1 (2%)	43,47,47	1.19	2 (4%)
3	NAP	227-A	202	-	50,52,52	1.71	8 (16%)	71,80,80	1.56	12 (16%)
3	NAP	91-A	202	-	50,52,52	1.74	11 (22%)	71,80,80	1.76	13 (18%)
3	NAP	30-A	202	-	50,52,52	1.89	6 (12%)	71,80,80	1.95	14 (19%)
2	FOL	32-A	201	-	34,34,34	0.88	0	43,47,47	1.37	6 (13%)
3	NAP	217-A	202	-	50,52,52	1.74	9 (18%)	71,80,80	1.56	13 (18%)
2	FOL	155-A	201	-	34,34,34	1.23	3 (8%)	43,47,47	1.59	8 (18%)
3	NAP	223-A	202	-	50,52,52	1.76	10 (20%)	71,80,80	1.79	13 (18%)
3	NAP	145-A	202	-	50,52,52	1.85	8 (16%)	71,80,80	1.53	12 (16%)
2	FOL	82-A	201	-	34,34,34	1.32	4 (11%)	43,47,47	1.68	6 (13%)
3	NAP	73-A	202	-	50,52,52	1.86	10 (20%)	71,80,80	1.78	11 (15%)
3	NAP	45-A	202	-	50,52,52	2.05	11 (22%)	71,80,80	1.87	17 (23%)
3	NAP	127-A	202	-	50,52,52	1.74	10 (20%)	71,80,80	1.55	10 (14%)
2	FOL	69-A	201	-	34,34,34	1.12	0	43,47,47	2.06	12 (27%)
2	FOL	227-A	201	-	34,34,34	0.88	1 (2%)	43,47,47	1.70	9 (20%)
2	FOL	225-A	201	-	34,34,34	1.05	2 (5%)	43,47,47	1.29	7 (16%)
2	FOL	56-A	201	-	34,34,34	1.29	3 (8%)	43,47,47	2.19	14 (32%)
3	NAP	52-A	202	-	50,52,52	1.75	10 (20%)	71,80,80	1.63	13 (18%)
2	FOL	120-A	201	-	34,34,34	1.10	2 (5%)	43,47,47	1.48	7 (16%)
3	NAP	101-A	202	-	50,52,52	1.76	9 (18%)	71,80,80	1.68	12 (16%)
3	NAP	114-A	202	-	50,52,52	1.70	11 (22%)	71,80,80	1.61	11 (15%)
2	FOL	164-A	201	-	34,34,34	1.02	1 (2%)	43,47,47	1.71	11 (25%)
3	NAP	66-A	202	-	50,52,52	1.75	9 (18%)	71,80,80	1.63	15 (21%)
2	FOL	158-A	201	-	34,34,34	1.11	2 (5%)	43,47,47	1.69	8 (18%)
2	FOL	28-A	201	-	34,34,34	0.96	0	43,47,47	1.30	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	243-A	201	-	34,34,34	1.11	2 (5%)	43,47,47	1.71	9 (20%)
3	NAP	82-A	202	-	50,52,52	1.73	8 (16%)	71,80,80	1.59	13 (18%)
2	FOL	84-A	201	-	34,34,34	0.98	1 (2%)	43,47,47	2.09	12 (27%)
3	NAP	172-A	202	-	50,52,52	1.74	11 (22%)	71,80,80	1.57	12 (16%)
3	NAP	153-A	202	-	50,52,52	1.80	7 (14%)	71,80,80	1.52	10 (14%)
3	NAP	34-A	202	-	50,52,52	1.72	8 (16%)	71,80,80	1.75	16 (22%)
2	FOL	29-A	201	-	34,34,34	1.09	3 (8%)	43,47,47	1.53	9 (20%)
3	NAP	89-A	202	-	50,52,52	1.76	10 (20%)	71,80,80	1.67	11 (15%)
3	NAP	99-A	202	-	50,52,52	1.74	8 (16%)	71,80,80	1.59	11 (15%)
3	NAP	76-A	202	-	50,52,52	1.71	9 (18%)	71,80,80	1.64	15 (21%)
3	NAP	205-A	202	-	50,52,52	1.94	9 (18%)	71,80,80	1.62	10 (14%)
2	FOL	79-A	201	-	34,34,34	1.30	3 (8%)	43,47,47	1.48	9 (20%)
3	NAP	161-A	202	-	50,52,52	1.72	7 (14%)	71,80,80	2.96	14 (19%)
3	NAP	213-A	202	-	50,52,52	2.00	9 (18%)	71,80,80	1.87	14 (19%)
2	FOL	9-A	201	-	34,34,34	1.10	3 (8%)	43,47,47	1.71	8 (18%)
2	FOL	66-A	201	-	34,34,34	1.03	1 (2%)	43,47,47	1.53	8 (18%)
3	NAP	5-A	202	-	50,52,52	1.81	10 (20%)	71,80,80	3.18	19 (26%)
2	FOL	215-A	201	-	34,34,34	1.10	2 (5%)	43,47,47	1.52	9 (20%)
3	NAP	67-A	202	-	50,52,52	1.76	9 (18%)	71,80,80	1.80	14 (19%)
2	FOL	237-A	201	-	34,34,34	1.13	2 (5%)	43,47,47	1.65	5 (11%)
3	NAP	49-A	202	-	50,52,52	1.72	8 (16%)	71,80,80	1.66	12 (16%)
3	NAP	112-A	202	-	50,52,52	1.75	10 (20%)	71,80,80	1.68	16 (22%)
3	NAP	163-A	202	-	50,52,52	1.99	8 (16%)	71,80,80	3.00	19 (26%)
2	FOL	141-A	201	-	34,34,34	1.13	2 (5%)	43,47,47	1.44	5 (11%)
2	FOL	76-A	201	-	34,34,34	1.26	1 (2%)	43,47,47	1.53	9 (20%)
2	FOL	242-A	201	-	34,34,34	1.00	1 (2%)	43,47,47	1.56	8 (18%)
2	FOL	6-A	201	-	34,34,34	1.03	0	43,47,47	1.74	7 (16%)
3	NAP	32-A	202	-	50,52,52	1.73	8 (16%)	71,80,80	1.68	12 (16%)
3	NAP	69-A	202	-	50,52,52	1.78	10 (20%)	71,80,80	1.76	15 (21%)
3	NAP	56-A	202	-	50,52,52	1.72	7 (14%)	71,80,80	1.56	10 (14%)
2	FOL	112-A	201	-	34,34,34	0.96	1 (2%)	43,47,47	1.75	8 (18%)
2	FOL	57-A	201	-	34,34,34	1.28	4 (11%)	43,47,47	2.06	8 (18%)
2	FOL	248-A	201	-	34,34,34	1.00	1 (2%)	43,47,47	1.41	7 (16%)
2	FOL	44-A	201	-	34,34,34	1.04	2 (5%)	43,47,47	1.50	6 (13%)
3	NAP	110-A	202	-	50,52,52	1.73	9 (18%)	71,80,80	1.73	15 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	231-A	202	-	50,52,52	1.73	9 (18%)	71,80,80	1.63	12 (16%)
3	NAP	1-A	202	-	50,52,52	1.93	7 (14%)	71,80,80	3.43	17 (23%)
2	FOL	17-A	201	-	34,34,34	1.10	2 (5%)	43,47,47	1.46	7 (16%)
2	FOL	40-A	201	-	34,34,34	1.28	3 (8%)	43,47,47	2.07	15 (34%)
3	NAP	154-A	202	-	50,52,52	1.74	8 (16%)	71,80,80	1.75	12 (16%)
3	NAP	54-A	202	-	50,52,52	1.75	7 (14%)	71,80,80	1.63	12 (16%)
2	FOL	21-A	201	-	34,34,34	1.01	2 (5%)	43,47,47	1.34	5 (11%)
2	FOL	127-A	201	-	34,34,34	1.07	2 (5%)	43,47,47	1.46	7 (16%)
3	NAP	33-A	202	-	50,52,52	1.72	8 (16%)	71,80,80	1.61	15 (21%)
3	NAP	129-A	202	-	50,52,52	1.71	9 (18%)	71,80,80	1.59	12 (16%)
3	NAP	182-A	202	-	50,52,52	1.72	8 (16%)	71,80,80	1.56	14 (19%)
3	NAP	225-A	202	-	50,52,52	1.74	11 (22%)	71,80,80	1.53	12 (16%)
2	FOL	25-A	201	-	34,34,34	1.35	3 (8%)	43,47,47	2.31	12 (27%)
3	NAP	209-A	202	-	50,52,52	1.78	9 (18%)	71,80,80	1.81	14 (19%)
2	FOL	165-A	201	-	34,34,34	1.02	2 (5%)	43,47,47	1.85	7 (16%)
2	FOL	202-A	201	-	34,34,34	1.26	2 (5%)	43,47,47	2.08	12 (27%)
2	FOL	95-A	201	-	34,34,34	1.22	3 (8%)	43,47,47	1.42	7 (16%)
2	FOL	172-A	201	-	34,34,34	1.21	2 (5%)	43,47,47	1.49	6 (13%)
2	FOL	149-A	201	-	34,34,34	1.09	2 (5%)	43,47,47	1.51	8 (18%)
3	NAP	28-A	202	-	50,52,52	1.70	8 (16%)	71,80,80	1.59	13 (18%)
2	FOL	150-A	201	-	34,34,34	1.09	1 (2%)	43,47,47	1.99	6 (13%)
3	NAP	245-A	202	-	50,52,52	1.64	8 (16%)	71,80,80	2.86	15 (21%)
2	FOL	38-A	201	-	34,34,34	1.27	4 (11%)	43,47,47	2.05	10 (23%)
3	NAP	84-A	202	-	50,52,52	1.70	8 (16%)	71,80,80	1.61	12 (16%)
2	FOL	59-A	201	-	34,34,34	1.15	1 (2%)	43,47,47	1.35	6 (13%)
3	NAP	168-A	202	-	50,52,52	1.72	8 (16%)	71,80,80	1.67	15 (21%)
3	NAP	215-A	202	-	50,52,52	1.69	9 (18%)	71,80,80	1.58	13 (18%)
2	FOL	128-A	201	-	34,34,34	0.98	1 (2%)	43,47,47	1.66	8 (18%)
3	NAP	98-A	202	-	50,52,52	1.72	10 (20%)	71,80,80	1.68	13 (18%)
3	NAP	142-A	202	-	50,52,52	1.94	11 (22%)	71,80,80	2.01	15 (21%)
2	FOL	74-A	201	-	34,34,34	1.22	2 (5%)	43,47,47	1.51	7 (16%)
3	NAP	176-A	202	-	50,52,52	1.70	8 (16%)	71,80,80	1.54	11 (15%)
2	FOL	136-A	201	-	34,34,34	1.24	4 (11%)	43,47,47	1.85	7 (16%)
3	NAP	79-A	202	-	50,52,52	1.76	9 (18%)	71,80,80	1.60	13 (18%)
2	FOL	156-A	201	-	34,34,34	0.92	0	43,47,47	2.02	12 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	209-A	201	-	34,34,34	1.28	2 (5%)	43,47,47	1.32	6 (13%)
2	FOL	221-A	201	-	34,34,34	2.06	9 (26%)	43,47,47	4.33	21 (48%)
3	NAP	188-A	202	-	50,52,52	1.74	7 (14%)	71,80,80	1.54	10 (14%)
3	NAP	24-A	202	-	50,52,52	1.73	8 (16%)	71,80,80	1.61	11 (15%)
2	FOL	122-A	201	-	34,34,34	0.98	1 (2%)	43,47,47	1.30	5 (11%)
3	NAP	247-A	202	-	50,52,52	1.67	12 (24%)	71,80,80	2.96	16 (22%)
3	NAP	238-A	202	-	50,52,52	1.94	9 (18%)	71,80,80	1.87	13 (18%)
3	NAP	240-A	202	-	50,52,52	1.70	11 (22%)	71,80,80	1.61	16 (22%)
2	FOL	31-A	201	-	34,34,34	1.01	1 (2%)	43,47,47	1.42	5 (11%)
2	FOL	170-A	201	-	34,34,34	0.98	1 (2%)	43,47,47	1.74	4 (9%)
3	NAP	120-A	202	-	50,52,52	2.85	11 (22%)	71,80,80	2.25	15 (21%)
2	FOL	146-A	201	-	34,34,34	1.08	2 (5%)	43,47,47	1.67	6 (13%)
3	NAP	70-A	202	-	50,52,52	1.71	10 (20%)	71,80,80	1.72	16 (22%)
2	FOL	132-A	201	-	34,34,34	1.11	1 (2%)	43,47,47	1.85	12 (27%)
3	NAP	26-A	202	-	50,52,52	1.73	9 (18%)	71,80,80	1.67	12 (16%)
2	FOL	192-A	201	-	34,34,34	1.43	5 (14%)	43,47,47	1.95	17 (39%)
3	NAP	116-A	202	-	50,52,52	1.78	9 (18%)	71,80,80	1.74	12 (16%)
3	NAP	248-A	202	-	50,52,52	1.68	11 (22%)	71,80,80	2.34	17 (23%)
3	NAP	72-A	202	-	50,52,52	1.74	10 (20%)	71,80,80	1.72	14 (19%)
3	NAP	151-A	202	-	50,52,52	1.77	9 (18%)	71,80,80	1.61	14 (19%)
2	FOL	52-A	201	-	34,34,34	1.05	1 (2%)	43,47,47	1.58	8 (18%)
2	FOL	125-A	201	-	34,34,34	1.28	2 (5%)	43,47,47	1.40	6 (13%)
3	NAP	97-A	202	-	50,52,52	1.73	9 (18%)	71,80,80	1.59	10 (14%)
2	FOL	234-A	201	-	34,34,34	1.17	2 (5%)	43,47,47	1.45	8 (18%)
2	FOL	169-A	201	-	34,34,34	0.91	0	43,47,47	1.39	7 (16%)
2	FOL	143-A	201	-	34,34,34	1.34	3 (8%)	43,47,47	1.85	10 (23%)
3	NAP	228-A	202	-	50,52,52	1.72	10 (20%)	71,80,80	1.53	14 (19%)
2	FOL	140-A	201	-	34,34,34	1.25	2 (5%)	43,47,47	1.89	9 (20%)
2	FOL	235-A	201	-	34,34,34	1.06	1 (2%)	43,47,47	1.54	9 (20%)
3	NAP	155-A	202	-	50,52,52	1.76	9 (18%)	71,80,80	1.72	13 (18%)
2	FOL	8-A	201	-	34,34,34	1.19	2 (5%)	43,47,47	1.49	9 (20%)
2	FOL	153-A	201	-	34,34,34	0.98	1 (2%)	43,47,47	1.50	8 (18%)
3	NAP	210-A	202	-	50,52,52	1.74	9 (18%)	71,80,80	1.67	12 (16%)
2	FOL	137-A	201	-	34,34,34	1.15	2 (5%)	43,47,47	1.65	7 (16%)
2	FOL	30-A	201	-	34,34,34	1.15	2 (5%)	43,47,47	1.87	12 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	164-A	202	-	50,52,52	2.74	11 (22%)	71,80,80	3.23	18 (25%)
2	FOL	98-A	201	-	34,34,34	0.99	1 (2%)	43,47,47	1.74	9 (20%)
3	NAP	243-A	202	-	50,52,52	2.07	11 (22%)	71,80,80	2.93	21 (29%)
3	NAP	131-A	202	-	50,52,52	1.73	7 (14%)	71,80,80	1.46	12 (16%)
2	FOL	138-A	201	-	34,34,34	1.07	2 (5%)	43,47,47	1.50	6 (13%)
2	FOL	166-A	201	-	34,34,34	1.24	2 (5%)	43,47,47	1.50	8 (18%)
2	FOL	111-A	201	-	34,34,34	1.02	2 (5%)	43,47,47	1.49	7 (16%)
3	NAP	6-A	202	-	50,52,52	1.80	9 (18%)	71,80,80	2.36	14 (19%)
3	NAP	75-A	202	-	50,52,52	1.68	7 (14%)	71,80,80	1.78	16 (22%)
2	FOL	73-A	201	-	34,34,34	1.24	2 (5%)	43,47,47	1.65	10 (23%)
3	NAP	12-A	202	-	50,52,52	1.73	8 (16%)	71,80,80	1.65	13 (18%)
3	NAP	136-A	202	-	50,52,52	1.66	8 (16%)	71,80,80	1.77	15 (21%)
2	FOL	71-A	201	-	34,34,34	1.18	4 (11%)	43,47,47	2.06	15 (34%)

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	187-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	17-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	24-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	119-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	180-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	222-A	201	-	-	7/22/22/22	0/3/3/3
3	NAP	122-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	247-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	29-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
3	NAP	218-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	43-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	159-A	202	-	-	7/35/67/67	0/5/5/5
2	FOL	189-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	181-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	185-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	117-A	201	-	-	2/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	10-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	90-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	244-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	229-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	83-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	78-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	177-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	234-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	169-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	23-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	125-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	139-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	68-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	87-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	36-A	201	-	-	8/22/22/22	0/3/3/3
3	NAP	197-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	103-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	129-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	115-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	162-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	94-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	147-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	138-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	200-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	204-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	103-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
2	FOL	61-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	71-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	80-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	114-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	183-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	99-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	220-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	93-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	47-A	201	-	-	3/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	16-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	38-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	23-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	177-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	115-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	246-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	57-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	96-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	104-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	46-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	208-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	135-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	43-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	223-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	203-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	152-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	62-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	173-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	90-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	228-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	139-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	249-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	207-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	55-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	9-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	179-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	13-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	157-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	108-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	65-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	192-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
2	FOL	238-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	116-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	239-A	202	-	1/1/12/12	5/35/67/67	0/5/5/5
3	NAP	130-A	202	-	-	4/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	222-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
2	FOL	126-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	93-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	180-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	48-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	26-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	14-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	181-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	156-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	58-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	10-A	201	-	-	8/22/22/22	0/3/3/3
3	NAP	140-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	27-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	133-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	217-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	117-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	72-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	151-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	147-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	242-A	202	-	-	7/35/67/67	0/5/5/5
2	FOL	97-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	233-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	244-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	196-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	86-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	203-A	202	-	-	6/35/67/67	0/5/5/5
2	FOL	236-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	2-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	167-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	178-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	77-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	12-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	208-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	166-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	111-A	202	-	-	4/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	104-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	75-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	202-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	211-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	178-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
3	NAP	198-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	142-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	191-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	163-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	196-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	20-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	39-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	85-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	206-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	224-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	249-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	44-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	241-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	189-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	101-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	37-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	199-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	1-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	35-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	19-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	185-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	184-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	197-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	88-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	187-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	226-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	159-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	83-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	41-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	190-A	201	-	-	5/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	102-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	48-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	241-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	160-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	42-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	53-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	81-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	58-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	128-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	7-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	193-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	219-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	106-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	113-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	133-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	121-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	77-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	175-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	4-A	202	-	-	6/35/67/67	0/5/5/5
3	NAP	86-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	211-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	55-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
3	NAP	236-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
3	NAP	179-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
2	FOL	176-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	13-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	50-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	108-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	63-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
3	NAP	123-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	193-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	110-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	107-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	132-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
3	NAP	191-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	161-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	21-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	113-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	149-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	170-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	39-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	20-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	85-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
3	NAP	59-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	206-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	67-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	224-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	92-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	174-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	2-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
2	FOL	37-A	201	-	-	9/22/22/22	0/3/3/3
2	FOL	218-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	16-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	64-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	62-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
3	NAP	81-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	80-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	118-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	167-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	88-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	226-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	18-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	190-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	173-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	229-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	41-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
2	FOL	160-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	92-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	171-A	202	-	-	4/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	18-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
2	FOL	216-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	232-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	121-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	22-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	106-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	152-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	33-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	182-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	4-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	11-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	119-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
3	NAP	14-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	65-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	214-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	200-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	63-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	245-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	8-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	144-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	233-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	168-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	60-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	109-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	199-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	15-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	78-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	102-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	183-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	70-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	175-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	7-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	124-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	198-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	240-A	201	-	-	3/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	64-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	45-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	207-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	165-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	60-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	131-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	40-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	134-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	219-A	201	-	-	11/22/22/22	0/3/3/3
3	NAP	105-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	68-A	202	-	-	6/35/67/67	0/5/5/5
2	FOL	15-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	130-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	162-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	22-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	51-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	250-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	204-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	54-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	19-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	216-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	107-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	212-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	239-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	61-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	174-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	49-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	232-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	74-A	202	-	1/1/12/12	3/35/67/67	0/5/5/5
2	FOL	91-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	105-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	11-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	221-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	96-A	202	-	1/1/12/12	3/35/67/67	0/5/5/5
3	NAP	53-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	42-A	201	-	-	1/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	94-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	235-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
3	NAP	47-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	201-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	141-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
3	NAP	194-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	144-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	31-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	186-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	146-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	118-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
2	FOL	148-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	201-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	194-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	213-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	87-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	195-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	100-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	186-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	3-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	135-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	124-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	143-A	202	-	1/1/12/12	5/35/67/67	0/5/5/5
2	FOL	154-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	237-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
2	FOL	50-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	51-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	171-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	188-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	210-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	126-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	230-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	205-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	137-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	46-A	202	-	-	4/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	148-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	27-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	150-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	109-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
3	NAP	36-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	184-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	158-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	157-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	250-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	95-A	202	-	1/1/12/12	3/35/67/67	0/5/5/5
2	FOL	34-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	89-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	212-A	202	-	1/1/12/12	5/35/67/67	0/5/5/5
3	NAP	25-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	231-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	246-A	202	-	-	7/35/67/67	0/5/5/5
3	NAP	214-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	145-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	5-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	195-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	230-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	134-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	3-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	35-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	220-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	123-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	227-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	91-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	30-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
2	FOL	32-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	217-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	155-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	223-A	202	-	1/1/12/12	5/35/67/67	0/5/5/5
3	NAP	145-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	82-A	201	-	-	3/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	73-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	45-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
3	NAP	127-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	69-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	227-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	225-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	56-A	201	-	-	8/22/22/22	0/3/3/3
3	NAP	52-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	120-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	101-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	114-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	164-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	66-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	158-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	28-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	243-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	82-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	84-A	201	-	-	9/22/22/22	0/3/3/3
3	NAP	172-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	153-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	34-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	29-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	89-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	99-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	76-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	205-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
2	FOL	79-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	161-A	202	-	-	6/35/67/67	0/5/5/5
3	NAP	213-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
2	FOL	9-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	66-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	5-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	215-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	67-A	202	-	-	4/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	237-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	49-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	112-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	163-A	202	-	1/1/12/12	6/35/67/67	0/5/5/5
2	FOL	141-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	76-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	242-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	6-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	32-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	69-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	56-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	112-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	57-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	248-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	44-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	110-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	231-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	1-A	202	-	1/1/12/12	5/35/67/67	0/5/5/5
3	NAP	154-A	202	-	1/1/12/12	3/35/67/67	0/5/5/5
2	FOL	17-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	40-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	54-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	21-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	127-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	33-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	129-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	182-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	225-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	25-A	201	-	-	8/22/22/22	0/3/3/3
3	NAP	209-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	165-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	202-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	95-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	172-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	149-A	201	-	-	3/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	28-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	150-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	245-A	202	-	-	7/35/67/67	0/5/5/5
2	FOL	38-A	201	-	-	8/22/22/22	0/3/3/3
3	NAP	84-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	59-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	168-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	215-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	128-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	98-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	142-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
2	FOL	74-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	176-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	136-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	79-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	156-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	209-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	221-A	201	-	-	12/22/22/22	0/3/3/3
3	NAP	188-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	24-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	122-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	247-A	202	-	-	6/35/67/67	0/5/5/5
3	NAP	238-A	202	-	1/1/12/12	4/35/67/67	0/5/5/5
3	NAP	240-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	31-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	170-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	120-A	202	-	1/1/12/12	3/35/67/67	0/5/5/5
2	FOL	146-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	70-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	132-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	26-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	192-A	201	-	-	9/22/22/22	0/3/3/3
3	NAP	116-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	248-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	72-A	202	-	-	4/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	151-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	52-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	125-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	97-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	234-A	201	-	-	9/22/22/22	0/3/3/3
2	FOL	169-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	143-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	228-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	140-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	235-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	155-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	8-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	153-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	210-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	137-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	30-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	164-A	202	-	1/1/12/12	6/35/67/67	0/5/5/5
2	FOL	98-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	243-A	202	-	-	7/35/67/67	0/5/5/5
3	NAP	131-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	138-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	166-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	111-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	6-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	75-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	73-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	12-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	136-A	202	-	-	5/35/67/67	0/5/5/5
2	FOL	71-A	201	-	-	3/22/22/22	0/3/3/3

The worst 5 of 2780 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	132-A	202	NAP	O3B-C3B	-16.51	1.02	1.43
3	143-A	202	NAP	O3B-C3B	-16.21	1.02	1.43
3	237-A	202	NAP	O3B-C3B	-16.18	1.02	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	120-A	202	NAP	O3B-C3B	-15.97	1.03	1.43
3	191-A	202	NAP	O3B-C3B	-15.82	1.03	1.43

The worst 5 of 5330 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5-A	202	NAP	O2N-PN-O3	-21.35	49.55	107.27
3	242-A	202	NAP	O2N-PN-O3	-19.51	54.54	107.27
3	165-A	202	NAP	O2N-PN-O3	-17.76	59.26	107.27
3	247-A	202	NAP	O2N-PN-O3	-17.39	60.26	107.27
3	4-A	202	NAP	O2N-PN-O3	-16.90	61.59	107.27

5 of 40 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	1-A	202	NAP	C3B
3	2-A	202	NAP	C3B
3	18-A	202	NAP	C3B
3	29-A	202	NAP	C3B
3	30-A	202	NAP	C3B

5 of 1838 torsion outliers are listed below:

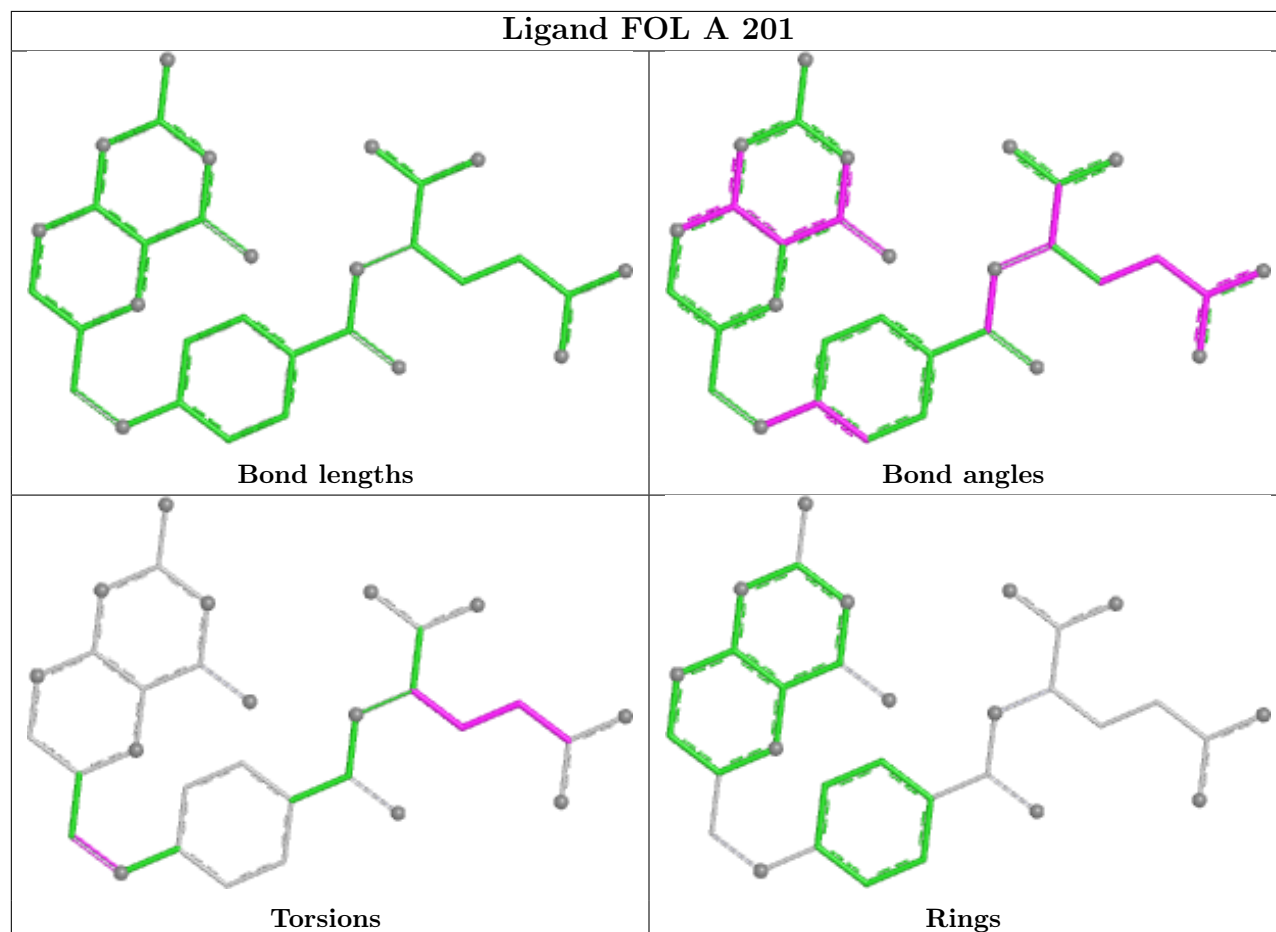
Mol	Chain	Res	Type	Atoms
2	6-A	201	FOL	C6-C9-N10-C14
2	13-A	201	FOL	N-CA-CB-CG
2	16-A	201	FOL	CT-CA-CB-CG
2	17-A	201	FOL	N-CA-CB-CG
2	17-A	201	FOL	CT-CA-CB-CG

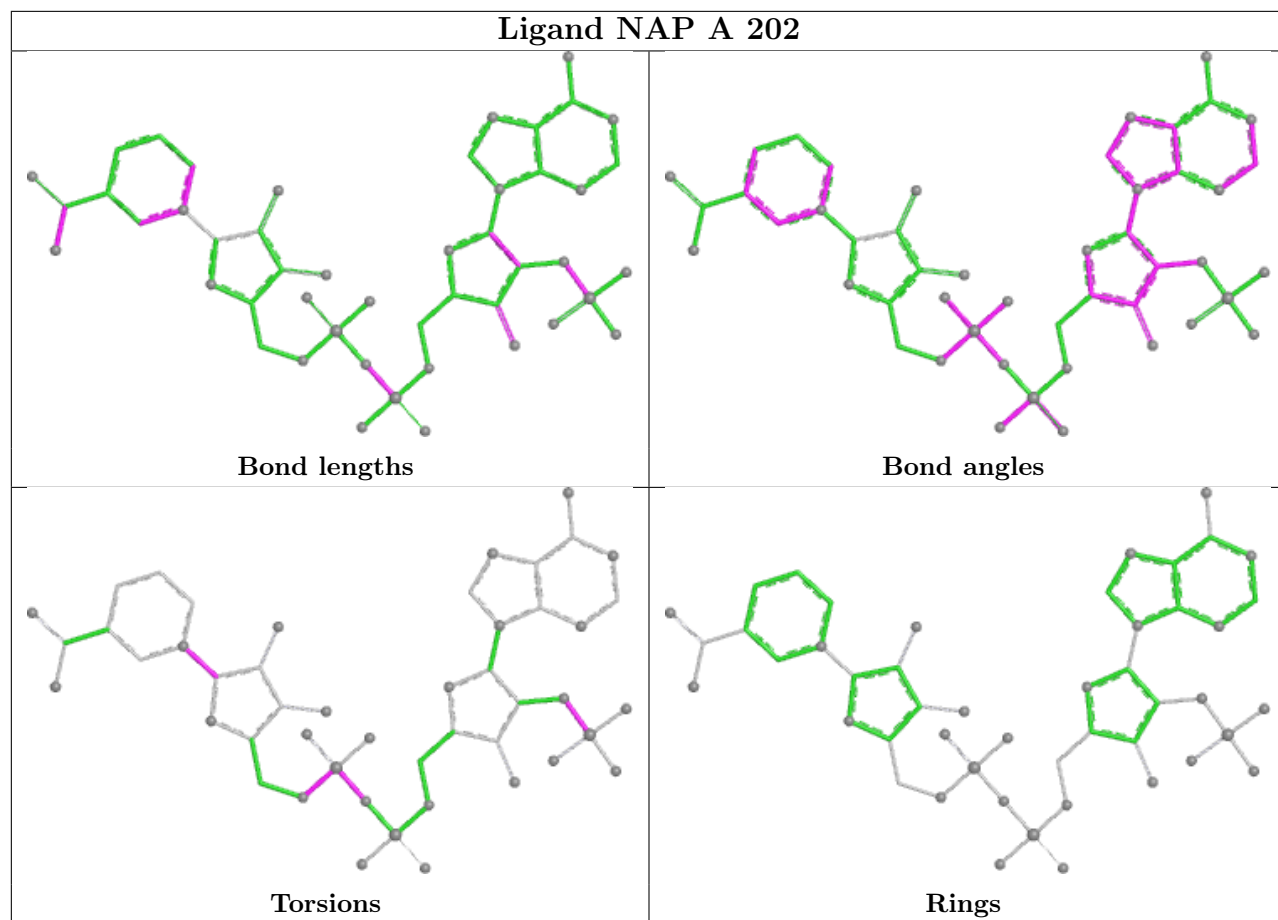
There are no ring outliers.

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	159/159 (100%)	2.72	94 (59%) 0 1	0, 0, 0, 0	159 (100%)
1	2-A	0/159	-	-	-	-
1	3-A	0/159	-	-	-	-
1	4-A	0/159	-	-	-	-
1	5-A	0/159	-	-	-	-
1	6-A	0/159	-	-	-	-
1	7-A	0/159	-	-	-	-
1	8-A	0/159	-	-	-	-
1	9-A	0/159	-	-	-	-
1	10-A	0/159	-	-	-	-
1	11-A	0/159	-	-	-	-
1	12-A	0/159	-	-	-	-
1	13-A	0/159	-	-	-	-
1	14-A	0/159	-	-	-	-
1	15-A	0/159	-	-	-	-
1	16-A	0/159	-	-	-	-
1	17-A	0/159	-	-	-	-
1	18-A	0/159	-	-	-	-
1	19-A	0/159	-	-	-	-
1	20-A	0/159	-	-	-	-
1	21-A	0/159	-	-	-	-
1	22-A	0/159	-	-	-	-
1	23-A	0/159	-	-	-	-
1	24-A	0/159	-	-	-	-
1	25-A	0/159	-	-	-	-
1	26-A	0/159	-	-	-	-
1	27-A	0/159	-	-	-	-
1	28-A	0/159	-	-	-	-
1	29-A	0/159	-	-	-	-
1	30-A	0/159	-	-	-	-
1	31-A	0/159	-	-	-	-
1	32-A	0/159	-	-	-	-

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

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

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

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	159-A	0/159	-	-	-	-
1	160-A	0/159	-	-	-	-
1	161-A	0/159	-	-	-	-
1	162-A	0/159	-	-	-	-
1	163-A	0/159	-	-	-	-
1	164-A	0/159	-	-	-	-
1	165-A	0/159	-	-	-	-
1	166-A	0/159	-	-	-	-
1	167-A	0/159	-	-	-	-
1	168-A	0/159	-	-	-	-
1	169-A	0/159	-	-	-	-
1	170-A	0/159	-	-	-	-
1	171-A	0/159	-	-	-	-
1	172-A	0/159	-	-	-	-
1	173-A	0/159	-	-	-	-
1	174-A	0/159	-	-	-	-
1	175-A	0/159	-	-	-	-
1	176-A	0/159	-	-	-	-
1	177-A	0/159	-	-	-	-
1	178-A	0/159	-	-	-	-
1	179-A	0/159	-	-	-	-
1	180-A	0/159	-	-	-	-
1	181-A	0/159	-	-	-	-
1	182-A	0/159	-	-	-	-
1	183-A	0/159	-	-	-	-
1	184-A	0/159	-	-	-	-
1	185-A	0/159	-	-	-	-
1	186-A	0/159	-	-	-	-
1	187-A	0/159	-	-	-	-
1	188-A	0/159	-	-	-	-
1	189-A	0/159	-	-	-	-
1	190-A	0/159	-	-	-	-
1	191-A	0/159	-	-	-	-
1	192-A	0/159	-	-	-	-
1	193-A	0/159	-	-	-	-
1	194-A	0/159	-	-	-	-
1	195-A	0/159	-	-	-	-
1	196-A	0/159	-	-	-	-
1	197-A	0/159	-	-	-	-
1	198-A	0/159	-	-	-	-
1	199-A	0/159	-	-	-	-
1	200-A	0/159	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	201-A	0/159	-	-	-	-
1	202-A	0/159	-	-	-	-
1	203-A	0/159	-	-	-	-
1	204-A	0/159	-	-	-	-
1	205-A	0/159	-	-	-	-
1	206-A	0/159	-	-	-	-
1	207-A	0/159	-	-	-	-
1	208-A	0/159	-	-	-	-
1	209-A	0/159	-	-	-	-
1	210-A	0/159	-	-	-	-
1	211-A	0/159	-	-	-	-
1	212-A	0/159	-	-	-	-
1	213-A	0/159	-	-	-	-
1	214-A	0/159	-	-	-	-
1	215-A	0/159	-	-	-	-
1	216-A	0/159	-	-	-	-
1	217-A	0/159	-	-	-	-
1	218-A	0/159	-	-	-	-
1	219-A	0/159	-	-	-	-
1	220-A	0/159	-	-	-	-
1	221-A	0/159	-	-	-	-
1	222-A	0/159	-	-	-	-
1	223-A	0/159	-	-	-	-
1	224-A	0/159	-	-	-	-
1	225-A	0/159	-	-	-	-
1	226-A	0/159	-	-	-	-
1	227-A	0/159	-	-	-	-
1	228-A	0/159	-	-	-	-
1	229-A	0/159	-	-	-	-
1	230-A	0/159	-	-	-	-
1	231-A	0/159	-	-	-	-
1	232-A	0/159	-	-	-	-
1	233-A	0/159	-	-	-	-
1	234-A	0/159	-	-	-	-
1	235-A	0/159	-	-	-	-
1	236-A	0/159	-	-	-	-
1	237-A	0/159	-	-	-	-
1	238-A	0/159	-	-	-	-
1	239-A	0/159	-	-	-	-
1	240-A	0/159	-	-	-	-
1	241-A	0/159	-	-	-	-
1	242-A	0/159	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	243-A	0/159	-	-	-	-
1	244-A	0/159	-	-	-	-
1	245-A	0/159	-	-	-	-
1	246-A	0/159	-	-	-	-
1	247-A	0/159	-	-	-	-
1	248-A	0/159	-	-	-	-
1	249-A	0/159	-	-	-	-
1	250-A	0/159	-	-	-	-
All	All	159/39750 (0%)	2.72	94 (59%) 0 1	0, 0, 0, 0	159 (100%)

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	1	MET	10.1
1	1-A	21	PRO	9.9
1	1-A	23	ASN	8.7
1	1-A	36	LEU	7.4
1	1-A	119	VAL	6.9

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

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

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FOL	1-A	201	32/32	0.71	0.13	4,4,5,5	49
2	FOL	2-A	201	32/32	-	-	4,4,5,6	49
2	FOL	3-A	201	32/32	-	-	4,4,5,5	49
2	FOL	4-A	201	32/32	-	-	4,4,5,5	49
2	FOL	5-A	201	32/32	-	-	4,4,5,5	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FOL	6-A	201	32/32	-	-	4,4,5,5	49
2	FOL	7-A	201	32/32	-	-	4,4,5,5	49
2	FOL	8-A	201	32/32	-	-	4,4,5,5	49
2	FOL	9-A	201	32/32	-	-	4,4,5,5	49
2	FOL	10-A	201	32/32	-	-	4,4,5,6	49
2	FOL	11-A	201	32/32	-	-	4,4,5,5	49
2	FOL	12-A	201	32/32	-	-	4,4,5,5	49
2	FOL	13-A	201	32/32	-	-	4,4,5,6	49
2	FOL	14-A	201	32/32	-	-	4,4,5,5	49
2	FOL	15-A	201	32/32	-	-	4,4,5,5	49
2	FOL	16-A	201	32/32	-	-	4,4,5,5	49
2	FOL	17-A	201	32/32	-	-	4,4,5,5	49
2	FOL	18-A	201	32/32	-	-	4,4,5,5	49
2	FOL	19-A	201	32/32	-	-	4,4,5,5	49
2	FOL	20-A	201	32/32	-	-	4,4,5,5	49
2	FOL	21-A	201	32/32	-	-	4,4,5,5	49
2	FOL	22-A	201	32/32	-	-	4,4,5,5	49
2	FOL	23-A	201	32/32	-	-	4,4,5,5	49
2	FOL	24-A	201	32/32	-	-	4,4,5,5	49
2	FOL	25-A	201	32/32	-	-	4,4,5,5	49
2	FOL	26-A	201	32/32	-	-	4,4,5,6	49
2	FOL	27-A	201	32/32	-	-	4,4,5,6	49
2	FOL	28-A	201	32/32	-	-	4,4,5,5	49
2	FOL	29-A	201	32/32	-	-	4,4,5,5	49
2	FOL	30-A	201	32/32	-	-	4,4,5,5	49
2	FOL	31-A	201	32/32	-	-	4,4,5,5	49
2	FOL	32-A	201	32/32	-	-	4,4,5,5	49
2	FOL	33-A	201	32/32	-	-	4,4,5,5	49
2	FOL	34-A	201	32/32	-	-	4,4,5,6	49
2	FOL	35-A	201	32/32	-	-	4,4,5,6	49
2	FOL	36-A	201	32/32	-	-	4,4,5,5	49
2	FOL	37-A	201	32/32	-	-	4,4,5,5	49
2	FOL	38-A	201	32/32	-	-	4,4,5,5	49
2	FOL	39-A	201	32/32	-	-	4,4,5,5	49
2	FOL	40-A	201	32/32	-	-	4,4,5,6	49
2	FOL	41-A	201	32/32	-	-	4,4,5,5	49
2	FOL	42-A	201	32/32	-	-	4,4,5,6	49
2	FOL	43-A	201	32/32	-	-	4,4,5,5	49
2	FOL	44-A	201	32/32	-	-	4,4,5,5	49
2	FOL	45-A	201	32/32	-	-	4,4,5,5	49
2	FOL	46-A	201	32/32	-	-	4,4,5,6	49
2	FOL	47-A	201	32/32	-	-	4,4,5,5	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FOL	48-A	201	32/32	-	-	4,4,5,6	49
2	FOL	49-A	201	32/32	-	-	4,4,5,6	49
2	FOL	50-A	201	32/32	-	-	4,4,5,6	49
2	FOL	51-A	201	32/32	-	-	4,4,5,5	49
2	FOL	52-A	201	32/32	-	-	4,4,5,6	49
2	FOL	53-A	201	32/32	-	-	4,4,5,5	49
2	FOL	54-A	201	32/32	-	-	4,4,5,5	49
2	FOL	55-A	201	32/32	-	-	4,4,5,5	49
2	FOL	56-A	201	32/32	-	-	4,4,5,6	49
2	FOL	57-A	201	32/32	-	-	4,4,5,5	49
2	FOL	58-A	201	32/32	-	-	4,4,5,5	49
2	FOL	59-A	201	32/32	-	-	4,4,5,6	49
2	FOL	60-A	201	32/32	-	-	4,4,5,5	49
2	FOL	61-A	201	32/32	-	-	4,4,5,5	49
2	FOL	62-A	201	32/32	-	-	4,4,5,5	49
2	FOL	63-A	201	32/32	-	-	4,4,5,5	49
2	FOL	64-A	201	32/32	-	-	4,4,5,5	49
2	FOL	65-A	201	32/32	-	-	4,4,5,5	49
2	FOL	66-A	201	32/32	-	-	4,4,5,6	49
2	FOL	67-A	201	32/32	-	-	4,4,5,6	49
2	FOL	68-A	201	32/32	-	-	4,4,5,6	49
2	FOL	69-A	201	32/32	-	-	4,4,5,6	49
2	FOL	70-A	201	32/32	-	-	4,4,5,6	49
2	FOL	71-A	201	32/32	-	-	4,4,5,6	49
2	FOL	72-A	201	32/32	-	-	4,4,5,5	49
2	FOL	73-A	201	32/32	-	-	4,4,5,5	49
2	FOL	74-A	201	32/32	-	-	4,4,5,6	49
2	FOL	75-A	201	32/32	-	-	4,4,5,5	49
2	FOL	76-A	201	32/32	-	-	4,4,5,5	49
2	FOL	77-A	201	32/32	-	-	4,4,5,6	49
2	FOL	78-A	201	32/32	-	-	4,4,5,5	49
2	FOL	79-A	201	32/32	-	-	4,4,5,5	49
2	FOL	80-A	201	32/32	-	-	4,4,5,6	49
2	FOL	81-A	201	32/32	-	-	4,4,5,6	49
2	FOL	82-A	201	32/32	-	-	4,4,5,6	49
2	FOL	83-A	201	32/32	-	-	4,4,5,6	49
2	FOL	84-A	201	32/32	-	-	4,4,5,6	49
2	FOL	85-A	201	32/32	-	-	4,4,5,6	49
2	FOL	86-A	201	32/32	-	-	4,4,5,6	49
2	FOL	87-A	201	32/32	-	-	4,4,5,5	49
2	FOL	88-A	201	32/32	-	-	4,4,5,5	49
2	FOL	89-A	201	32/32	-	-	4,4,5,5	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FOL	90-A	201	32/32	-	-	4,4,5,5	49
2	FOL	91-A	201	32/32	-	-	4,4,5,5	49
2	FOL	92-A	201	32/32	-	-	4,4,5,5	49
2	FOL	93-A	201	32/32	-	-	4,4,5,5	49
2	FOL	94-A	201	32/32	-	-	4,4,5,5	49
2	FOL	95-A	201	32/32	-	-	4,4,5,6	49
2	FOL	96-A	201	32/32	-	-	4,4,5,5	49
2	FOL	97-A	201	32/32	-	-	4,4,5,5	49
2	FOL	98-A	201	32/32	-	-	4,4,5,5	49
2	FOL	99-A	201	32/32	-	-	4,4,5,5	49
2	FOL	100-A	201	32/32	-	-	4,4,5,6	49
2	FOL	101-A	201	32/32	-	-	4,4,5,5	49
2	FOL	102-A	201	32/32	-	-	4,4,5,6	49
2	FOL	103-A	201	32/32	-	-	4,4,5,6	49
2	FOL	104-A	201	32/32	-	-	4,4,5,6	49
2	FOL	105-A	201	32/32	-	-	4,4,5,5	49
2	FOL	106-A	201	32/32	-	-	4,4,5,5	49
2	FOL	107-A	201	32/32	-	-	4,4,5,6	49
2	FOL	108-A	201	32/32	-	-	4,4,5,5	49
2	FOL	109-A	201	32/32	-	-	4,4,5,5	49
2	FOL	110-A	201	32/32	-	-	4,4,5,5	49
2	FOL	111-A	201	32/32	-	-	4,4,5,5	49
2	FOL	112-A	201	32/32	-	-	4,4,5,5	49
2	FOL	113-A	201	32/32	-	-	4,4,5,5	49
2	FOL	114-A	201	32/32	-	-	4,4,5,5	49
2	FOL	115-A	201	32/32	-	-	4,4,5,5	49
2	FOL	116-A	201	32/32	-	-	4,4,5,6	49
2	FOL	117-A	201	32/32	-	-	4,4,5,5	49
2	FOL	118-A	201	32/32	-	-	4,4,5,6	49
2	FOL	119-A	201	32/32	-	-	4,4,5,6	49
2	FOL	120-A	201	32/32	-	-	4,4,5,6	49
2	FOL	121-A	201	32/32	-	-	4,4,5,5	49
2	FOL	122-A	201	32/32	-	-	4,4,5,5	49
2	FOL	123-A	201	32/32	-	-	4,4,5,5	49
2	FOL	124-A	201	32/32	-	-	4,4,5,5	49
2	FOL	125-A	201	32/32	-	-	4,4,5,5	49
2	FOL	126-A	201	32/32	-	-	4,4,5,5	49
2	FOL	127-A	201	32/32	-	-	4,4,5,5	49
2	FOL	128-A	201	32/32	-	-	4,4,5,5	49
2	FOL	129-A	201	32/32	-	-	4,4,5,5	49
2	FOL	130-A	201	32/32	-	-	4,4,5,5	49
2	FOL	131-A	201	32/32	-	-	4,4,5,5	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FOL	132-A	201	32/32	-	-	4,4,5,5	49
2	FOL	133-A	201	32/32	-	-	4,4,5,5	49
2	FOL	134-A	201	32/32	-	-	4,4,5,5	49
2	FOL	135-A	201	32/32	-	-	4,4,5,5	49
2	FOL	136-A	201	32/32	-	-	4,4,5,5	49
2	FOL	137-A	201	32/32	-	-	4,4,5,6	49
2	FOL	138-A	201	32/32	-	-	4,4,5,5	49
2	FOL	139-A	201	32/32	-	-	4,4,5,6	49
2	FOL	140-A	201	32/32	-	-	4,4,5,5	49
2	FOL	141-A	201	32/32	-	-	4,4,5,5	49
2	FOL	142-A	201	32/32	-	-	4,4,5,5	49
2	FOL	143-A	201	32/32	-	-	4,4,5,5	49
2	FOL	144-A	201	32/32	-	-	4,4,5,5	49
2	FOL	145-A	201	32/32	-	-	4,4,5,5	49
2	FOL	146-A	201	32/32	-	-	4,4,5,6	49
2	FOL	147-A	201	32/32	-	-	4,4,5,6	49
2	FOL	148-A	201	32/32	-	-	4,4,5,5	49
2	FOL	149-A	201	32/32	-	-	4,4,5,5	49
2	FOL	150-A	201	32/32	-	-	4,4,5,5	49
2	FOL	151-A	201	32/32	-	-	4,4,5,5	49
2	FOL	152-A	201	32/32	-	-	4,4,5,5	49
2	FOL	153-A	201	32/32	-	-	4,4,5,6	49
2	FOL	154-A	201	32/32	-	-	4,4,5,5	49
2	FOL	155-A	201	32/32	-	-	4,4,5,5	49
2	FOL	156-A	201	32/32	-	-	4,4,5,5	49
2	FOL	157-A	201	32/32	-	-	4,4,5,5	49
2	FOL	158-A	201	32/32	-	-	4,4,5,5	49
2	FOL	159-A	201	32/32	-	-	4,4,5,5	49
2	FOL	160-A	201	32/32	-	-	4,4,5,6	49
2	FOL	161-A	201	32/32	-	-	4,4,5,5	49
2	FOL	162-A	201	32/32	-	-	4,4,5,6	49
2	FOL	163-A	201	32/32	-	-	4,4,5,6	49
2	FOL	164-A	201	32/32	-	-	4,4,5,6	49
2	FOL	165-A	201	32/32	-	-	4,4,5,6	49
2	FOL	166-A	201	32/32	-	-	4,4,5,5	49
2	FOL	167-A	201	32/32	-	-	4,4,5,5	49
2	FOL	168-A	201	32/32	-	-	4,4,5,5	49
2	FOL	169-A	201	32/32	-	-	4,4,5,5	49
2	FOL	170-A	201	32/32	-	-	4,4,5,5	49
2	FOL	171-A	201	32/32	-	-	4,4,5,6	49
2	FOL	172-A	201	32/32	-	-	4,4,5,6	49
2	FOL	173-A	201	32/32	-	-	4,4,5,6	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FOL	174-A	201	32/32	-	-	4,4,5,6	49
2	FOL	175-A	201	32/32	-	-	4,4,5,6	49
2	FOL	176-A	201	32/32	-	-	4,4,5,6	49
2	FOL	177-A	201	32/32	-	-	4,4,5,6	49
2	FOL	178-A	201	32/32	-	-	4,4,5,5	49
2	FOL	179-A	201	32/32	-	-	4,4,5,5	49
2	FOL	180-A	201	32/32	-	-	4,4,5,5	49
2	FOL	181-A	201	32/32	-	-	4,4,5,5	49
2	FOL	182-A	201	32/32	-	-	4,4,5,6	49
2	FOL	183-A	201	32/32	-	-	4,4,5,6	49
2	FOL	184-A	201	32/32	-	-	4,4,5,6	49
2	FOL	185-A	201	32/32	-	-	4,4,5,6	49
2	FOL	186-A	201	32/32	-	-	4,4,5,6	49
2	FOL	187-A	201	32/32	-	-	4,4,5,5	49
2	FOL	188-A	201	32/32	-	-	4,4,5,5	49
2	FOL	189-A	201	32/32	-	-	4,4,5,5	49
2	FOL	190-A	201	32/32	-	-	4,4,5,5	49
2	FOL	191-A	201	32/32	-	-	4,4,5,6	49
2	FOL	192-A	201	32/32	-	-	4,4,5,6	49
2	FOL	193-A	201	32/32	-	-	4,4,5,6	49
2	FOL	194-A	201	32/32	-	-	4,4,5,6	49
2	FOL	195-A	201	32/32	-	-	4,4,5,6	49
2	FOL	196-A	201	32/32	-	-	4,4,5,6	49
2	FOL	197-A	201	32/32	-	-	4,4,5,5	49
2	FOL	198-A	201	32/32	-	-	4,4,5,5	49
2	FOL	199-A	201	32/32	-	-	4,4,5,5	49
2	FOL	200-A	201	32/32	-	-	4,4,5,5	49
2	FOL	201-A	201	32/32	-	-	4,4,5,5	49
2	FOL	202-A	201	32/32	-	-	4,4,5,5	49
2	FOL	203-A	201	32/32	-	-	4,4,5,5	49
2	FOL	204-A	201	32/32	-	-	4,4,5,6	49
2	FOL	205-A	201	32/32	-	-	4,4,5,5	49
2	FOL	206-A	201	32/32	-	-	4,4,5,5	49
2	FOL	207-A	201	32/32	-	-	4,4,5,5	49
2	FOL	208-A	201	32/32	-	-	4,4,5,6	49
2	FOL	209-A	201	32/32	-	-	4,4,5,6	49
2	FOL	210-A	201	32/32	-	-	4,4,5,5	49
2	FOL	211-A	201	32/32	-	-	4,4,5,5	49
2	FOL	212-A	201	32/32	-	-	4,4,5,5	49
2	FOL	213-A	201	32/32	-	-	4,4,5,6	49
2	FOL	214-A	201	32/32	-	-	4,4,5,5	49
2	FOL	215-A	201	32/32	-	-	4,4,5,6	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FOL	216-A	201	32/32	-	-	4,4,5,5	49
2	FOL	217-A	201	32/32	-	-	4,4,5,6	49
2	FOL	218-A	201	32/32	-	-	4,4,5,6	49
2	FOL	219-A	201	32/32	-	-	4,4,5,6	49
2	FOL	220-A	201	32/32	-	-	4,4,5,5	49
2	FOL	221-A	201	32/32	-	-	4,4,5,6	49
2	FOL	222-A	201	32/32	-	-	4,4,5,6	49
2	FOL	223-A	201	32/32	-	-	4,4,5,6	49
2	FOL	224-A	201	32/32	-	-	4,4,5,5	49
2	FOL	225-A	201	32/32	-	-	4,4,5,5	49
2	FOL	226-A	201	32/32	-	-	4,4,5,5	49
2	FOL	227-A	201	32/32	-	-	4,4,5,5	49
2	FOL	228-A	201	32/32	-	-	4,4,5,6	49
2	FOL	229-A	201	32/32	-	-	4,4,5,6	49
2	FOL	230-A	201	32/32	-	-	4,4,5,6	49
2	FOL	231-A	201	32/32	-	-	4,4,5,5	49
2	FOL	232-A	201	32/32	-	-	4,4,5,5	49
2	FOL	233-A	201	32/32	-	-	4,4,5,5	49
2	FOL	234-A	201	32/32	-	-	4,4,5,6	49
2	FOL	235-A	201	32/32	-	-	4,4,5,5	49
2	FOL	236-A	201	32/32	-	-	4,4,5,5	49
2	FOL	237-A	201	32/32	-	-	4,4,5,5	49
2	FOL	238-A	201	32/32	-	-	4,4,5,5	49
2	FOL	239-A	201	32/32	-	-	4,4,5,5	49
2	FOL	240-A	201	32/32	-	-	4,4,5,5	49
2	FOL	241-A	201	32/32	-	-	4,4,5,5	49
2	FOL	242-A	201	32/32	-	-	4,4,5,5	49
2	FOL	243-A	201	32/32	-	-	4,4,5,5	49
2	FOL	244-A	201	32/32	-	-	4,4,5,6	49
2	FOL	245-A	201	32/32	-	-	4,4,5,6	49
2	FOL	246-A	201	32/32	-	-	4,4,5,5	49
2	FOL	247-A	201	32/32	-	-	4,4,5,5	49
2	FOL	248-A	201	32/32	-	-	4,4,5,5	49
2	FOL	249-A	201	32/32	-	-	4,4,5,5	49
2	FOL	250-A	201	32/32	-	-	4,4,5,6	49
3	NAP	1-A	202	48/48	0.86	0.13	4,5,5,6	69
3	NAP	2-A	202	48/48	-	-	4,5,5,6	69
3	NAP	3-A	202	48/48	-	-	4,5,5,6	69
3	NAP	4-A	202	48/48	-	-	4,5,5,6	69
3	NAP	5-A	202	48/48	-	-	4,5,5,6	69
3	NAP	6-A	202	48/48	-	-	4,5,5,6	69
3	NAP	7-A	202	48/48	-	-	4,5,5,6	69

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	8-A	202	48/48	-	-	4,5,5,6	69
3	NAP	9-A	202	48/48	-	-	4,5,5,6	69
3	NAP	10-A	202	48/48	-	-	4,5,5,6	69
3	NAP	11-A	202	48/48	-	-	4,5,5,6	69
3	NAP	12-A	202	48/48	-	-	4,5,5,6	69
3	NAP	13-A	202	48/48	-	-	4,5,5,6	69
3	NAP	14-A	202	48/48	-	-	4,5,5,6	69
3	NAP	15-A	202	48/48	-	-	4,5,5,6	69
3	NAP	16-A	202	48/48	-	-	4,5,5,6	69
3	NAP	17-A	202	48/48	-	-	4,5,5,6	69
3	NAP	18-A	202	48/48	-	-	4,5,5,6	69
3	NAP	19-A	202	48/48	-	-	4,5,5,6	69
3	NAP	20-A	202	48/48	-	-	4,5,5,6	69
3	NAP	21-A	202	48/48	-	-	4,5,5,6	69
3	NAP	22-A	202	48/48	-	-	4,5,5,6	69
3	NAP	23-A	202	48/48	-	-	4,5,5,6	69
3	NAP	24-A	202	48/48	-	-	4,5,5,6	69
3	NAP	25-A	202	48/48	-	-	4,5,5,6	69
3	NAP	26-A	202	48/48	-	-	4,5,5,6	69
3	NAP	27-A	202	48/48	-	-	4,5,5,6	69
3	NAP	28-A	202	48/48	-	-	4,5,5,6	69
3	NAP	29-A	202	48/48	-	-	4,5,5,6	69
3	NAP	30-A	202	48/48	-	-	4,5,5,6	69
3	NAP	31-A	202	48/48	-	-	4,5,5,6	69
3	NAP	32-A	202	48/48	-	-	4,5,5,6	69
3	NAP	33-A	202	48/48	-	-	4,5,5,6	69
3	NAP	34-A	202	48/48	-	-	4,5,5,6	69
3	NAP	35-A	202	48/48	-	-	4,5,5,6	69
3	NAP	36-A	202	48/48	-	-	4,5,5,6	69
3	NAP	37-A	202	48/48	-	-	4,5,5,6	69
3	NAP	38-A	202	48/48	-	-	4,5,5,6	69
3	NAP	39-A	202	48/48	-	-	4,5,5,6	69
3	NAP	40-A	202	48/48	-	-	4,5,5,6	69
3	NAP	41-A	202	48/48	-	-	4,5,5,6	69
3	NAP	42-A	202	48/48	-	-	4,5,5,6	69
3	NAP	43-A	202	48/48	-	-	4,5,5,6	69
3	NAP	44-A	202	48/48	-	-	4,5,5,6	69
3	NAP	45-A	202	48/48	-	-	4,5,5,6	69
3	NAP	46-A	202	48/48	-	-	4,5,5,6	69
3	NAP	47-A	202	48/48	-	-	4,5,5,6	69
3	NAP	48-A	202	48/48	-	-	4,5,5,6	69
3	NAP	49-A	202	48/48	-	-	4,5,5,6	69

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	50-A	202	48/48	-	-	4,5,5,6	69
3	NAP	51-A	202	48/48	-	-	4,5,5,6	69
3	NAP	52-A	202	48/48	-	-	4,5,5,6	69
3	NAP	53-A	202	48/48	-	-	4,5,5,6	69
3	NAP	54-A	202	48/48	-	-	4,5,5,6	69
3	NAP	55-A	202	48/48	-	-	4,5,5,6	69
3	NAP	56-A	202	48/48	-	-	4,5,5,6	69
3	NAP	57-A	202	48/48	-	-	4,5,5,6	69
3	NAP	58-A	202	48/48	-	-	4,5,5,6	69
3	NAP	59-A	202	48/48	-	-	4,5,5,6	69
3	NAP	60-A	202	48/48	-	-	4,5,5,6	69
3	NAP	61-A	202	48/48	-	-	4,5,5,6	69
3	NAP	62-A	202	48/48	-	-	4,5,5,6	69
3	NAP	63-A	202	48/48	-	-	4,5,5,6	69
3	NAP	64-A	202	48/48	-	-	4,5,5,6	69
3	NAP	65-A	202	48/48	-	-	4,5,5,6	69
3	NAP	66-A	202	48/48	-	-	4,5,5,6	69
3	NAP	67-A	202	48/48	-	-	4,5,5,6	69
3	NAP	68-A	202	48/48	-	-	4,5,5,6	69
3	NAP	69-A	202	48/48	-	-	4,5,5,6	69
3	NAP	70-A	202	48/48	-	-	4,5,5,6	69
3	NAP	71-A	202	48/48	-	-	4,5,5,6	69
3	NAP	72-A	202	48/48	-	-	4,5,5,6	69
3	NAP	73-A	202	48/48	-	-	4,5,5,6	69
3	NAP	74-A	202	48/48	-	-	4,5,5,6	69
3	NAP	75-A	202	48/48	-	-	4,5,5,6	69
3	NAP	76-A	202	48/48	-	-	4,5,5,6	69
3	NAP	77-A	202	48/48	-	-	4,5,5,6	69
3	NAP	78-A	202	48/48	-	-	4,5,5,6	69
3	NAP	79-A	202	48/48	-	-	4,5,5,6	69
3	NAP	80-A	202	48/48	-	-	4,5,5,6	69
3	NAP	81-A	202	48/48	-	-	4,5,5,6	69
3	NAP	82-A	202	48/48	-	-	4,5,5,6	69
3	NAP	83-A	202	48/48	-	-	4,5,5,6	69
3	NAP	84-A	202	48/48	-	-	4,5,5,6	69
3	NAP	85-A	202	48/48	-	-	4,5,5,6	69
3	NAP	86-A	202	48/48	-	-	4,5,5,6	69
3	NAP	87-A	202	48/48	-	-	4,5,5,6	69
3	NAP	88-A	202	48/48	-	-	4,5,5,6	69
3	NAP	89-A	202	48/48	-	-	4,5,5,6	69
3	NAP	90-A	202	48/48	-	-	4,5,5,6	69
3	NAP	91-A	202	48/48	-	-	4,5,5,6	69

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	92-A	202	48/48	-	-	4,5,5,6	69
3	NAP	93-A	202	48/48	-	-	4,5,5,6	69
3	NAP	94-A	202	48/48	-	-	4,5,5,6	69
3	NAP	95-A	202	48/48	-	-	4,5,5,6	69
3	NAP	96-A	202	48/48	-	-	4,5,5,6	69
3	NAP	97-A	202	48/48	-	-	4,5,5,6	69
3	NAP	98-A	202	48/48	-	-	4,5,5,6	69
3	NAP	99-A	202	48/48	-	-	4,5,5,6	69
3	NAP	100-A	202	48/48	-	-	4,5,5,6	69
3	NAP	101-A	202	48/48	-	-	4,5,5,6	69
3	NAP	102-A	202	48/48	-	-	4,5,5,6	69
3	NAP	103-A	202	48/48	-	-	4,5,5,6	69
3	NAP	104-A	202	48/48	-	-	4,5,5,6	69
3	NAP	105-A	202	48/48	-	-	4,5,5,6	69
3	NAP	106-A	202	48/48	-	-	4,5,5,6	69
3	NAP	107-A	202	48/48	-	-	4,5,5,6	69
3	NAP	108-A	202	48/48	-	-	4,5,5,6	69
3	NAP	109-A	202	48/48	-	-	4,5,5,6	69
3	NAP	110-A	202	48/48	-	-	4,5,5,6	69
3	NAP	111-A	202	48/48	-	-	4,5,5,6	69
3	NAP	112-A	202	48/48	-	-	4,5,5,6	69
3	NAP	113-A	202	48/48	-	-	4,5,5,6	69
3	NAP	114-A	202	48/48	-	-	4,5,5,6	69
3	NAP	115-A	202	48/48	-	-	4,5,5,6	69
3	NAP	116-A	202	48/48	-	-	4,5,5,6	69
3	NAP	117-A	202	48/48	-	-	4,5,5,6	69
3	NAP	118-A	202	48/48	-	-	4,5,5,6	69
3	NAP	119-A	202	48/48	-	-	4,5,5,6	69
3	NAP	120-A	202	48/48	-	-	4,5,5,6	69
3	NAP	121-A	202	48/48	-	-	4,5,5,6	69
3	NAP	122-A	202	48/48	-	-	4,5,5,6	69
3	NAP	123-A	202	48/48	-	-	4,5,5,6	69
3	NAP	124-A	202	48/48	-	-	4,5,5,6	69
3	NAP	125-A	202	48/48	-	-	4,5,5,6	69
3	NAP	126-A	202	48/48	-	-	4,5,5,6	69
3	NAP	127-A	202	48/48	-	-	4,5,5,6	69
3	NAP	128-A	202	48/48	-	-	4,5,5,6	69
3	NAP	129-A	202	48/48	-	-	4,5,5,6	69
3	NAP	130-A	202	48/48	-	-	4,5,5,6	69
3	NAP	131-A	202	48/48	-	-	4,5,5,6	69
3	NAP	132-A	202	48/48	-	-	4,5,5,6	69
3	NAP	133-A	202	48/48	-	-	4,5,5,6	69

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	134-A	202	48/48	-	-	4,5,5,6	69
3	NAP	135-A	202	48/48	-	-	4,5,5,6	69
3	NAP	136-A	202	48/48	-	-	4,5,5,6	69
3	NAP	137-A	202	48/48	-	-	4,5,5,6	69
3	NAP	138-A	202	48/48	-	-	4,5,5,6	69
3	NAP	139-A	202	48/48	-	-	4,5,5,6	69
3	NAP	140-A	202	48/48	-	-	4,5,5,6	69
3	NAP	141-A	202	48/48	-	-	4,5,5,6	69
3	NAP	142-A	202	48/48	-	-	4,5,5,6	69
3	NAP	143-A	202	48/48	-	-	4,5,5,6	69
3	NAP	144-A	202	48/48	-	-	4,5,5,6	69
3	NAP	145-A	202	48/48	-	-	4,5,5,6	69
3	NAP	146-A	202	48/48	-	-	4,5,5,6	69
3	NAP	147-A	202	48/48	-	-	4,5,5,6	69
3	NAP	148-A	202	48/48	-	-	4,5,5,6	69
3	NAP	149-A	202	48/48	-	-	4,5,5,6	69
3	NAP	150-A	202	48/48	-	-	4,5,5,6	69
3	NAP	151-A	202	48/48	-	-	4,5,5,6	69
3	NAP	152-A	202	48/48	-	-	4,5,5,6	69
3	NAP	153-A	202	48/48	-	-	4,5,5,6	69
3	NAP	154-A	202	48/48	-	-	4,5,5,6	69
3	NAP	155-A	202	48/48	-	-	4,5,5,6	69
3	NAP	156-A	202	48/48	-	-	4,5,5,6	69
3	NAP	157-A	202	48/48	-	-	4,5,5,6	69
3	NAP	158-A	202	48/48	-	-	4,5,5,6	69
3	NAP	159-A	202	48/48	-	-	4,5,5,6	69
3	NAP	160-A	202	48/48	-	-	4,5,5,6	69
3	NAP	161-A	202	48/48	-	-	4,5,5,6	69
3	NAP	162-A	202	48/48	-	-	4,5,5,6	69
3	NAP	163-A	202	48/48	-	-	4,5,5,6	69
3	NAP	164-A	202	48/48	-	-	4,5,5,6	69
3	NAP	165-A	202	48/48	-	-	4,5,5,6	69
3	NAP	166-A	202	48/48	-	-	4,5,5,6	69
3	NAP	167-A	202	48/48	-	-	4,5,5,6	69
3	NAP	168-A	202	48/48	-	-	4,5,5,6	69
3	NAP	169-A	202	48/48	-	-	4,5,5,6	69
3	NAP	170-A	202	48/48	-	-	4,5,5,6	69
3	NAP	171-A	202	48/48	-	-	4,5,5,6	69
3	NAP	172-A	202	48/48	-	-	4,5,5,6	69
3	NAP	173-A	202	48/48	-	-	4,5,5,6	69
3	NAP	174-A	202	48/48	-	-	4,5,5,6	69
3	NAP	175-A	202	48/48	-	-	4,5,5,6	69

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	176-A	202	48/48	-	-	4,5,5,6	69
3	NAP	177-A	202	48/48	-	-	4,5,5,6	69
3	NAP	178-A	202	48/48	-	-	4,5,5,6	69
3	NAP	179-A	202	48/48	-	-	4,5,5,6	69
3	NAP	180-A	202	48/48	-	-	4,5,5,6	69
3	NAP	181-A	202	48/48	-	-	4,5,5,6	69
3	NAP	182-A	202	48/48	-	-	4,5,5,6	69
3	NAP	183-A	202	48/48	-	-	4,5,5,6	69
3	NAP	184-A	202	48/48	-	-	4,5,5,6	69
3	NAP	185-A	202	48/48	-	-	4,5,5,6	69
3	NAP	186-A	202	48/48	-	-	4,5,5,6	69
3	NAP	187-A	202	48/48	-	-	4,5,5,6	69
3	NAP	188-A	202	48/48	-	-	4,5,5,6	69
3	NAP	189-A	202	48/48	-	-	4,5,5,6	69
3	NAP	190-A	202	48/48	-	-	4,5,5,6	69
3	NAP	191-A	202	48/48	-	-	4,5,5,6	69
3	NAP	192-A	202	48/48	-	-	4,5,5,6	69
3	NAP	193-A	202	48/48	-	-	4,5,5,6	69
3	NAP	194-A	202	48/48	-	-	4,5,5,6	69
3	NAP	195-A	202	48/48	-	-	4,5,5,6	69
3	NAP	196-A	202	48/48	-	-	4,5,5,6	69
3	NAP	197-A	202	48/48	-	-	4,5,5,6	69
3	NAP	198-A	202	48/48	-	-	4,5,5,6	69
3	NAP	199-A	202	48/48	-	-	4,5,5,6	69
3	NAP	200-A	202	48/48	-	-	4,5,5,6	69
3	NAP	201-A	202	48/48	-	-	4,5,5,6	69
3	NAP	202-A	202	48/48	-	-	4,5,5,6	69
3	NAP	203-A	202	48/48	-	-	4,5,5,6	69
3	NAP	204-A	202	48/48	-	-	4,5,5,6	69
3	NAP	205-A	202	48/48	-	-	4,5,5,6	69
3	NAP	206-A	202	48/48	-	-	4,5,5,6	69
3	NAP	207-A	202	48/48	-	-	4,5,5,6	69
3	NAP	208-A	202	48/48	-	-	4,5,5,6	69
3	NAP	209-A	202	48/48	-	-	4,5,5,6	69
3	NAP	210-A	202	48/48	-	-	4,5,5,6	69
3	NAP	211-A	202	48/48	-	-	4,5,5,6	69
3	NAP	212-A	202	48/48	-	-	4,5,5,6	69
3	NAP	213-A	202	48/48	-	-	4,5,5,6	69
3	NAP	214-A	202	48/48	-	-	4,5,5,6	69
3	NAP	215-A	202	48/48	-	-	4,5,5,6	69
3	NAP	216-A	202	48/48	-	-	4,5,5,6	69
3	NAP	217-A	202	48/48	-	-	4,5,5,6	69

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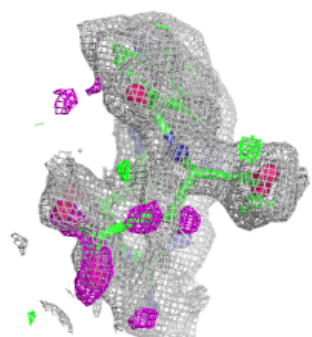
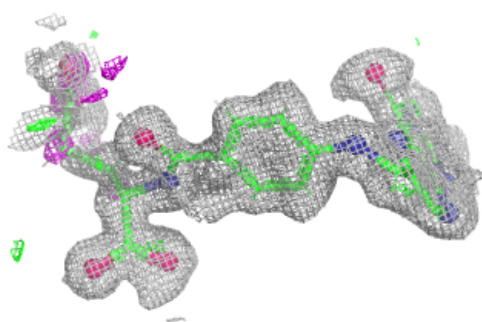
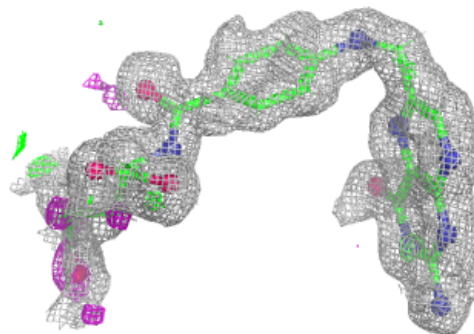
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAP	218-A	202	48/48	-	-	4,5,5,6	69
3	NAP	219-A	202	48/48	-	-	4,5,5,6	69
3	NAP	220-A	202	48/48	-	-	4,5,5,6	69
3	NAP	221-A	202	48/48	-	-	4,5,5,6	69
3	NAP	222-A	202	48/48	-	-	4,5,5,6	69
3	NAP	223-A	202	48/48	-	-	4,5,5,6	69
3	NAP	224-A	202	48/48	-	-	4,5,5,6	69
3	NAP	225-A	202	48/48	-	-	4,5,5,6	69
3	NAP	226-A	202	48/48	-	-	4,5,5,6	69
3	NAP	227-A	202	48/48	-	-	4,5,5,6	69
3	NAP	228-A	202	48/48	-	-	4,5,5,6	69
3	NAP	229-A	202	48/48	-	-	4,5,5,6	69
3	NAP	230-A	202	48/48	-	-	4,5,5,6	69
3	NAP	231-A	202	48/48	-	-	4,5,5,6	69
3	NAP	232-A	202	48/48	-	-	4,5,5,6	69
3	NAP	233-A	202	48/48	-	-	4,5,5,6	69
3	NAP	234-A	202	48/48	-	-	4,5,5,6	69
3	NAP	235-A	202	48/48	-	-	4,5,5,6	69
3	NAP	236-A	202	48/48	-	-	4,5,5,6	69
3	NAP	237-A	202	48/48	-	-	4,5,5,6	69
3	NAP	238-A	202	48/48	-	-	4,5,5,6	69
3	NAP	239-A	202	48/48	-	-	4,5,5,6	69
3	NAP	240-A	202	48/48	-	-	4,5,5,6	69
3	NAP	241-A	202	48/48	-	-	4,5,5,6	69
3	NAP	242-A	202	48/48	-	-	4,5,5,6	69
3	NAP	243-A	202	48/48	-	-	4,5,5,6	69
3	NAP	244-A	202	48/48	-	-	4,5,5,6	69
3	NAP	245-A	202	48/48	-	-	4,5,5,6	69
3	NAP	246-A	202	48/48	-	-	4,5,5,6	69
3	NAP	247-A	202	48/48	-	-	4,5,5,6	69
3	NAP	248-A	202	48/48	-	-	4,5,5,6	69
3	NAP	249-A	202	48/48	-	-	4,5,5,6	69
3	NAP	250-A	202	48/48	-	-	4,5,5,6	69

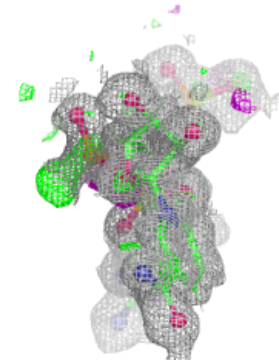
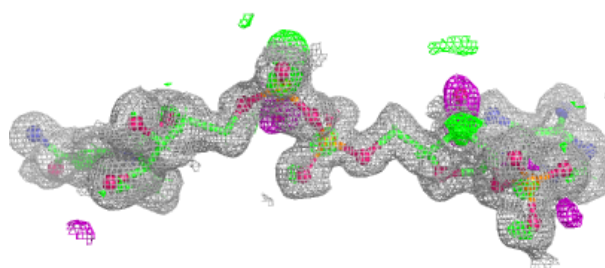
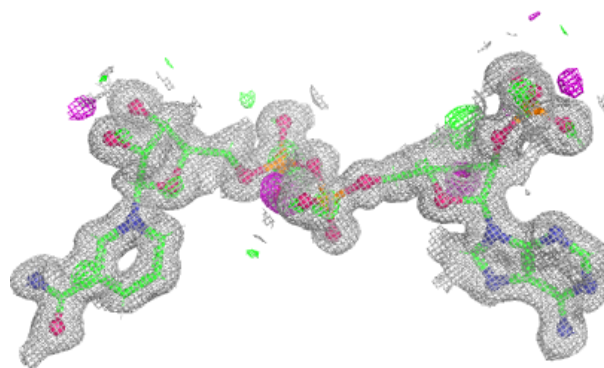
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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