



wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2024 – 06:15 PM EDT

PDB ID : 4P3R
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

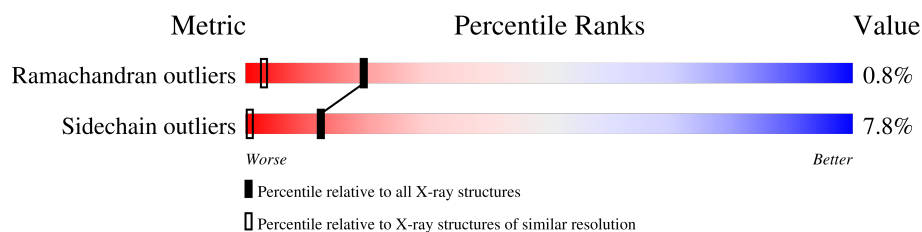
1 Overall quality at a glance

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))
Ramachandran outliers	138981	1483 (1.18-1.10)
Sidechain outliers	138945	1480 (1.18-1.10)














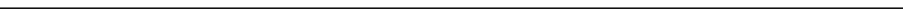











The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	159	92% 5% . .
1	10-A	159	92% 6% .
1	100-A	159	92% 7% .
1	101-A	159	90% 8% . .
1	102-A	159	89% 9% .
1	103-A	159	87% 12% .
1	104-A	159	89% 9% .
1	105-A	159	91% 9%
1	106-A	159	92% 6% .














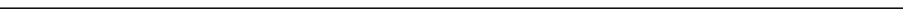





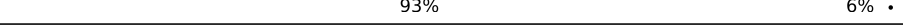
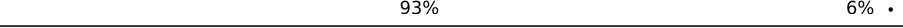




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Mol	Chain	Length	Quality of chain
1	107-A	159	 91% 8% .
1	108-A	159	 91% 8% .
1	109-A	159	 89% 9% ..
1	11-A	159	 93% 6% .
1	110-A	159	 88% 10% .
1	111-A	159	 88% 11% .
1	112-A	159	 90% 9% .
1	113-A	159	 89% 11% .
1	114-A	159	 92% 8% .
1	115-A	159	 92% 5% ..
1	116-A	159	 95% . .
1	117-A	159	 93% 7%
1	118-A	159	 94% 6% .
1	119-A	159	 94% 5% .
1	12-A	159	 91% 9%
1	120-A	159	 91% 7% .
1	121-A	159	 88% 9% ..
1	122-A	159	 92% 6% ..
1	123-A	159	 91% 7% .
1	124-A	159	 89% 9% .
1	125-A	159	 92% 7% ..
1	126-A	159	 91% 8% .
1	127-A	159	 91% 6% ..
1	128-A	159	 92% 5% ..
1	129-A	159	 88% 12%














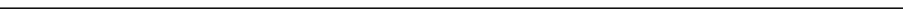


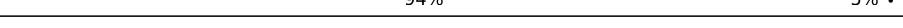
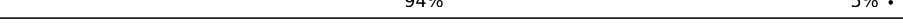

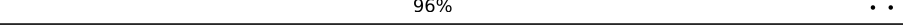





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Mol	Chain	Length	Quality of chain
1	13-A	159	 89% 9% ..
1	130-A	159	 91% 8% .
1	131-A	159	 89% 8% ..
1	132-A	159	 87% 10% ..
1	133-A	159	 91% 6% ..
1	134-A	159	 93% 5% ..
1	135-A	159	 92% 6% .
1	136-A	159	 89% 10% ..
1	137-A	159	 89% 8% ..
1	138-A	159	 91% 9% .
1	139-A	159	 92% 6% .
1	14-A	159	 92% 6% .
1	140-A	159	 87% 10% ..
1	141-A	159	 89% 9% ..
1	142-A	159	 88% 9% ..
1	143-A	159	 89% 7% ..
1	144-A	159	 89% 8% ..
1	145-A	159	 91% 9% .
1	146-A	159	 93% 6% .
1	147-A	159	 93% 6% .
1	148-A	159	 93% 5% ..
1	149-A	159	 89% 9% ..
1	15-A	159	 93% 6% .
1	150-A	159	 90% 9% .
1	151-A	159	 91% 6% ..




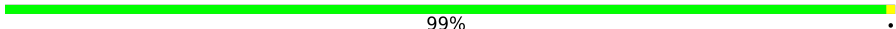
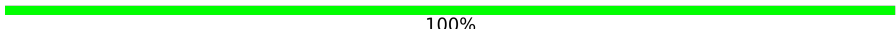

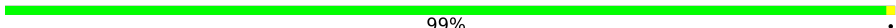
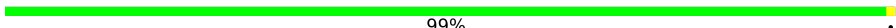
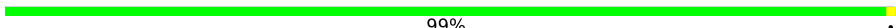
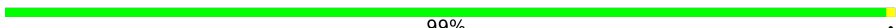
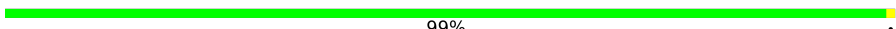
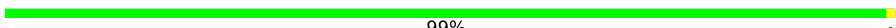
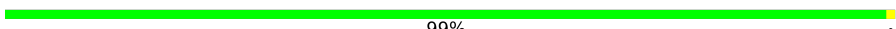
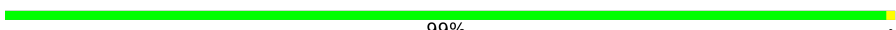
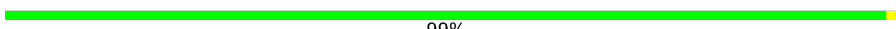
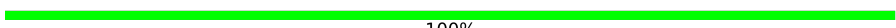

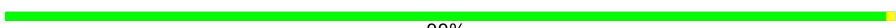
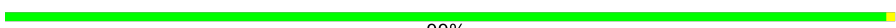
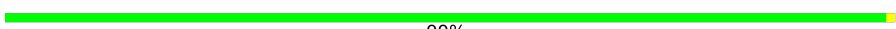
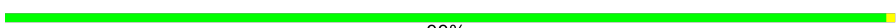

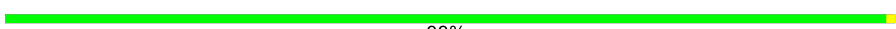


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Mol	Chain	Length	Quality of chain
1	152-A	159	 91% 9% .
1	153-A	159	 89% 9% .
1	154-A	159	 88% 11% .
1	155-A	159	 92% 6% .
1	156-A	159	 91% 7% .
1	157-A	159	 90% 9% .
1	158-A	159	 94% 5% ..
1	159-A	159	 94% 6% .
1	16-A	159	 94% 6% .
1	160-A	159	 89% 9% .
1	161-A	159	 94% 5% .
1	162-A	159	 91% 9% .
1	163-A	159	 89% 10% .
1	164-A	159	 91% 8% .
1	165-A	159	 92% 6% .
1	166-A	159	 94% 5% .
1	167-A	159	 94% 5% .
1	168-A	159	 89% 9% .
1	169-A	159	 96% ..
1	17-A	159	 92% 8%
1	170-A	159	 93% 6% .
1	171-A	159	 92% 6% .
1	172-A	159	 89% 9% .
1	173-A	159	 89% 9% .
1	174-A	159	 90% 8% .

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Mol	Chain	Length	Quality of chain
1	175-A	159	 90% 8% .
1	176-A	159	 92% 8% .
1	177-A	159	 94% . .
1	178-A	159	 99% .
1	179-A	159	 100%
1	18-A	159	 91% 8% .
1	180-A	159	 99% .
1	181-A	159	 99% .
1	182-A	159	 99% .
1	183-A	159	 99% .
1	184-A	159	 99% .
1	185-A	159	 99% .
1	186-A	159	 99% .
1	187-A	159	 99% .
1	188-A	159	 99% .
1	189-A	159	 100%
1	19-A	159	 89% 9% .
1	190-A	159	 99% .
1	191-A	159	 99% .
1	192-A	159	 99% .
1	193-A	159	 99% .
1	194-A	159	 99% .
1	195-A	159	 99% .
1	196-A	159	 100%
1	197-A	159	 99% .


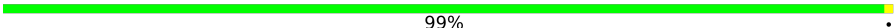
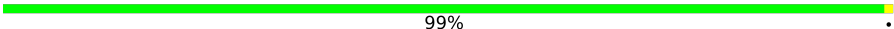
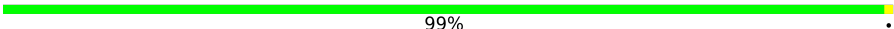
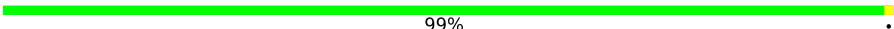

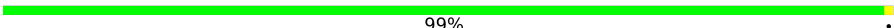
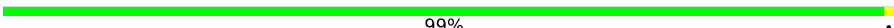
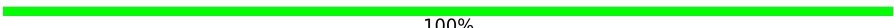
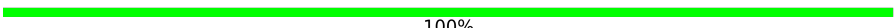
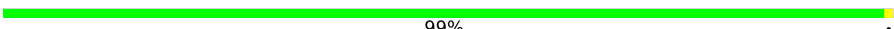

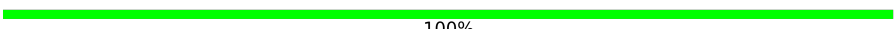
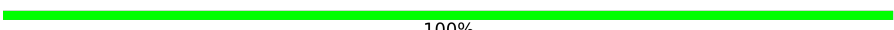
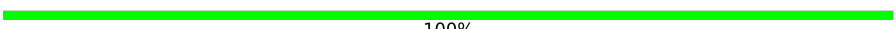
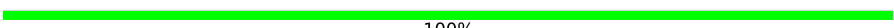
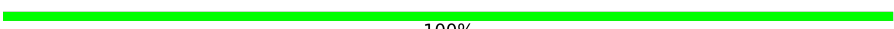
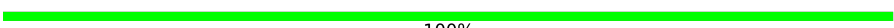
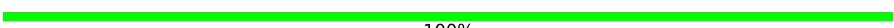
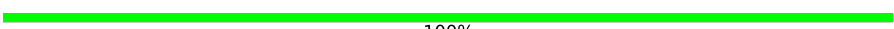
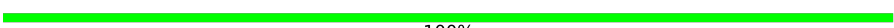
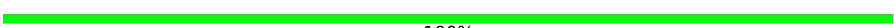



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Mol	Chain	Length	Quality of chain
1	198-A	159	100%
1	199-A	159	100%
1	2-A	159	91% 8% .
1	20-A	159	89% 9% .
1	200-A	159	100%
1	201-A	159	100%
1	202-A	159	100%
1	203-A	159	100%
1	204-A	159	100%
1	205-A	159	99% .
1	206-A	159	100%
1	207-A	159	100%
1	208-A	159	100%
1	209-A	159	99% .
1	21-A	159	92% 8% .
1	210-A	159	99% .
1	211-A	159	100%
1	212-A	159	99% .
1	213-A	159	99% .
1	214-A	159	99% .
1	215-A	159	99% .
1	216-A	159	99% .
1	217-A	159	99% .
1	218-A	159	99% .
1	219-A	159	99% .

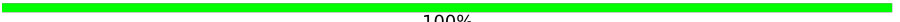

















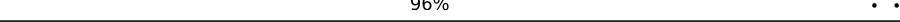






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Mol	Chain	Length	Quality of chain
1	22-A	159	 93% 5% .
1	220-A	159	 99% .
1	221-A	159	 99% .
1	222-A	159	 99% .
1	223-A	159	 99% .
1	224-A	159	 98% .
1	225-A	159	 99% .
1	226-A	159	 99% .
1	227-A	159	 100%
1	228-A	159	 100%
1	229-A	159	 99% .
1	23-A	159	 92% 6% .
1	230-A	159	 100%
1	231-A	159	 100%
1	232-A	159	 100%
1	233-A	159	 100%
1	234-A	159	 100%
1	235-A	159	 100%
1	236-A	159	 100%
1	237-A	159	 100%
1	238-A	159	 100%
1	239-A	159	 100%
1	24-A	159	 89% 10% .
1	240-A	159	 100%
1	241-A	159	 100%





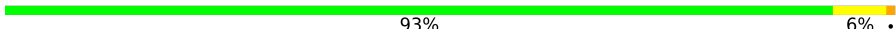

















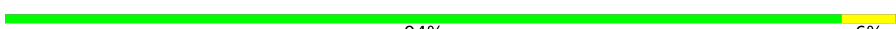


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Mol	Chain	Length	Quality of chain
1	242-A	159	 100%
1	243-A	159	 100%
1	244-A	159	 100%
1	245-A	159	 100%
1	246-A	159	 100%
1	247-A	159	 99% .
1	248-A	159	 100%
1	249-A	159	 100%
1	25-A	159	 91% 8% .
1	250-A	159	 100%
1	26-A	159	 91% 8% .
1	27-A	159	 94% 6%
1	28-A	159	 91% 8% .
1	29-A	159	 94% 6% .
1	3-A	159	 89% 7% .
1	30-A	159	 93% 6% .
1	31-A	159	 93% 6% .
1	32-A	159	 96% . .
1	33-A	159	 93% 6% .
1	34-A	159	 91% 9% .
1	35-A	159	 89% 9% . .
1	36-A	159	 91% 7% .
1	37-A	159	 93% 7%
1	38-A	159	 91% 8% . .
1	39-A	159	 92% 8% .














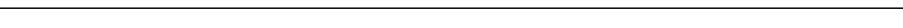











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Mol	Chain	Length	Quality of chain
1	4-A	159	 92% 6% .
1	40-A	159	 91% 6% .
1	41-A	159	 89% 9% ..
1	42-A	159	 91% 7% .
1	43-A	159	 93% 6% .
1	44-A	159	 92% 7% .
1	45-A	159	 94% 6% .
1	46-A	159	 92% 6% .
1	47-A	159	 89% 8% .
1	48-A	159	 90% 8% .
1	49-A	159	 89% 9% .
1	5-A	159	 93% . .
1	50-A	159	 90% 8% .
1	51-A	159	 89% 9% .
1	52-A	159	 88% 10% .
1	53-A	159	 88% 9% ..
1	54-A	159	 88% 11% .
1	55-A	159	 90% 8% .
1	56-A	159	 91% 8% .
1	57-A	159	 87% 8% .
1	58-A	159	 89% 9% .
1	59-A	159	 89% 8% .
1	6-A	159	 94% 6% .
1	60-A	159	 90% 8% .
1	61-A	159	 91% 8% .











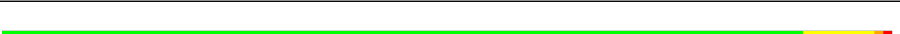


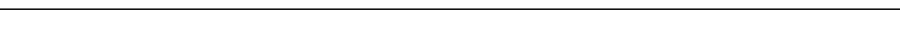
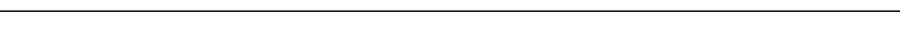
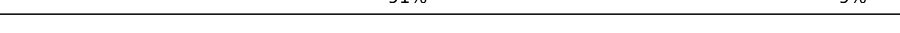
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Mol	Chain	Length	Quality of chain
1	62-A	159	 87% 10% ..
1	63-A	159	 89% 8% ..
1	64-A	159	 89% 9% ..
1	65-A	159	 91% 7% ..
1	66-A	159	 86% 10% ..
1	67-A	159	 89% 8% .
1	68-A	159	 91% 6% .
1	69-A	159	 89% 9% ..
1	7-A	159	 93% 5% .
1	70-A	159	 87% 9% .
1	71-A	159	 89% 7% .
1	72-A	159	 92% 6% .
1	73-A	159	 91% 7% .
1	74-A	159	 89% 11% .
1	75-A	159	 90% 7% .
1	76-A	159	 88% 8% .
1	77-A	159	 91% 6% .
1	78-A	159	 89% 9% .
1	79-A	159	 92% 8% .
1	8-A	159	 91% 8% .
1	80-A	159	 93% 6% .
1	81-A	159	 92% 6% .
1	82-A	159	 93% . .
1	83-A	159	 88% 9% .
1	84-A	159	 88% 10% ..

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Mol	Chain	Length	Quality of chain
1	85-A	159	 88% 11% .
1	86-A	159	 91% 8% .
1	87-A	159	 91% 8% .
1	88-A	159	 89% 9% .
1	89-A	159	 94% 6% .
1	9-A	159	 91% 7% .
1	90-A	159	 91% 7% ..
1	91-A	159	 91% 8% .
1	92-A	159	 92% 7% .
1	93-A	159	 91% 9% .
1	94-A	159	 90% 8% ..
1	95-A	159	 92% 6% .
1	96-A	159	 91% 8% .
1	97-A	159	 88% 11% .
1	98-A	159	 91% 9%
1	99-A	159	 91% 8% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FOL	221-A	201	-	X	-	-

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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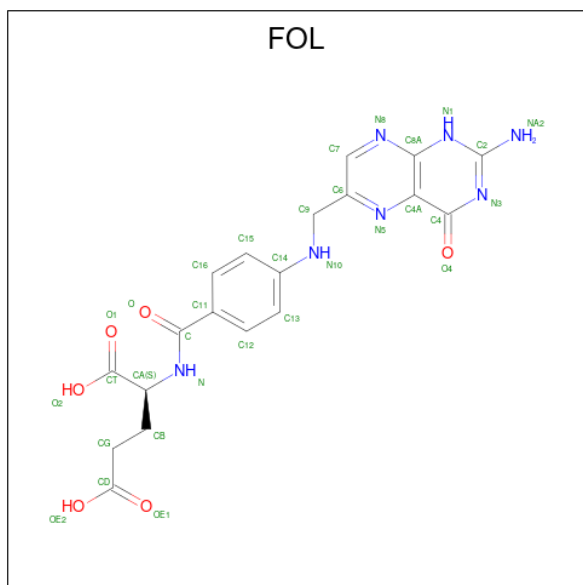
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	227-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	228-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	229-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	7			
1	230-A	159	Total	C	H	N	O	S	0	0	0
			2492	805	1224	217	239	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 (three-letter code: 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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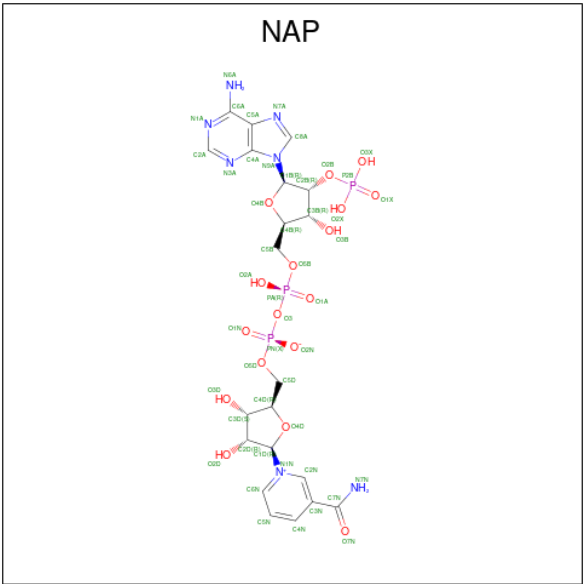
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	219-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	220-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	221-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	222-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	223-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	224-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	225-A	1	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	C	H	N	O	0	0
			49	19	17	7	6		
2	241-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	242-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	243-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	244-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	245-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	246-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	247-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	248-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	249-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		
2	250-A	1	Total	C	H	N	O	0	0
			49	19	17	7	6		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

- Molecule 1: Dihydrofolate reductase

Chain 1-A:  92% 5% . .



- Molecule 1: Dihydrofolate reductase

Chain 2-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 3-A:  89% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 4-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 5-A:  93% . .



- Molecule 1: Dihydrofolate reductase

Chain 6-A:  94% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 7-A:  93% 5% .



- Molecule 1: Dihydrofolate reductase

Chain 8-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 9-A:  91% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 10-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 11-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 12-A:  91% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 13-A:  89% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 14-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 15-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 16-A:  94% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 17-A:  92% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 18-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 19-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 20-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 21-A:  92% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 22-A:  93% 5% .



- Molecule 1: Dihydrofolate reductase

Chain 23-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 24-A:  89% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 25-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 26-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 27-A:  94% 6%



- Molecule 1: Dihydrofolate reductase

Chain 28-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 29-A:  94% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 30-A:  93% 6% .



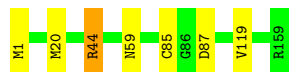
- Molecule 1: Dihydrofolate reductase

Chain 31-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 32-A:  96% . .



- Molecule 1: Dihydrofolate reductase

Chain 33-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 34-A:  91% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 35-A:  89% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 36-A:  91% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 37-A:  93% 7%



- Molecule 1: Dihydrofolate reductase

Chain 38-A:  91% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 39-A:  92% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 40-A:  91% 6% .



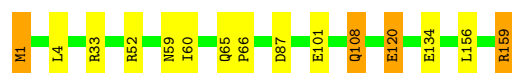
- Molecule 1: Dihydrofolate reductase

Chain 41-A:  89% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 42-A:  91% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 43-A:  93% 6% .



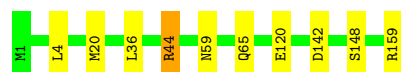
- Molecule 1: Dihydrofolate reductase

Chain 44-A:  92% 7% .



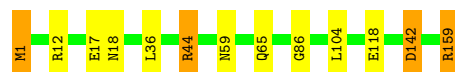
- Molecule 1: Dihydrofolate reductase

Chain 45-A:  94% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 46-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 47-A:  89% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 48-A:  90% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 49-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 50-A:  90% 8% .



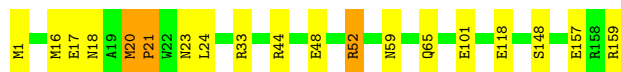
- Molecule 1: Dihydrofolate reductase

Chain 51-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 52-A:  88% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 53-A:  88% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 54-A:  88% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 55-A:  90% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 56-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 57-A:  87% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 58-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 59-A:  89% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 60-A:  90% 8% .




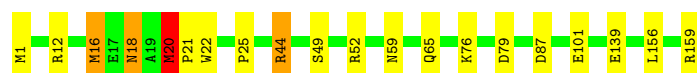
- Molecule 1: Dihydrofolate reductase

Chain 61-A:  91% 8% .



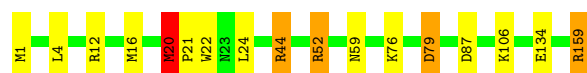
- Molecule 1: Dihydrofolate reductase

Chain 62-A:  87% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 63-A:  89% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 64-A:  89% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 65-A:  91% 7% ..



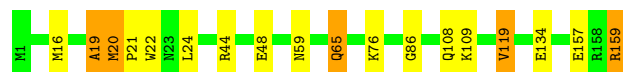
- Molecule 1: Dihydrofolate reductase

Chain 66-A:  86% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 67-A:  89% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 68-A:  91% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 69-A:  89% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 70-A:  87% 9% .



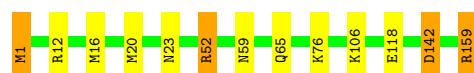
- Molecule 1: Dihydrofolate reductase

Chain 71-A:  89% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 72-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 73-A:  91% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 74-A:  89% 11% .



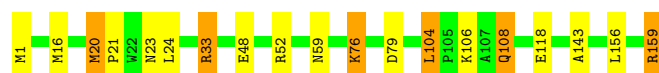
- Molecule 1: Dihydrofolate reductase

Chain 75-A:  90% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 76-A:  88% 8% .



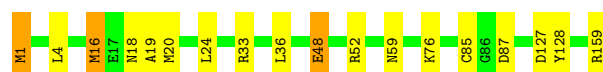
- Molecule 1: Dihydrofolate reductase

Chain 77-A:  91% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 78-A:  89% 9% .



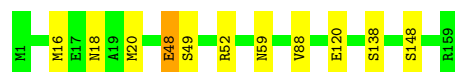
- Molecule 1: Dihydrofolate reductase

Chain 79-A:  92% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 80-A:  93% 6% .



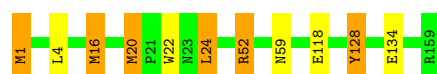
- Molecule 1: Dihydrofolate reductase

Chain 81-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 82-A:  93% . .



- Molecule 1: Dihydrofolate reductase

Chain 83-A:  88% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 84-A:  88% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 85-A:  88% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 86-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 87-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 88-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 89-A:  94% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 90-A:  91% 7% ..



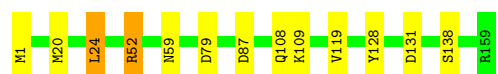
- Molecule 1: Dihydrofolate reductase

Chain 91-A:  91% 8% .



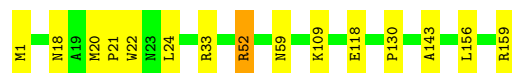
- Molecule 1: Dihydrofolate reductase

Chain 92-A:  92% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 93-A:  91% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 94-A:  90% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 95-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 96-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 97-A:  88% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 98-A:  91% 9%



- Molecule 1: Dihydrofolate reductase

Chain 99-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 100-A:  92% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 101-A:  90% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 102-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 103-A:  87% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 104-A:  89% 9% .



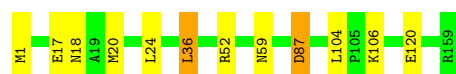
• Molecule 1: Dihydrofolate reductase

Chain 105-A:  91% 9%



• Molecule 1: Dihydrofolate reductase

Chain 106-A:  92% 6% .



• Molecule 1: Dihydrofolate reductase

Chain 107-A:  91% 8% .



• Molecule 1: Dihydrofolate reductase

Chain 108-A:  91% 8% .



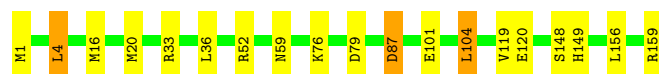
• Molecule 1: Dihydrofolate reductase

Chain 109-A:  89% 9% ..



• Molecule 1: Dihydrofolate reductase

Chain 110-A:  88% 10% .



• Molecule 1: Dihydrofolate reductase

Chain 111-A:  88% 11% .



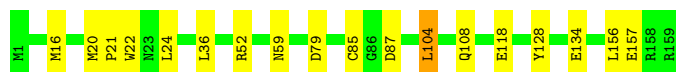
- Molecule 1: Dihydrofolate reductase

Chain 112-A:  90% 9% .



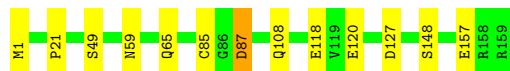
- Molecule 1: Dihydrofolate reductase

Chain 113-A:  89% 11% .



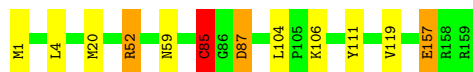
- Molecule 1: Dihydrofolate reductase

Chain 114-A:  92% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 115-A:  92% 5% ..



- Molecule 1: Dihydrofolate reductase

Chain 116-A:  95% ..



- Molecule 1: Dihydrofolate reductase

Chain 117-A:  93% 7%



- Molecule 1: Dihydrofolate reductase

Chain 118-A:  94% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 119-A:  94% 5% .



- Molecule 1: Dihydrofolate reductase

Chain 120-A:  91% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 121-A:  88% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 122-A:  92% 6% ..



- Molecule 1: Dihydrofolate reductase

Chain 123-A:  91% 7% .



- Molecule 1: Dihydrofolate reductase

Chain 124-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 125-A:  92% 7% ..



- Molecule 1: Dihydrofolate reductase

Chain 126-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 127-A:  91% 6% ..



- Molecule 1: Dihydrofolate reductase

Chain 128-A:  92% 5% ..



- Molecule 1: Dihydrofolate reductase

Chain 129-A:  88% 12%



- Molecule 1: Dihydrofolate reductase

Chain 130-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 131-A:  89% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 132-A:  87% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 133-A:  91% 6% ..



- Molecule 1: Dihydrofolate reductase

Chain 134-A:  93% 5% ..



- Molecule 1: Dihydrofolate reductase

Chain 135-A:  92% 6% .



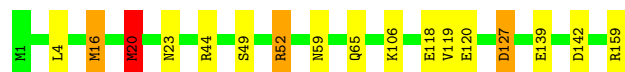
- Molecule 1: Dihydrofolate reductase

Chain 136-A:  89% 10% ..



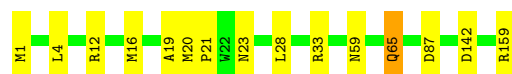
- Molecule 1: Dihydrofolate reductase

Chain 137-A:  89% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 138-A:  91% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 139-A:  92% 6% .



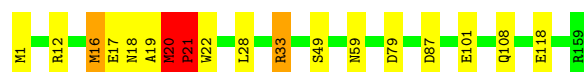
- Molecule 1: Dihydrofolate reductase

Chain 140-A:  87% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 141-A:  89% 9% ..



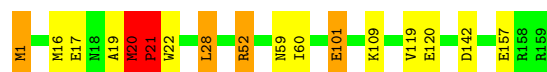
- Molecule 1: Dihydrofolate reductase

Chain 142-A:  88% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 143-A:  89% 7% ..



- Molecule 1: Dihydrofolate reductase

Chain 144-A:  89% 8% ..



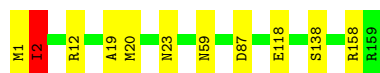
- Molecule 1: Dihydrofolate reductase

Chain 145-A:  91% 9% .



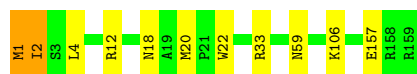
- Molecule 1: Dihydrofolate reductase

Chain 146-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 147-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 148-A:  93% 5% ..



- Molecule 1: Dihydrofolate reductase

Chain 149-A:  89% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 150-A:  90% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 151-A:  91% 6% ..



- Molecule 1: Dihydrofolate reductase

Chain 152-A:  91% 9% .



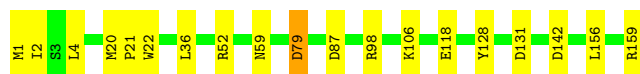
- Molecule 1: Dihydrofolate reductase

Chain 153-A:  89% 9% .



• Molecule 1: Dihydrofolate reductase

Chain 154-A:  88% 11% .



• Molecule 1: Dihydrofolate reductase

Chain 155-A:  92% 6% .



• Molecule 1: Dihydrofolate reductase

Chain 156-A:  91% 7% .



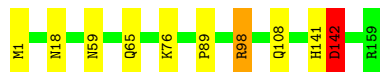
• Molecule 1: Dihydrofolate reductase

Chain 157-A:  90% 9% .



• Molecule 1: Dihydrofolate reductase

Chain 158-A:  94% 5% ..



• Molecule 1: Dihydrofolate reductase

Chain 159-A:  94% 6% .



• Molecule 1: Dihydrofolate reductase

Chain 160-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 161-A:  94% 5% .



- Molecule 1: Dihydrofolate reductase

Chain 162-A:  91% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 163-A:  89% 10% .



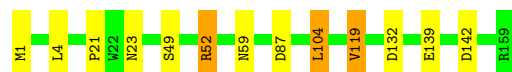
- Molecule 1: Dihydrofolate reductase

Chain 164-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 165-A:  92% 6% .



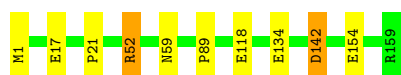
- Molecule 1: Dihydrofolate reductase

Chain 166-A:  94% 5% .



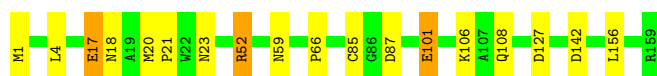
- Molecule 1: Dihydrofolate reductase

Chain 167-A:  94% 5% .



- Molecule 1: Dihydrofolate reductase

Chain 168-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 169-A:  96% . .



- Molecule 1: Dihydrofolate reductase

Chain 170-A:  93% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 171-A:  92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 172-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 173-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 174-A:  90% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 175-A:  90% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 176-A:  92% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 177-A:  94% . .



- Molecule 1: Dihydrofolate reductase

Chain 178-A:  99% .



- Molecule 1: Dihydrofolate reductase

Chain 179-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 180-A:  99% .



- Molecule 1: Dihydrofolate reductase

Chain 181-A:  99% .



- Molecule 1: Dihydrofolate reductase

Chain 182-A:  99%



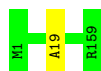
- Molecule 1: Dihydrofolate reductase

Chain 183-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 184-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 185-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 186-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 187-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 188-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 189-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 190-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 191-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 192-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 193-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 194-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 195-A:  99%



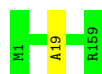
- Molecule 1: Dihydrofolate reductase

Chain 196-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 197-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 198-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 199-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 200-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 201-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 202-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 203-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 204-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 205-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 206-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 207-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 208-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 209-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 210-A:  99%



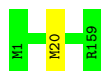
- Molecule 1: Dihydrofolate reductase

Chain 211-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 212-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 213-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 214-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 215-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 216-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 217-A:  99%



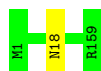
- Molecule 1: Dihydrofolate reductase

Chain 218-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 219-A:  99%



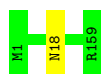
- Molecule 1: Dihydrofolate reductase

Chain 220-A:  99%



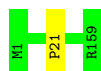
- Molecule 1: Dihydrofolate reductase

Chain 221-A:  99%



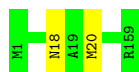
- Molecule 1: Dihydrofolate reductase

Chain 222-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 223-A:  99%



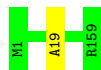
- Molecule 1: Dihydrofolate reductase

Chain 224-A:  98%



- Molecule 1: Dihydrofolate reductase

Chain 225-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 226-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 227-A:  100%

There are no outlier residues recorded for this chain.

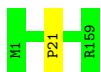
- Molecule 1: Dihydrofolate reductase

Chain 228-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 229-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 230-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 231-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 232-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 233-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 234-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 235-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 236-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 237-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 238-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 239-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 240-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 241-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 242-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 243-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 244-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 245-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 246-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 247-A:  99%



- Molecule 1: Dihydrofolate reductase

Chain 248-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 249-A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: Dihydrofolate reductase

Chain 250-A:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	34.04Å 44.82Å 98.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.77 – 1.15	Depositor
% Data completeness (in resolution range)	94.4 (40.77-1.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.99 (at 1.15Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement: 1.8.4_1496)	Depositor
R, R_{free}	0.109 , 0.136	Depositor
Wilson B-factor (Å ²)	6.9	Xtriage
Anisotropy	0.279	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	699653	wwPDB-VP
Average B, all atoms (Å ²)	5.0	wwPDB-VP

Xtriage'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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1-A	0.82	3/1302 (0.2%)	1.13	7/1770 (0.4%)
1	2-A	0.78	1/1302 (0.1%)	1.00	6/1770 (0.3%)
1	3-A	0.80	2/1302 (0.2%)	0.95	6/1770 (0.3%)
1	4-A	0.71	1/1302 (0.1%)	0.96	3/1770 (0.2%)
1	5-A	0.77	1/1302 (0.1%)	0.97	6/1770 (0.3%)
1	6-A	0.76	0/1302	0.95	5/1770 (0.3%)
1	7-A	0.77	2/1302 (0.2%)	0.92	3/1770 (0.2%)
1	8-A	0.83	3/1302 (0.2%)	0.97	8/1770 (0.5%)
1	9-A	0.79	2/1302 (0.2%)	1.02	5/1770 (0.3%)
1	10-A	0.88	6/1302 (0.5%)	0.93	3/1770 (0.2%)
1	11-A	0.75	2/1302 (0.2%)	0.95	5/1770 (0.3%)
1	12-A	0.78	2/1302 (0.2%)	0.98	4/1770 (0.2%)
1	13-A	0.91	4/1302 (0.3%)	1.01	8/1770 (0.5%)
1	14-A	0.76	1/1302 (0.1%)	0.99	5/1770 (0.3%)
1	15-A	0.77	2/1302 (0.2%)	0.91	1/1770 (0.1%)
1	16-A	0.66	0/1302	0.91	1/1770 (0.1%)
1	17-A	0.70	0/1302	0.88	0/1770
1	18-A	0.72	2/1302 (0.2%)	0.95	3/1770 (0.2%)
1	19-A	0.71	2/1302 (0.2%)	0.94	3/1770 (0.2%)
1	20-A	0.75	2/1302 (0.2%)	0.97	4/1770 (0.2%)
1	21-A	0.77	1/1302 (0.1%)	0.89	2/1770 (0.1%)
1	22-A	0.76	1/1302 (0.1%)	1.03	6/1770 (0.3%)
1	23-A	0.74	1/1302 (0.1%)	1.00	6/1770 (0.3%)
1	24-A	0.88	5/1302 (0.4%)	1.27	10/1770 (0.6%)
1	25-A	0.78	2/1302 (0.2%)	0.96	4/1770 (0.2%)
1	26-A	0.81	3/1302 (0.2%)	1.04	7/1770 (0.4%)
1	27-A	0.73	0/1302	0.88	2/1770 (0.1%)
1	28-A	0.73	1/1302 (0.1%)	0.97	7/1770 (0.4%)
1	29-A	0.78	3/1302 (0.2%)	0.91	2/1770 (0.1%)
1	30-A	0.71	1/1302 (0.1%)	0.92	4/1770 (0.2%)
1	31-A	0.89	5/1302 (0.4%)	0.97	4/1770 (0.2%)
1	32-A	0.70	1/1302 (0.1%)	0.89	1/1770 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	33-A	0.70	0/1302	0.94	4/1770 (0.2%)
1	34-A	0.84	3/1302 (0.2%)	0.99	3/1770 (0.2%)
1	35-A	0.77	2/1302 (0.2%)	1.00	5/1770 (0.3%)
1	36-A	0.79	2/1302 (0.2%)	1.02	9/1770 (0.5%)
1	37-A	0.77	2/1302 (0.2%)	0.87	0/1770
1	38-A	0.83	3/1302 (0.2%)	0.96	5/1770 (0.3%)
1	39-A	0.81	5/1302 (0.4%)	0.95	3/1770 (0.2%)
1	40-A	0.93	9/1302 (0.7%)	0.99	5/1770 (0.3%)
1	41-A	0.95	4/1302 (0.3%)	0.98	4/1770 (0.2%)
1	42-A	0.88	5/1302 (0.4%)	0.95	5/1770 (0.3%)
1	43-A	0.78	3/1302 (0.2%)	0.91	3/1770 (0.2%)
1	44-A	0.84	5/1302 (0.4%)	0.91	2/1770 (0.1%)
1	45-A	0.70	1/1302 (0.1%)	1.03	4/1770 (0.2%)
1	46-A	0.78	2/1302 (0.2%)	1.18	10/1770 (0.6%)
1	47-A	0.75	1/1302 (0.1%)	1.00	7/1770 (0.4%)
1	48-A	0.73	0/1302	0.95	3/1770 (0.2%)
1	49-A	0.83	3/1302 (0.2%)	1.04	5/1770 (0.3%)
1	50-A	0.76	0/1302	0.93	5/1770 (0.3%)
1	51-A	0.88	5/1302 (0.4%)	1.01	4/1770 (0.2%)
1	52-A	0.76	1/1302 (0.1%)	1.00	6/1770 (0.3%)
1	53-A	0.81	1/1302 (0.1%)	0.98	5/1770 (0.3%)
1	54-A	0.75	0/1302	0.90	2/1770 (0.1%)
1	55-A	0.75	0/1302	0.96	4/1770 (0.2%)
1	56-A	0.76	2/1302 (0.2%)	1.06	7/1770 (0.4%)
1	57-A	0.90	6/1302 (0.5%)	1.08	5/1770 (0.3%)
1	58-A	0.78	1/1302 (0.1%)	1.00	6/1770 (0.3%)
1	59-A	0.84	5/1302 (0.4%)	1.00	9/1770 (0.5%)
1	60-A	0.84	6/1302 (0.5%)	0.98	5/1770 (0.3%)
1	61-A	0.75	3/1302 (0.2%)	0.99	7/1770 (0.4%)
1	62-A	0.74	1/1302 (0.1%)	0.99	9/1770 (0.5%)
1	63-A	0.85	1/1302 (0.1%)	1.03	10/1770 (0.6%)
1	64-A	0.89	5/1302 (0.4%)	1.01	6/1770 (0.3%)
1	65-A	0.75	1/1302 (0.1%)	1.00	6/1770 (0.3%)
1	66-A	0.92	5/1302 (0.4%)	1.12	10/1770 (0.6%)
1	67-A	0.83	3/1302 (0.2%)	1.06	8/1770 (0.5%)
1	68-A	0.78	0/1302	1.06	8/1770 (0.5%)
1	69-A	0.87	2/1302 (0.2%)	1.21	9/1770 (0.5%)
1	70-A	0.89	4/1302 (0.3%)	1.05	6/1770 (0.3%)
1	71-A	0.80	1/1302 (0.1%)	1.06	7/1770 (0.4%)
1	72-A	0.74	1/1302 (0.1%)	0.99	7/1770 (0.4%)
1	73-A	0.77	2/1302 (0.2%)	0.95	8/1770 (0.5%)
1	74-A	0.74	2/1302 (0.2%)	0.95	5/1770 (0.3%)
1	75-A	0.75	2/1302 (0.2%)	1.04	8/1770 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	76-A	0.82	2/1302 (0.2%)	1.08	12/1770 (0.7%)
1	77-A	0.77	2/1302 (0.2%)	0.98	5/1770 (0.3%)
1	78-A	0.82	3/1302 (0.2%)	1.08	12/1770 (0.7%)
1	79-A	0.84	5/1302 (0.4%)	1.00	7/1770 (0.4%)
1	80-A	0.75	1/1302 (0.1%)	0.87	2/1770 (0.1%)
1	81-A	0.76	1/1302 (0.1%)	0.95	4/1770 (0.2%)
1	82-A	0.79	1/1302 (0.1%)	1.02	6/1770 (0.3%)
1	83-A	0.77	1/1302 (0.1%)	1.03	5/1770 (0.3%)
1	84-A	0.80	2/1302 (0.2%)	1.10	13/1770 (0.7%)
1	85-A	0.82	3/1302 (0.2%)	0.97	7/1770 (0.4%)
1	86-A	0.79	3/1302 (0.2%)	0.97	5/1770 (0.3%)
1	87-A	0.80	2/1302 (0.2%)	0.97	1/1770 (0.1%)
1	88-A	0.92	6/1302 (0.5%)	1.05	8/1770 (0.5%)
1	89-A	0.76	1/1302 (0.1%)	0.98	5/1770 (0.3%)
1	90-A	0.84	3/1302 (0.2%)	0.96	8/1770 (0.5%)
1	91-A	0.95	5/1302 (0.4%)	1.04	7/1770 (0.4%)
1	92-A	0.69	0/1302	0.91	4/1770 (0.2%)
1	93-A	0.74	0/1302	0.94	3/1770 (0.2%)
1	94-A	0.82	3/1302 (0.2%)	1.02	8/1770 (0.5%)
1	95-A	0.70	1/1302 (0.1%)	0.94	7/1770 (0.4%)
1	96-A	0.80	3/1302 (0.2%)	0.93	3/1770 (0.2%)
1	97-A	0.81	6/1302 (0.5%)	0.98	5/1770 (0.3%)
1	98-A	0.71	0/1302	0.93	2/1770 (0.1%)
1	99-A	0.77	3/1302 (0.2%)	1.00	6/1770 (0.3%)
1	100-A	0.75	0/1302	0.94	4/1770 (0.2%)
1	101-A	0.83	2/1302 (0.2%)	1.06	9/1770 (0.5%)
1	102-A	0.81	3/1302 (0.2%)	0.97	6/1770 (0.3%)
1	103-A	0.78	2/1302 (0.2%)	1.05	8/1770 (0.5%)
1	104-A	0.71	0/1302	0.94	3/1770 (0.2%)
1	105-A	0.74	1/1302 (0.1%)	0.94	3/1770 (0.2%)
1	106-A	0.79	2/1302 (0.2%)	1.01	5/1770 (0.3%)
1	107-A	0.76	2/1302 (0.2%)	0.96	4/1770 (0.2%)
1	108-A	0.72	1/1302 (0.1%)	1.05	4/1770 (0.2%)
1	109-A	0.76	0/1302	1.01	4/1770 (0.2%)
1	110-A	0.78	1/1302 (0.1%)	1.08	9/1770 (0.5%)
1	111-A	0.81	2/1302 (0.2%)	1.01	7/1770 (0.4%)
1	112-A	0.74	2/1302 (0.2%)	0.99	3/1770 (0.2%)
1	113-A	0.73	1/1302 (0.1%)	1.00	4/1770 (0.2%)
1	114-A	0.75	1/1302 (0.1%)	0.93	2/1770 (0.1%)
1	115-A	0.81	3/1302 (0.2%)	0.91	2/1770 (0.1%)
1	116-A	0.70	0/1302	0.90	2/1770 (0.1%)
1	117-A	0.75	3/1302 (0.2%)	0.87	0/1770
1	118-A	0.78	1/1302 (0.1%)	0.97	3/1770 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	119-A	0.81	1/1302 (0.1%)	0.96	1/1770 (0.1%)
1	120-A	0.75	1/1302 (0.1%)	0.99	6/1770 (0.3%)
1	121-A	0.75	2/1302 (0.2%)	1.06	10/1770 (0.6%)
1	122-A	0.77	3/1302 (0.2%)	0.99	6/1770 (0.3%)
1	123-A	0.75	1/1302 (0.1%)	0.98	7/1770 (0.4%)
1	124-A	0.82	2/1302 (0.2%)	1.04	13/1770 (0.7%)
1	125-A	0.84	6/1302 (0.5%)	1.06	7/1770 (0.4%)
1	126-A	0.83	7/1302 (0.5%)	0.93	2/1770 (0.1%)
1	127-A	0.79	3/1302 (0.2%)	1.00	4/1770 (0.2%)
1	128-A	0.75	2/1302 (0.2%)	0.97	3/1770 (0.2%)
1	129-A	0.81	2/1302 (0.2%)	0.95	6/1770 (0.3%)
1	130-A	0.77	0/1302	1.03	10/1770 (0.6%)
1	131-A	0.79	1/1302 (0.1%)	1.08	10/1770 (0.6%)
1	132-A	0.77	0/1302	1.04	10/1770 (0.6%)
1	133-A	0.74	1/1302 (0.1%)	1.00	7/1770 (0.4%)
1	134-A	0.74	0/1302	1.00	6/1770 (0.3%)
1	135-A	0.74	0/1302	0.99	3/1770 (0.2%)
1	136-A	0.77	1/1302 (0.1%)	1.02	8/1770 (0.5%)
1	137-A	0.74	0/1302	1.04	9/1770 (0.5%)
1	138-A	0.76	1/1302 (0.1%)	1.04	8/1770 (0.5%)
1	139-A	0.71	1/1302 (0.1%)	0.95	5/1770 (0.3%)
1	140-A	0.78	4/1302 (0.3%)	1.02	10/1770 (0.6%)
1	141-A	0.78	1/1302 (0.1%)	1.04	9/1770 (0.5%)
1	142-A	0.88	2/1302 (0.2%)	1.07	10/1770 (0.6%)
1	143-A	0.93	9/1302 (0.7%)	1.15	12/1770 (0.7%)
1	144-A	0.84	4/1302 (0.3%)	1.03	8/1770 (0.5%)
1	145-A	0.83	4/1302 (0.3%)	1.11	10/1770 (0.6%)
1	146-A	0.73	1/1302 (0.1%)	0.97	3/1770 (0.2%)
1	147-A	0.75	0/1302	0.90	3/1770 (0.2%)
1	148-A	0.74	1/1302 (0.1%)	0.92	3/1770 (0.2%)
1	149-A	0.85	1/1302 (0.1%)	1.04	6/1770 (0.3%)
1	150-A	0.82	3/1302 (0.2%)	1.08	7/1770 (0.4%)
1	151-A	0.77	2/1302 (0.2%)	0.96	7/1770 (0.4%)
1	152-A	0.77	0/1302	0.95	4/1770 (0.2%)
1	153-A	0.72	0/1302	0.94	5/1770 (0.3%)
1	154-A	0.74	0/1302	1.01	5/1770 (0.3%)
1	155-A	0.82	4/1302 (0.3%)	0.97	4/1770 (0.2%)
1	156-A	0.88	6/1302 (0.5%)	0.98	7/1770 (0.4%)
1	157-A	0.75	1/1302 (0.1%)	0.96	5/1770 (0.3%)
1	158-A	0.73	0/1302	0.92	3/1770 (0.2%)
1	159-A	0.75	1/1302 (0.1%)	0.93	3/1770 (0.2%)
1	160-A	0.74	1/1302 (0.1%)	1.03	8/1770 (0.5%)
1	161-A	0.69	0/1302	0.97	4/1770 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	162-A	0.76	2/1302 (0.2%)	0.93	5/1770 (0.3%)
1	163-A	0.93	6/1302 (0.5%)	0.93	5/1770 (0.3%)
1	164-A	0.72	1/1302 (0.1%)	1.01	6/1770 (0.3%)
1	165-A	0.81	0/1302	1.01	4/1770 (0.2%)
1	166-A	0.74	0/1302	0.96	4/1770 (0.2%)
1	167-A	0.78	1/1302 (0.1%)	1.03	7/1770 (0.4%)
1	168-A	0.79	4/1302 (0.3%)	0.93	3/1770 (0.2%)
1	169-A	0.67	0/1302	0.92	3/1770 (0.2%)
1	170-A	0.73	1/1302 (0.1%)	0.95	2/1770 (0.1%)
1	171-A	0.77	2/1302 (0.2%)	0.98	7/1770 (0.4%)
1	172-A	0.71	1/1302 (0.1%)	0.88	3/1770 (0.2%)
1	173-A	0.82	3/1302 (0.2%)	0.98	6/1770 (0.3%)
1	174-A	0.80	3/1302 (0.2%)	1.03	7/1770 (0.4%)
1	175-A	0.89	1/1302 (0.1%)	1.02	8/1770 (0.5%)
1	176-A	0.79	2/1302 (0.2%)	0.94	2/1770 (0.1%)
1	177-A	0.59	0/570	1.00	4/774 (0.5%)
All	All	0.79	363/229722 (0.2%)	0.99	970/312294 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	1
1	3-A	0	1
1	4-A	0	1
1	5-A	0	1
1	8-A	0	1
1	13-A	0	1
1	22-A	0	1
1	25-A	0	1
1	34-A	0	1
1	35-A	0	1
1	41-A	0	1
1	46-A	0	1
1	47-A	0	1
1	48-A	0	1
1	53-A	0	1
1	57-A	0	2
1	58-A	0	1
1	59-A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	62-A	0	1
1	65-A	0	2
1	66-A	0	3
1	67-A	0	3
1	68-A	0	2
1	69-A	0	1
1	70-A	0	1
1	71-A	0	1
1	78-A	0	1
1	82-A	0	1
1	83-A	0	1
1	84-A	0	1
1	85-A	0	1
1	94-A	0	1
1	96-A	0	2
1	100-A	0	1
1	101-A	0	1
1	109-A	0	2
1	113-A	0	1
1	114-A	0	1
1	115-A	0	2
1	120-A	0	2
1	121-A	0	2
1	122-A	0	3
1	123-A	0	1
1	124-A	0	3
1	125-A	0	1
1	126-A	0	2
1	127-A	0	1
1	128-A	0	2
1	129-A	0	2
1	130-A	0	1
1	131-A	0	2
1	133-A	0	2
1	134-A	0	2
1	138-A	0	2
1	140-A	0	2
1	141-A	0	1
1	142-A	0	2
1	143-A	0	1
1	144-A	0	2
1	146-A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	147-A	0	1
1	148-A	0	1
1	149-A	0	1
1	151-A	0	1
1	152-A	0	1
1	154-A	0	1
1	155-A	0	1
1	157-A	0	1
1	158-A	0	1
1	160-A	0	1
1	164-A	0	1
1	173-A	0	1
1	174-A	0	1
1	175-A	0	2
1	176-A	0	1
1	177-A	0	1
1	178-A	0	2
1	180-A	0	1
1	181-A	0	1
1	182-A	0	2
1	183-A	0	1
1	184-A	0	1
1	185-A	0	2
1	186-A	0	1
1	187-A	0	3
1	188-A	0	2
1	190-A	0	1
1	191-A	0	1
1	192-A	0	1
1	193-A	0	1
1	194-A	0	2
1	195-A	0	1
1	197-A	0	1
1	205-A	0	1
1	209-A	0	1
1	210-A	0	2
1	212-A	0	1
1	213-A	0	2
1	214-A	0	2
1	215-A	0	1
1	216-A	0	1
1	217-A	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	218-A	0	1
1	219-A	0	1
1	220-A	0	1
1	221-A	0	1
1	222-A	0	1
1	223-A	0	2
1	224-A	0	3
1	225-A	0	1
1	226-A	0	2
1	229-A	0	1
1	247-A	0	1
All	All	0	155

The worst 5 of 363 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	175-A	152	CYS	CB-SG	-17.08	1.53	1.82
1	41-A	120	GLU	CB-CG	12.46	1.75	1.52
1	13-A	120	GLU	CB-CG	-12.39	1.28	1.52
1	101-A	85	CYS	CB-SG	-11.88	1.62	1.82
1	40-A	101	GLU	CB-CG	11.72	1.74	1.52

The worst 5 of 970 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	69-A	44	ARG	NE-CZ-NH2	-22.77	108.92	120.30
1	24-A	44	ARG	NE-CZ-NH2	-21.25	109.67	120.30
1	46-A	44	ARG	NE-CZ-NH2	-21.14	109.73	120.30
1	24-A	44	ARG	NE-CZ-NH1	19.11	129.85	120.30
1	56-A	44	ARG	NE-CZ-NH2	-17.13	111.74	120.30

There are no chirality outliers.

5 of 155 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	1	MET	Peptide
1	3-A	1	MET	Peptide
1	4-A	1	MET	Peptide
1	5-A	1	MET	Peptide
1	8-A	1	MET	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1268	1224	1223	0	0
1	2-A	1268	1224	1223	0	0
1	3-A	1268	1224	1223	0	0
1	4-A	1268	1224	1223	0	0
1	5-A	1268	1224	1223	0	0
1	6-A	1268	1224	1223	0	0
1	7-A	1268	1224	1223	0	0
1	8-A	1268	1224	1223	0	0
1	9-A	1268	1224	1223	0	0
1	10-A	1268	1224	1223	0	0
1	11-A	1268	1224	1223	0	0
1	12-A	1268	1224	1223	0	0
1	13-A	1268	1224	1223	0	0
1	14-A	1268	1224	1223	0	0
1	15-A	1268	1224	1223	0	0
1	16-A	1268	1224	1223	0	0
1	17-A	1268	1224	1223	0	0
1	18-A	1268	1224	1223	0	0
1	19-A	1268	1224	1223	0	0
1	20-A	1268	1224	1223	0	0
1	21-A	1268	1224	1223	0	0
1	22-A	1268	1224	1223	0	0
1	23-A	1268	1224	1223	0	0
1	24-A	1268	1224	1223	0	0
1	25-A	1268	1224	1223	0	0
1	26-A	1268	1224	1223	0	0
1	27-A	1268	1224	1223	0	0
1	28-A	1268	1224	1223	0	0
1	29-A	1268	1224	1223	0	0
1	30-A	1268	1224	1223	0	0
1	31-A	1268	1224	1223	0	0
1	32-A	1268	1224	1223	0	0
1	33-A	1268	1224	1223	0	0
1	34-A	1268	1224	1223	0	0
1	35-A	1268	1224	1223	0	0
1	36-A	1268	1224	1223	0	0
1	37-A	1268	1224	1223	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	38-A	1268	1224	1223	0	0
1	39-A	1268	1224	1223	0	0
1	40-A	1268	1224	1223	0	0
1	41-A	1268	1224	1223	0	0
1	42-A	1268	1224	1223	0	0
1	43-A	1268	1224	1223	0	0
1	44-A	1268	1224	1223	0	0
1	45-A	1268	1224	1223	0	0
1	46-A	1268	1224	1223	0	0
1	47-A	1268	1224	1223	0	0
1	48-A	1268	1224	1223	0	0
1	49-A	1268	1224	1223	0	0
1	50-A	1268	1224	1223	0	0
1	51-A	1268	1224	1223	0	0
1	52-A	1268	1224	1223	0	0
1	53-A	1268	1224	1223	0	0
1	54-A	1268	1224	1223	0	0
1	55-A	1268	1224	1223	0	0
1	56-A	1268	1224	1223	0	0
1	57-A	1268	1224	1223	0	0
1	58-A	1268	1224	1223	0	0
1	59-A	1268	1224	1223	0	0
1	60-A	1268	1224	1223	0	0
1	61-A	1268	1224	1223	0	0
1	62-A	1268	1224	1223	0	0
1	63-A	1268	1224	1223	0	0
1	64-A	1268	1224	1223	0	0
1	65-A	1268	1224	1223	0	0
1	66-A	1268	1224	1223	0	0
1	67-A	1268	1224	1223	0	0
1	68-A	1268	1224	1223	0	0
1	69-A	1268	1224	1223	0	0
1	70-A	1268	1224	1223	0	0
1	71-A	1268	1224	1223	0	0
1	72-A	1268	1224	1223	0	0
1	73-A	1268	1224	1223	0	0
1	74-A	1268	1224	1223	0	0
1	75-A	1268	1224	1223	0	0
1	76-A	1268	1224	1223	0	0
1	77-A	1268	1224	1223	0	0
1	78-A	1268	1224	1223	0	0
1	79-A	1268	1224	1223	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	80-A	1268	1224	1223	0	0
1	81-A	1268	1224	1223	0	0
1	82-A	1268	1224	1223	0	0
1	83-A	1268	1224	1223	0	0
1	84-A	1268	1224	1223	0	0
1	85-A	1268	1224	1223	0	0
1	86-A	1268	1224	1223	0	0
1	87-A	1268	1224	1223	0	0
1	88-A	1268	1224	1223	0	0
1	89-A	1268	1224	1223	0	0
1	90-A	1268	1224	1223	0	0
1	91-A	1268	1224	1223	0	0
1	92-A	1268	1224	1223	0	0
1	93-A	1268	1224	1223	0	0
1	94-A	1268	1224	1223	0	0
1	95-A	1268	1224	1223	0	0
1	96-A	1268	1224	1223	0	0
1	97-A	1268	1224	1223	0	0
1	98-A	1268	1224	1223	0	0
1	99-A	1268	1224	1223	0	0
1	100-A	1268	1224	1223	0	0
1	101-A	1268	1224	1223	0	0
1	102-A	1268	1224	1223	0	0
1	103-A	1268	1224	1223	0	0
1	104-A	1268	1224	1223	0	0
1	105-A	1268	1224	1223	0	0
1	106-A	1268	1224	1223	0	0
1	107-A	1268	1224	1223	0	0
1	108-A	1268	1224	1223	0	0
1	109-A	1268	1224	1223	0	0
1	110-A	1268	1224	1223	0	0
1	111-A	1268	1224	1223	0	0
1	112-A	1268	1224	1223	0	0
1	113-A	1268	1224	1223	0	0
1	114-A	1268	1224	1223	0	0
1	115-A	1268	1224	1223	0	0
1	116-A	1268	1224	1223	0	0
1	117-A	1268	1224	1223	0	0
1	118-A	1268	1224	1223	0	0
1	119-A	1268	1224	1223	0	0
1	120-A	1268	1224	1223	0	0
1	121-A	1268	1224	1223	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	122-A	1268	1224	1223	0	0
1	123-A	1268	1224	1223	0	0
1	124-A	1268	1224	1223	0	0
1	125-A	1268	1224	1223	0	0
1	126-A	1268	1224	1223	0	0
1	127-A	1268	1224	1223	0	0
1	128-A	1268	1224	1223	0	0
1	129-A	1268	1224	1223	0	0
1	130-A	1268	1224	1223	0	0
1	131-A	1268	1224	1223	0	0
1	132-A	1268	1224	1223	0	0
1	133-A	1268	1224	1223	0	0
1	134-A	1268	1224	1223	0	0
1	135-A	1268	1224	1223	0	0
1	136-A	1268	1224	1223	0	0
1	137-A	1268	1224	1223	0	0
1	138-A	1268	1224	1223	0	0
1	139-A	1268	1224	1223	0	0
1	140-A	1268	1224	1223	0	0
1	141-A	1268	1224	1223	0	0
1	142-A	1268	1224	1223	0	0
1	143-A	1268	1224	1223	0	0
1	144-A	1268	1224	1223	0	0
1	145-A	1268	1224	1223	0	0
1	146-A	1268	1224	1223	0	0
1	147-A	1268	1224	1223	0	0
1	148-A	1268	1224	1223	0	0
1	149-A	1268	1224	1223	0	0
1	150-A	1268	1224	1223	0	0
1	151-A	1268	1224	1223	0	0
1	152-A	1268	1224	1223	0	0
1	153-A	1268	1224	1223	0	0
1	154-A	1268	1224	1223	0	0
1	155-A	1268	1224	1223	0	0
1	156-A	1268	1224	1223	0	0
1	157-A	1268	1224	1223	0	0
1	158-A	1268	1224	1223	0	0
1	159-A	1268	1224	1223	0	0
1	160-A	1268	1224	1223	0	0
1	161-A	1268	1224	1223	0	0
1	162-A	1268	1224	1223	0	0
1	163-A	1268	1224	1223	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	164-A	1268	1224	1223	0	0
1	165-A	1268	1224	1223	0	0
1	166-A	1268	1224	1223	0	0
1	167-A	1268	1224	1223	0	0
1	168-A	1268	1224	1223	0	0
1	169-A	1268	1224	1223	0	0
1	170-A	1268	1224	1223	0	0
1	171-A	1268	1224	1223	0	0
1	172-A	1268	1224	1223	0	0
1	173-A	1268	1224	1223	0	0
1	174-A	1268	1224	1223	0	0
1	175-A	1268	1224	1223	0	0
1	176-A	1268	1224	1223	0	0
1	177-A	1268	1224	576	0	0
1	178-A	1268	1224	0	0	0
1	179-A	1268	1224	0	0	0
1	180-A	1268	1224	0	0	0
1	181-A	1268	1224	0	0	0
1	182-A	1268	1224	0	0	0
1	183-A	1268	1224	0	0	0
1	184-A	1268	1224	0	0	0
1	185-A	1268	1224	0	0	0
1	186-A	1268	1224	0	0	0
1	187-A	1268	1224	0	0	0
1	188-A	1268	1224	0	0	0
1	189-A	1268	1224	0	0	0
1	190-A	1268	1224	0	0	0
1	191-A	1268	1224	0	0	0
1	192-A	1268	1224	0	0	0
1	193-A	1268	1224	0	0	0
1	194-A	1268	1224	0	0	0
1	195-A	1268	1224	0	0	0
1	196-A	1268	1224	0	0	0
1	197-A	1268	1224	0	0	0
1	198-A	1268	1224	0	0	0
1	199-A	1268	1224	0	0	0
1	200-A	1268	1224	0	0	0
1	201-A	1268	1224	0	0	0
1	202-A	1268	1224	0	0	0
1	203-A	1268	1224	0	0	0
1	204-A	1268	1224	0	0	0
1	205-A	1268	1224	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	206-A	1268	1224	0	0	0
1	207-A	1268	1224	0	0	0
1	208-A	1268	1224	0	0	0
1	209-A	1268	1224	0	0	0
1	210-A	1268	1224	0	0	0
1	211-A	1268	1224	0	0	0
1	212-A	1268	1224	0	0	0
1	213-A	1268	1224	0	0	0
1	214-A	1268	1224	0	0	0
1	215-A	1268	1224	0	0	0
1	216-A	1268	1224	0	0	0
1	217-A	1268	1224	0	0	0
1	218-A	1268	1224	0	0	0
1	219-A	1268	1224	0	0	0
1	220-A	1268	1224	0	0	0
1	221-A	1268	1224	0	0	0
1	222-A	1268	1224	0	0	0
1	223-A	1268	1224	0	0	0
1	224-A	1268	1224	0	0	0
1	225-A	1268	1224	0	0	0
1	226-A	1268	1224	0	0	0
1	227-A	1268	1224	0	0	0
1	228-A	1268	1224	0	0	0
1	229-A	1268	1224	0	0	0
1	230-A	1268	1224	0	0	0
1	231-A	1268	1224	0	0	0
1	232-A	1268	1224	0	0	0
1	233-A	1268	1224	0	0	0
1	234-A	1268	1224	0	0	0
1	235-A	1268	1224	0	0	0
1	236-A	1268	1224	0	0	0
1	237-A	1268	1224	0	0	0
1	238-A	1268	1224	0	0	0
1	239-A	1268	1224	0	0	0
1	240-A	1268	1224	0	0	0
1	241-A	1268	1224	0	0	0
1	242-A	1268	1224	0	0	0
1	243-A	1268	1224	0	0	0
1	244-A	1268	1224	0	0	0
1	245-A	1268	1224	0	0	0
1	246-A	1268	1224	0	0	0
1	247-A	1268	1224	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	248-A	1268	1224	0	0	0
1	249-A	1268	1224	0	0	0
1	250-A	1268	1224	0	0	0
2	1-A	32	17	17	0	0
2	2-A	32	17	17	0	0
2	3-A	32	17	17	0	0
2	4-A	32	17	17	0	0
2	5-A	32	17	17	0	0
2	6-A	32	17	17	0	0
2	7-A	32	17	17	0	0
2	8-A	32	17	17	0	0
2	9-A	32	17	17	0	0
2	10-A	32	17	17	0	0
2	11-A	32	17	17	0	0
2	12-A	32	17	17	0	0
2	13-A	32	17	17	0	0
2	14-A	32	17	17	0	0
2	15-A	32	17	17	0	0
2	16-A	32	17	17	0	0
2	17-A	32	17	17	0	0
2	18-A	32	17	17	0	0
2	19-A	32	17	17	0	0
2	20-A	32	17	17	0	0
2	21-A	32	17	17	0	0
2	22-A	32	17	17	0	0
2	23-A	32	17	17	0	0
2	24-A	32	17	17	0	0
2	25-A	32	17	17	0	0
2	26-A	32	17	17	0	0
2	27-A	32	17	17	0	0
2	28-A	32	17	17	0	0
2	29-A	32	17	17	0	0
2	30-A	32	17	17	0	0
2	31-A	32	17	17	0	0
2	32-A	32	17	17	0	0
2	33-A	32	17	17	0	0
2	34-A	32	17	17	0	0
2	35-A	32	17	17	0	0
2	36-A	32	17	17	0	0
2	37-A	32	17	16	0	0
2	38-A	32	17	17	0	0
2	39-A	32	17	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	40-A	32	17	17	0	0
2	41-A	32	17	17	0	0
2	42-A	32	17	17	0	0
2	43-A	32	17	17	0	0
2	44-A	32	17	17	0	0
2	45-A	32	17	17	0	0
2	46-A	32	17	17	0	0
2	47-A	32	17	17	0	0
2	48-A	32	17	17	0	0
2	49-A	32	17	17	0	0
2	50-A	32	17	17	0	0
2	51-A	32	17	17	0	0
2	52-A	32	17	17	0	0
2	53-A	32	17	17	0	0
2	54-A	32	17	17	0	0
2	55-A	32	17	17	0	0
2	56-A	32	17	17	0	0
2	57-A	32	17	17	0	0
2	58-A	32	17	17	0	0
2	59-A	32	17	17	0	0
2	60-A	32	17	17	0	0
2	61-A	32	17	17	0	0
2	62-A	32	17	17	0	0
2	63-A	32	17	17	0	0
2	64-A	32	17	17	0	0
2	65-A	32	17	17	0	0
2	66-A	32	17	17	0	0
2	67-A	32	17	17	0	0
2	68-A	32	17	17	0	0
2	69-A	32	17	17	0	0
2	70-A	32	17	17	0	0
2	71-A	32	17	17	0	0
2	72-A	32	17	17	0	0
2	73-A	32	17	17	0	0
2	74-A	32	17	17	0	0
2	75-A	32	17	17	0	0
2	76-A	32	17	17	0	0
2	77-A	32	17	17	0	0
2	78-A	32	17	17	0	0
2	79-A	32	17	17	0	0
2	80-A	32	17	17	0	0
2	81-A	32	17	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	82-A	32	17	17	0	0
2	83-A	32	17	17	0	0
2	84-A	32	17	17	0	0
2	85-A	32	17	17	0	0
2	86-A	32	17	17	0	0
2	87-A	32	17	17	0	0
2	88-A	32	17	17	0	0
2	89-A	32	17	17	0	0
2	90-A	32	17	17	0	0
2	91-A	32	17	17	0	0
2	92-A	32	17	17	0	0
2	93-A	32	17	17	0	0
2	94-A	32	17	17	0	0
2	95-A	32	17	17	0	0
2	96-A	32	17	17	0	0
2	97-A	32	17	17	0	0
2	98-A	32	17	17	0	0
2	99-A	32	17	17	0	0
2	100-A	32	17	17	0	0
2	101-A	32	17	17	0	0
2	102-A	32	17	17	0	0
2	103-A	32	17	17	0	0
2	104-A	32	17	17	0	0
2	105-A	32	17	17	0	0
2	106-A	32	17	17	0	0
2	107-A	32	17	17	0	0
2	108-A	32	17	17	0	0
2	109-A	32	17	17	0	0
2	110-A	32	17	17	0	0
2	111-A	32	17	17	0	0
2	112-A	32	17	17	0	0
2	113-A	32	17	17	0	0
2	114-A	32	17	17	0	0
2	115-A	32	17	17	0	0
2	116-A	32	17	17	0	0
2	117-A	32	17	17	0	0
2	118-A	32	17	17	0	0
2	119-A	32	17	17	0	0
2	120-A	32	17	17	0	0
2	121-A	32	17	17	0	0
2	122-A	32	17	17	0	0
2	123-A	32	17	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	124-A	32	17	17	0	0
2	125-A	32	17	17	0	0
2	126-A	32	17	17	0	0
2	127-A	32	17	17	0	0
2	128-A	32	17	17	0	0
2	129-A	32	17	17	0	0
2	130-A	32	17	17	0	0
2	131-A	32	17	17	0	0
2	132-A	32	17	17	0	0
2	133-A	32	17	17	0	0
2	134-A	32	17	17	0	0
2	135-A	32	17	17	0	0
2	136-A	32	17	17	0	0
2	137-A	32	17	17	0	0
2	138-A	32	17	17	0	0
2	139-A	32	17	17	0	0
2	140-A	32	17	17	0	0
2	141-A	32	17	17	0	0
2	142-A	32	17	17	0	0
2	143-A	32	17	17	0	0
2	144-A	32	17	17	0	0
2	145-A	32	17	17	0	0
2	146-A	32	17	17	0	0
2	147-A	32	17	17	0	0
2	148-A	32	17	17	0	0
2	149-A	32	17	17	0	0
2	150-A	32	17	17	0	0
2	151-A	32	17	17	0	0
2	152-A	32	17	17	0	0
2	153-A	32	17	17	0	0
2	154-A	32	17	17	0	0
2	155-A	32	17	17	0	0
2	156-A	32	17	17	0	0
2	157-A	32	17	17	0	0
2	158-A	32	17	17	0	0
2	159-A	32	17	17	0	0
2	160-A	32	17	17	0	0
2	161-A	32	17	17	0	0
2	162-A	32	17	17	0	0
2	163-A	32	17	17	0	0
2	164-A	32	17	17	0	0
2	165-A	32	17	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	166-A	32	17	17	0	0
2	167-A	32	17	17	0	0
2	168-A	32	17	17	0	0
2	169-A	32	17	17	0	0
2	170-A	32	17	17	0	0
2	171-A	32	17	17	0	0
2	172-A	32	17	17	0	0
2	173-A	32	17	17	0	0
2	174-A	32	17	17	0	0
2	175-A	32	17	17	0	0
2	176-A	32	17	17	0	0
2	177-A	32	17	0	0	0
2	178-A	32	17	0	0	0
2	179-A	32	17	0	0	0
2	180-A	32	17	0	0	0
2	181-A	32	17	0	0	0
2	182-A	32	17	0	0	0
2	183-A	32	17	0	0	0
2	184-A	32	17	0	0	0
2	185-A	32	17	0	0	0
2	186-A	32	17	0	0	0
2	187-A	32	17	0	0	0
2	188-A	32	17	0	0	0
2	189-A	32	17	0	0	0
2	190-A	32	17	0	0	0
2	191-A	32	17	0	0	0
2	192-A	32	17	0	0	0
2	193-A	32	17	0	0	0
2	194-A	32	17	0	0	0
2	195-A	32	17	0	0	0
2	196-A	32	17	0	0	0
2	197-A	32	17	0	0	0
2	198-A	32	17	0	0	0
2	199-A	32	17	0	0	0
2	200-A	32	17	0	0	0
2	201-A	32	17	0	0	0
2	202-A	32	17	0	0	0
2	203-A	32	17	0	0	0
2	204-A	32	17	0	0	0
2	205-A	32	17	0	0	0
2	206-A	32	17	0	0	0
2	207-A	32	17	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	208-A	32	17	0	0	0
2	209-A	32	17	0	0	0
2	210-A	32	17	0	0	0
2	211-A	32	17	0	0	0
2	212-A	32	17	0	0	0
2	213-A	32	17	0	0	0
2	214-A	32	17	0	0	0
2	215-A	32	17	0	0	0
2	216-A	32	17	0	0	0
2	217-A	32	17	0	0	0
2	218-A	32	17	0	0	0
2	219-A	32	17	0	0	0
2	220-A	32	17	0	0	0
2	221-A	32	17	0	0	0
2	222-A	32	17	0	0	0
2	223-A	32	17	0	0	0
2	224-A	32	17	0	0	0
2	225-A	32	17	0	0	0
2	226-A	32	17	0	0	0
2	227-A	32	17	0	0	0
2	228-A	32	17	0	0	0
2	229-A	32	17	0	0	0
2	230-A	32	17	0	0	0
2	231-A	32	17	0	0	0
2	232-A	32	17	0	0	0
2	233-A	32	17	0	0	0
2	234-A	32	17	0	0	0
2	235-A	32	17	0	0	0
2	236-A	32	17	0	0	0
2	237-A	32	17	0	0	0
2	238-A	32	17	0	0	0
2	239-A	32	17	0	0	0
2	240-A	32	17	0	0	0
2	241-A	32	17	0	0	0
2	242-A	32	17	0	0	0
2	243-A	32	17	0	0	0
2	244-A	32	17	0	0	0
2	245-A	32	17	0	0	0
2	246-A	32	17	0	0	0
2	247-A	32	17	0	0	0
2	248-A	32	17	0	0	0
2	249-A	32	17	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	250-A	32	17	0	0	0
3	1-A	48	21	23	0	0
3	2-A	48	21	23	0	0
3	3-A	48	21	23	0	0
3	4-A	48	21	23	0	0
3	5-A	48	21	23	0	0
3	6-A	48	21	23	0	0
3	7-A	48	21	23	0	0
3	8-A	48	21	23	0	0
3	9-A	48	21	23	0	0
3	10-A	48	21	23	0	0
3	11-A	48	21	23	0	0
3	12-A	48	21	23	0	0
3	13-A	48	21	23	0	0
3	14-A	48	21	23	0	0
3	15-A	48	21	23	0	0
3	16-A	48	21	23	0	0
3	17-A	48	21	23	0	0
3	18-A	48	21	23	0	0
3	19-A	48	21	23	0	0
3	20-A	48	21	23	0	0
3	21-A	48	21	23	0	0
3	22-A	48	21	23	0	0
3	23-A	48	21	23	0	0
3	24-A	48	21	23	0	0
3	25-A	48	21	23	0	0
3	26-A	48	21	23	0	0
3	27-A	48	21	23	0	0
3	28-A	48	21	23	0	0
3	29-A	48	21	23	0	0
3	30-A	48	21	23	0	0
3	31-A	48	21	23	0	0
3	32-A	48	21	23	0	0
3	33-A	48	21	23	0	0
3	34-A	48	21	23	0	0
3	35-A	48	21	23	0	0
3	36-A	48	21	23	0	0
3	37-A	48	21	23	0	0
3	38-A	48	21	23	0	0
3	39-A	48	21	23	0	0
3	40-A	48	21	23	0	0
3	41-A	48	21	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	42-A	48	21	23	0	0
3	43-A	48	21	23	0	0
3	44-A	48	21	23	0	0
3	45-A	48	21	23	0	0
3	46-A	48	21	23	0	0
3	47-A	48	21	23	0	0
3	48-A	48	21	23	0	0
3	49-A	48	21	23	0	0
3	50-A	48	21	23	0	0
3	51-A	48	21	23	0	0
3	52-A	48	21	23	0	0
3	53-A	48	21	23	0	0
3	54-A	48	21	23	0	0
3	55-A	48	21	23	0	0
3	56-A	48	21	23	0	0
3	57-A	48	21	23	0	0
3	58-A	48	21	23	0	0
3	59-A	48	21	23	0	0
3	60-A	48	21	23	0	0
3	61-A	48	21	23	0	0
3	62-A	48	21	23	0	0
3	63-A	48	21	23	0	0
3	64-A	48	21	23	0	0
3	65-A	48	21	23	0	0
3	66-A	48	21	23	0	0
3	67-A	48	21	23	0	0
3	68-A	48	21	23	0	0
3	69-A	48	21	23	0	0
3	70-A	48	21	23	0	0
3	71-A	48	21	23	0	0
3	72-A	48	21	23	0	0
3	73-A	48	21	23	0	0
3	74-A	48	21	23	0	0
3	75-A	48	21	23	0	0
3	76-A	48	21	23	0	0
3	77-A	48	21	23	0	0
3	78-A	48	21	23	0	0
3	79-A	48	21	23	0	0
3	80-A	48	21	23	0	0
3	81-A	48	21	23	0	0
3	82-A	48	21	23	0	0
3	83-A	48	21	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	84-A	48	21	23	0	0
3	85-A	48	21	23	0	0
3	86-A	48	21	23	0	0
3	87-A	48	21	23	0	0
3	88-A	48	21	23	0	0
3	89-A	48	21	23	0	0
3	90-A	48	21	23	0	0
3	91-A	48	21	23	0	0
3	92-A	48	21	23	0	0
3	93-A	48	21	23	0	0
3	94-A	48	21	23	0	0
3	95-A	48	21	23	0	0
3	96-A	48	21	23	0	0
3	97-A	48	21	23	0	0
3	98-A	48	21	23	0	0
3	99-A	48	21	23	0	0
3	100-A	48	21	23	0	0
3	101-A	48	21	23	0	0
3	102-A	48	21	23	0	0
3	103-A	48	21	23	0	0
3	104-A	48	21	23	0	0
3	105-A	48	21	23	0	0
3	106-A	48	21	23	0	0
3	107-A	48	21	23	0	0
3	108-A	48	21	23	0	0
3	109-A	48	21	23	0	0
3	110-A	48	21	23	0	0
3	111-A	48	21	23	0	0
3	112-A	48	21	23	0	0
3	113-A	48	21	23	0	0
3	114-A	48	21	23	0	0
3	115-A	48	21	23	0	0
3	116-A	48	21	23	0	0
3	117-A	48	21	23	0	0
3	118-A	48	21	23	0	0
3	119-A	48	21	23	0	0
3	120-A	48	21	23	0	0
3	121-A	48	21	23	0	0
3	122-A	48	21	23	0	0
3	123-A	48	21	23	0	0
3	124-A	48	21	23	0	0
3	125-A	48	21	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	126-A	48	21	23	0	0
3	127-A	48	21	23	0	0
3	128-A	48	21	23	0	0
3	129-A	48	21	23	0	0
3	130-A	48	21	23	0	0
3	131-A	48	21	23	0	0
3	132-A	48	21	23	0	0
3	133-A	48	21	23	0	0
3	134-A	48	21	23	0	0
3	135-A	48	21	23	0	0
3	136-A	48	21	23	0	0
3	137-A	48	21	23	0	0
3	138-A	48	21	23	0	0
3	139-A	48	21	23	0	0
3	140-A	48	21	23	0	0
3	141-A	48	21	23	0	0
3	142-A	48	21	23	0	0
3	143-A	48	21	23	0	0
3	144-A	48	21	23	0	0
3	145-A	48	21	23	0	0
3	146-A	48	21	23	0	0
3	147-A	48	21	23	0	0
3	148-A	48	21	23	0	0
3	149-A	48	21	23	0	0
3	150-A	48	21	23	0	0
3	151-A	48	21	23	0	0
3	152-A	48	21	23	0	0
3	153-A	48	21	23	0	0
3	154-A	48	21	23	0	0
3	155-A	48	21	23	0	0
3	156-A	48	21	23	0	0
3	157-A	48	21	23	0	0
3	158-A	48	21	23	0	0
3	159-A	48	21	23	0	0
3	160-A	48	21	23	0	0
3	161-A	48	21	23	0	0
3	162-A	48	21	23	0	0
3	163-A	48	21	23	0	0
3	164-A	48	21	23	0	0
3	165-A	48	21	23	0	0
3	166-A	48	21	23	0	0
3	167-A	48	21	23	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	168-A	48	21	23	0	0
3	169-A	48	21	23	0	0
3	170-A	48	21	23	0	0
3	171-A	48	21	23	0	0
3	172-A	48	21	23	0	0
3	173-A	48	21	23	0	0
3	174-A	48	21	23	0	0
3	175-A	48	21	23	0	0
3	176-A	48	21	23	0	0
3	177-A	48	21	0	0	0
3	178-A	48	21	0	0	0
3	179-A	48	21	0	0	0
3	180-A	48	21	0	0	0
3	181-A	48	21	0	0	0
3	182-A	48	21	0	0	0
3	183-A	48	21	0	0	0
3	184-A	48	21	0	0	0
3	185-A	48	21	0	0	0
3	186-A	48	21	0	0	0
3	187-A	48	21	0	0	0
3	188-A	48	21	0	0	0
3	189-A	48	21	0	0	0
3	190-A	48	21	0	0	0
3	191-A	48	21	0	0	0
3	192-A	48	21	0	0	0
3	193-A	48	21	0	0	0
3	194-A	48	21	0	0	0
3	195-A	48	21	0	0	0
3	196-A	48	21	0	0	0
3	197-A	48	21	0	0	0
3	198-A	48	21	0	0	0
3	199-A	48	21	0	0	0
3	200-A	48	21	0	0	0
3	201-A	48	21	0	0	0
3	202-A	48	21	0	0	0
3	203-A	48	21	0	0	0
3	204-A	48	21	0	0	0
3	205-A	48	21	0	0	0
3	206-A	48	21	0	0	0
3	207-A	48	21	0	0	0
3	208-A	48	21	0	0	0
3	209-A	48	21	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	210-A	48	21	0	0	0
3	211-A	48	21	0	0	0
3	212-A	48	21	0	0	0
3	213-A	48	21	0	0	0
3	214-A	48	21	0	0	0
3	215-A	48	21	0	0	0
3	216-A	48	21	0	0	0
3	217-A	48	21	0	0	0
3	218-A	48	21	0	0	0
3	219-A	48	21	0	0	0
3	220-A	48	21	0	0	0
3	221-A	48	21	0	0	0
3	222-A	48	21	0	0	0
3	223-A	48	21	0	0	0
3	224-A	48	21	0	0	0
3	225-A	48	21	0	0	0
3	226-A	48	21	0	0	0
3	227-A	48	21	0	0	0
3	228-A	48	21	0	0	0
3	229-A	48	21	0	0	0
3	230-A	48	21	0	0	0
3	231-A	48	21	0	0	0
3	232-A	48	21	0	0	0
3	233-A	48	21	0	0	0
3	234-A	48	21	0	0	0
3	235-A	48	21	0	0	0
3	236-A	48	21	0	0	0
3	237-A	48	21	0	0	0
3	238-A	48	21	0	0	0
3	239-A	48	21	0	0	0
3	240-A	48	21	0	0	0
3	241-A	48	21	0	0	0
3	242-A	48	21	0	0	0
3	243-A	48	21	0	0	0
3	244-A	48	21	0	0	0
3	245-A	48	21	0	0	0
3	246-A	48	21	0	0	0
3	247-A	48	21	0	0	0
3	248-A	48	21	0	0	0
3	249-A	48	21	0	0	0
3	250-A	48	21	0	0	0
4	1-A	200	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	2-A	206	0	0	0	0
4	3-A	185	0	0	0	0
4	4-A	175	0	0	0	0
4	5-A	186	0	0	0	0
4	6-A	185	0	0	0	0
4	7-A	202	0	0	0	0
4	8-A	200	0	0	0	0
4	9-A	201	0	0	0	0
4	10-A	204	0	0	0	0
4	11-A	205	0	0	0	0
4	12-A	197	0	0	0	0
4	13-A	192	0	0	0	0
4	14-A	189	0	0	0	0
4	15-A	173	0	0	0	0
4	16-A	176	0	0	0	0
4	17-A	188	0	0	0	0
4	18-A	195	0	0	0	0
4	19-A	196	0	0	0	0
4	20-A	211	0	0	0	0
4	21-A	189	0	0	0	0
4	22-A	191	0	0	0	0
4	23-A	173	0	0	0	0
4	24-A	183	0	0	0	0
4	25-A	174	0	0	0	0
4	26-A	195	0	0	0	0
4	27-A	188	0	0	0	0
4	28-A	181	0	0	0	0
4	29-A	183	0	0	0	0
4	30-A	186	0	0	0	0
4	31-A	191	0	0	0	0
4	32-A	187	0	0	0	0
4	33-A	190	0	0	0	0
4	34-A	194	0	0	0	0
4	35-A	201	0	0	0	0
4	36-A	197	0	0	0	0
4	37-A	196	0	0	0	0
4	38-A	203	0	0	0	0
4	39-A	181	0	0	0	0
4	40-A	171	0	0	0	0
4	41-A	179	0	0	0	0
4	42-A	176	0	0	0	0
4	43-A	176	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	44-A	183	0	0	0	0
4	45-A	187	0	0	0	0
4	46-A	197	0	0	0	0
4	47-A	191	0	0	0	0
4	48-A	184	0	0	0	0
4	49-A	195	0	0	0	0
4	50-A	189	0	0	0	0
4	51-A	198	0	0	0	0
4	52-A	190	0	0	0	0
4	53-A	182	0	0	0	0
4	54-A	180	0	0	0	0
4	55-A	185	0	0	0	0
4	56-A	184	0	0	0	0
4	57-A	191	0	0	0	0
4	58-A	187	0	0	0	0
4	59-A	192	0	0	0	0
4	60-A	173	0	0	0	0
4	61-A	186	0	0	0	0
4	62-A	201	0	0	0	0
4	63-A	201	0	0	0	0
4	64-A	188	0	0	0	0
4	65-A	187	0	0	0	0
4	66-A	174	0	0	0	0
4	67-A	184	0	0	0	0
4	68-A	178	0	0	0	0
4	69-A	173	0	0	0	0
4	70-A	171	0	0	0	0
4	71-A	171	0	0	0	0
4	72-A	196	0	0	0	0
4	73-A	207	0	0	0	0
4	74-A	191	0	0	0	0
4	75-A	193	0	0	0	0
4	76-A	182	0	0	0	0
4	77-A	176	0	0	0	0
4	78-A	184	0	0	0	0
4	79-A	193	0	0	0	0
4	80-A	201	0	0	0	0
4	81-A	187	0	0	0	0
4	82-A	175	0	0	0	0
4	83-A	175	0	0	0	0
4	84-A	172	0	0	0	0
4	85-A	186	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	86-A	199	0	0	0	0
4	87-A	200	0	0	0	0
4	88-A	191	0	0	0	0
4	89-A	189	0	0	0	0
4	90-A	180	0	0	0	0
4	91-A	190	0	0	0	0
4	92-A	181	0	0	0	0
4	93-A	177	0	0	0	0
4	94-A	189	0	0	0	0
4	95-A	173	0	0	0	0
4	96-A	182	0	0	0	0
4	97-A	188	0	0	0	0
4	98-A	191	0	0	0	0
4	99-A	198	0	0	0	0
4	100-A	200	0	0	0	0
4	101-A	204	0	0	0	0
4	102-A	189	0	0	0	0
4	103-A	211	0	0	0	0
4	104-A	202	0	0	0	0
4	105-A	196	0	0	0	0
4	106-A	189	0	0	0	0
4	107-A	179	0	0	0	0
4	108-A	185	0	0	0	0
4	109-A	186	0	0	0	0
4	110-A	186	0	0	0	0
4	111-A	181	0	0	0	0
4	112-A	175	0	0	0	0
4	113-A	183	0	0	0	0
4	114-A	189	0	0	0	0
4	115-A	183	0	0	0	0
4	116-A	194	0	0	0	0
4	117-A	190	0	0	0	0
4	118-A	194	0	0	0	0
4	119-A	194	0	0	0	0
4	120-A	204	0	0	0	0
4	121-A	191	0	0	0	0
4	122-A	192	0	0	0	0
4	123-A	195	0	0	0	0
4	124-A	186	0	0	0	0
4	125-A	185	0	0	0	0
4	126-A	178	0	0	0	0
4	127-A	185	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	128-A	175	0	0	0	0
4	129-A	180	0	0	0	0
4	130-A	186	0	0	0	0
4	131-A	201	0	0	0	0
4	132-A	205	0	0	0	0
4	133-A	205	0	0	0	0
4	134-A	209	0	0	0	0
4	135-A	195	0	0	0	0
4	136-A	205	0	0	0	0
4	137-A	190	0	0	0	0
4	138-A	174	0	0	0	0
4	139-A	186	0	0	0	0
4	140-A	186	0	0	0	0
4	141-A	196	0	0	0	0
4	142-A	203	0	0	0	0
4	143-A	192	0	0	0	0
4	144-A	187	0	0	0	0
4	145-A	176	0	0	0	0
4	146-A	176	0	0	0	0
4	147-A	162	0	0	0	0
4	148-A	163	0	0	0	0
4	149-A	178	0	0	0	0
4	150-A	190	0	0	0	0
4	151-A	204	0	0	0	0
4	152-A	187	0	0	0	0
4	153-A	191	0	0	0	0
4	154-A	190	0	0	0	0
4	155-A	187	0	0	0	0
4	156-A	190	0	0	0	0
4	157-A	193	0	0	0	0
4	158-A	181	0	0	0	0
4	159-A	176	0	0	0	0
4	160-A	185	0	0	0	0
4	161-A	187	0	0	0	0
4	162-A	196	0	0	0	0
4	163-A	204	0	0	0	0
4	164-A	198	0	0	0	0
4	165-A	215	0	0	0	0
4	166-A	194	0	0	0	0
4	167-A	175	0	0	0	0
4	168-A	176	0	0	0	0
4	169-A	184	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	170-A	190	0	0	0	0
4	171-A	187	0	0	0	0
4	172-A	187	0	0	0	0
4	173-A	191	0	0	0	0
4	174-A	199	0	0	0	0
4	175-A	196	0	0	0	0
4	176-A	194	0	0	0	0
4	177-A	203	0	0	0	0
4	178-A	188	0	0	0	0
4	179-A	175	0	0	0	0
4	180-A	169	0	0	0	0
4	181-A	192	0	0	0	0
4	182-A	187	0	0	0	0
4	183-A	185	0	0	0	0
4	184-A	179	0	0	0	0
4	185-A	197	0	0	0	0
4	186-A	187	0	0	0	0
4	187-A	191	0	0	0	0
4	188-A	203	0	0	0	0
4	189-A	209	0	0	0	0
4	190-A	197	0	0	0	0
4	191-A	179	0	0	0	0
4	192-A	185	0	0	0	0
4	193-A	183	0	0	0	0
4	194-A	182	0	0	0	0
4	195-A	173	0	0	0	0
4	196-A	184	0	0	0	0
4	197-A	181	0	0	0	0
4	198-A	181	0	0	0	0
4	199-A	184	0	0	0	0
4	200-A	192	0	0	0	0
4	201-A	207	0	0	0	0
4	202-A	194	0	0	0	0
4	203-A	184	0	0	0	0
4	204-A	182	0	0	0	0
4	205-A	193	0	0	0	0
4	206-A	190	0	0	0	0
4	207-A	180	0	0	0	0
4	208-A	178	0	0	0	0
4	209-A	185	0	0	0	0
4	210-A	184	0	0	0	0
4	211-A	184	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	212-A	191	0	0	0	0
4	213-A	202	0	0	0	0
4	214-A	190	0	0	0	0
4	215-A	193	0	0	0	0
4	216-A	195	0	0	0	0
4	217-A	197	0	0	0	0
4	218-A	197	0	0	0	0
4	219-A	192	0	0	0	0
4	220-A	177	0	0	0	0
4	221-A	183	0	0	0	0
4	222-A	182	0	0	0	0
4	223-A	181	0	0	0	0
4	224-A	203	0	0	0	0
4	225-A	205	0	0	0	0
4	226-A	202	0	0	0	0
4	227-A	189	0	0	0	0
4	228-A	162	0	0	0	0
4	229-A	180	0	0	0	0
4	230-A	174	0	0	0	0
4	231-A	206	0	0	0	0
4	232-A	211	0	0	0	0
4	233-A	195	0	0	0	0
4	234-A	184	0	0	0	0
4	235-A	167	0	0	0	0
4	236-A	172	0	0	0	0
4	237-A	184	0	0	0	0
4	238-A	198	0	0	0	0
4	239-A	194	0	0	0	0
4	240-A	206	0	0	0	0
4	241-A	208	0	0	0	0
4	242-A	179	0	0	0	0
4	243-A	184	0	0	0	0
4	244-A	181	0	0	0	0
4	245-A	178	0	0	0	0
4	246-A	197	0	0	0	0
4	247-A	186	0	0	0	0
4	248-A	182	0	0	0	0
4	249-A	195	0	0	0	0
4	250-A	202	0	0	0	0
All	All	384153	315500	222863	0	0

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

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	157/159 (99%)	154 (98%)	2 (1%)	1 (1%)	25	5
1	2-A	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	3-A	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	25	5
1	4-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	5
1	5-A	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	6-A	157/159 (99%)	153 (98%)	2 (1%)	2 (1%)	12	0
1	7-A	157/159 (99%)	155 (99%)	1 (1%)	1 (1%)	25	5
1	8-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	5
1	9-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	10-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	11-A	157/159 (99%)	155 (99%)	2 (1%)	0	100	100
1	12-A	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	25	5
1	13-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	5
1	14-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	0
1	15-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	16-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	17-A	157/159 (99%)	153 (98%)	2 (1%)	2 (1%)	12	0
1	18-A	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	25	5
1	19-A	157/159 (99%)	153 (98%)	2 (1%)	2 (1%)	12	0
1	20-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	5
1	21-A	157/159 (99%)	155 (99%)	1 (1%)	1 (1%)	25	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	22-A	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	23-A	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	25	5
1	24-A	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
1	25-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	26-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	5
1	27-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	28-A	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	25	5
1	29-A	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
1	30-A	157/159 (99%)	153 (98%)	3 (2%)	1 (1%)	25	5
1	31-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	32-A	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
1	33-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	5
1	34-A	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	25	5
1	35-A	157/159 (99%)	154 (98%)	2 (1%)	1 (1%)	25	5
1	36-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	37-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	38-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	12	0
1	39-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	40-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	41-A	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	25	5
1	42-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	43-A	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
1	44-A	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
1	45-A	157/159 (99%)	155 (99%)	2 (1%)	0	100	100
1	46-A	157/159 (99%)	148 (94%)	7 (4%)	2 (1%)	12	0
1	47-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	5
1	48-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	25	5
1	49-A	157/159 (99%)	153 (98%)	3 (2%)	1 (1%)	25	5
1	50-A	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	25	5
1	51-A	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	25	5
1	52-A	157/159 (99%)	148 (94%)	8 (5%)	1 (1%)	25	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	53-A	157/159 (99%)	151 (96%)	2 (1%)	4 (2%)	5	0
1	54-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	5
1	55-A	157/159 (99%)	153 (98%)	3 (2%)	1 (1%)	25	5
1	56-A	157/159 (99%)	147 (94%)	8 (5%)	2 (1%)	12	0
1	57-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	58-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	12	0
1	59-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	12	0
1	60-A	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	61-A	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
1	62-A	157/159 (99%)	148 (94%)	5 (3%)	4 (2%)	5	0
1	63-A	157/159 (99%)	150 (96%)	4 (2%)	3 (2%)	8	0
1	64-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	5
1	65-A	157/159 (99%)	152 (97%)	3 (2%)	2 (1%)	12	0
1	66-A	157/159 (99%)	152 (97%)	3 (2%)	2 (1%)	12	0
1	67-A	157/159 (99%)	151 (96%)	3 (2%)	3 (2%)	8	0
1	68-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	0
1	69-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	12	0
1	70-A	157/159 (99%)	153 (98%)	3 (2%)	1 (1%)	25	5
1	71-A	157/159 (99%)	155 (99%)	1 (1%)	1 (1%)	25	5
1	72-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	73-A	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	74-A	157/159 (99%)	151 (96%)	3 (2%)	3 (2%)	8	0
1	75-A	157/159 (99%)	153 (98%)	3 (2%)	1 (1%)	25	5
1	76-A	157/159 (99%)	146 (93%)	9 (6%)	2 (1%)	12	0
1	77-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	78-A	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
1	79-A	157/159 (99%)	153 (98%)	3 (2%)	1 (1%)	25	5
1	80-A	157/159 (99%)	153 (98%)	3 (2%)	1 (1%)	25	5
1	81-A	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	25	5
1	82-A	157/159 (99%)	148 (94%)	8 (5%)	1 (1%)	25	5
1	83-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	12	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	84-A	157/159 (99%)	145 (92%)	10 (6%)	2 (1%)	12	0
1	85-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	86-A	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
1	87-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	5
1	88-A	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	89-A	157/159 (99%)	150 (96%)	4 (2%)	3 (2%)	8	0
1	90-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	12	0
1	91-A	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	25	5
1	92-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	93-A	157/159 (99%)	149 (95%)	5 (3%)	3 (2%)	8	0
1	94-A	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
1	95-A	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
1	96-A	157/159 (99%)	153 (98%)	3 (2%)	1 (1%)	25	5
1	97-A	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	98-A	157/159 (99%)	155 (99%)	1 (1%)	1 (1%)	25	5
1	99-A	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	100-A	157/159 (99%)	151 (96%)	3 (2%)	3 (2%)	8	0
1	101-A	157/159 (99%)	154 (98%)	2 (1%)	1 (1%)	25	5
1	102-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	103-A	157/159 (99%)	154 (98%)	1 (1%)	2 (1%)	12	0
1	104-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	105-A	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
1	106-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	107-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	108-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	5
1	109-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	25	5
1	110-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	5
1	111-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	0
1	112-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	12	0
1	113-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	25	5
1	114-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	115-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	12	0
1	116-A	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
1	117-A	157/159 (99%)	148 (94%)	9 (6%)	0	100	100
1	118-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	5
1	119-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	0
1	120-A	157/159 (99%)	153 (98%)	2 (1%)	2 (1%)	12	0
1	121-A	157/159 (99%)	152 (97%)	3 (2%)	2 (1%)	12	0
1	122-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	12	0
1	123-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	25	5
1	124-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	125-A	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	126-A	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	25	5
1	127-A	157/159 (99%)	151 (96%)	3 (2%)	3 (2%)	8	0
1	128-A	157/159 (99%)	153 (98%)	3 (2%)	1 (1%)	25	5
1	129-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	5
1	130-A	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
1	131-A	157/159 (99%)	152 (97%)	3 (2%)	2 (1%)	12	0
1	132-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	4	0
1	133-A	157/159 (99%)	148 (94%)	8 (5%)	1 (1%)	25	5
1	134-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	12	0
1	135-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	12	0
1	136-A	157/159 (99%)	146 (93%)	10 (6%)	1 (1%)	25	5
1	137-A	157/159 (99%)	154 (98%)	2 (1%)	1 (1%)	25	5
1	138-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	0
1	139-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	12	0
1	140-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	0
1	141-A	157/159 (99%)	149 (95%)	4 (2%)	4 (2%)	5	0
1	142-A	157/159 (99%)	145 (92%)	7 (4%)	5 (3%)	4	0
1	143-A	157/159 (99%)	150 (96%)	4 (2%)	3 (2%)	8	0
1	144-A	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	8	0
1	145-A	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	8	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	146-A	157/159 (99%)	152 (97%)	3 (2%)	2 (1%)	12	0
1	147-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	12	0
1	148-A	157/159 (99%)	148 (94%)	7 (4%)	2 (1%)	12	0
1	149-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	12	0
1	150-A	157/159 (99%)	148 (94%)	7 (4%)	2 (1%)	12	0
1	151-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	5
1	152-A	157/159 (99%)	153 (98%)	3 (2%)	1 (1%)	25	5
1	153-A	157/159 (99%)	151 (96%)	3 (2%)	3 (2%)	8	0
1	154-A	157/159 (99%)	153 (98%)	3 (2%)	1 (1%)	25	5
1	155-A	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
1	156-A	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
1	157-A	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	158-A	157/159 (99%)	150 (96%)	4 (2%)	3 (2%)	8	0
1	159-A	157/159 (99%)	155 (99%)	2 (1%)	0	100	100
1	160-A	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	25	5
1	161-A	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	162-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	5
1	163-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	25	5
1	164-A	157/159 (99%)	155 (99%)	2 (1%)	0	100	100
1	165-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	5
1	166-A	157/159 (99%)	155 (99%)	2 (1%)	0	100	100
1	167-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	5
1	168-A	157/159 (99%)	149 (95%)	4 (2%)	4 (2%)	5	0
1	169-A	157/159 (99%)	154 (98%)	2 (1%)	1 (1%)	25	5
1	170-A	157/159 (99%)	151 (96%)	3 (2%)	3 (2%)	8	0
1	171-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	12	0
1	172-A	157/159 (99%)	151 (96%)	3 (2%)	3 (2%)	8	0
1	173-A	157/159 (99%)	150 (96%)	4 (2%)	3 (2%)	8	0
1	174-A	157/159 (99%)	145 (92%)	6 (4%)	6 (4%)	3	0
1	175-A	157/159 (99%)	149 (95%)	3 (2%)	5 (3%)	4	0
1	176-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	5	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	177-A	69/159 (43%)	63 (91%)	4 (6%)	2 (3%)	4	0
All	All	27701/28143 (98%)	26679 (96%)	798 (3%)	224 (1%)	19	3

5 of 224 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	4-A	87	ASP
1	6-A	21	PRO
1	28-A	22	TRP
1	38-A	121	GLY
1	48-A	22	TRP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	2-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	3-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	4-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	5-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	6-A	136/136 (100%)	130 (96%)	6 (4%)	28	3
1	7-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	8-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	9-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	10-A	136/136 (100%)	130 (96%)	6 (4%)	28	3
1	11-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	12-A	136/136 (100%)	129 (95%)	7 (5%)	24	2
1	13-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	14-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	15-A	136/136 (100%)	127 (93%)	9 (7%)	16	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	16-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	17-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	18-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	19-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	20-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	21-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	22-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	23-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	24-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	25-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	26-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	27-A	136/136 (100%)	129 (95%)	7 (5%)	24	2
1	28-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	29-A	136/136 (100%)	129 (95%)	7 (5%)	24	2
1	30-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	31-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	32-A	136/136 (100%)	130 (96%)	6 (4%)	28	3
1	33-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	34-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	35-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	36-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	37-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	38-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	39-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	40-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	41-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	42-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	43-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	44-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	45-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	46-A	136/136 (100%)	129 (95%)	7 (5%)	24	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	47-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	48-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	49-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	50-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	51-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	52-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	53-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	54-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	55-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	56-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	57-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	58-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	59-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	60-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	61-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	62-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	63-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	64-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	65-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	66-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	67-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	68-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	69-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	70-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	71-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	72-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	73-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	74-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	75-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	76-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	77-A	136/136 (100%)	124 (91%)	12 (9%)	10	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	78-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	79-A	136/136 (100%)	129 (95%)	7 (5%)	24	2
1	80-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	81-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	82-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	83-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	84-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	85-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	86-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	87-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	88-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	89-A	136/136 (100%)	131 (96%)	5 (4%)	34	4
1	90-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	91-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	92-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	93-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	94-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	95-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	96-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	97-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	98-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	99-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	100-A	136/136 (100%)	129 (95%)	7 (5%)	24	2
1	101-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	102-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	103-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	104-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	105-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	106-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	107-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	108-A	136/136 (100%)	126 (93%)	10 (7%)	13	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	109-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	110-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	111-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	112-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	113-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	114-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	115-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	116-A	136/136 (100%)	129 (95%)	7 (5%)	24	2
1	117-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	118-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	119-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	120-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	121-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	122-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	123-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	124-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	125-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	126-A	136/136 (100%)	130 (96%)	6 (4%)	28	3
1	127-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	128-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	129-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	130-A	136/136 (100%)	129 (95%)	7 (5%)	24	2
1	131-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	132-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	133-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	134-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	135-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	136-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	137-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	138-A	136/136 (100%)	131 (96%)	5 (4%)	34	4
1	139-A	136/136 (100%)	128 (94%)	8 (6%)	19	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	140-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	141-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	142-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	143-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	144-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	145-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	146-A	136/136 (100%)	129 (95%)	7 (5%)	24	2
1	147-A	136/136 (100%)	129 (95%)	7 (5%)	24	2
1	148-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	149-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	150-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	151-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	152-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	153-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	154-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	155-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	156-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	157-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	158-A	136/136 (100%)	129 (95%)	7 (5%)	24	2
1	159-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	160-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	161-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	162-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	163-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	164-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	165-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	166-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	167-A	136/136 (100%)	129 (95%)	7 (5%)	24	2
1	168-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	169-A	136/136 (100%)	131 (96%)	5 (4%)	34	4
1	170-A	136/136 (100%)	129 (95%)	7 (5%)	24	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	171-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	172-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	173-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	174-A	136/136 (100%)	131 (96%)	5 (4%)	34	4
1	175-A	136/136 (100%)	131 (96%)	5 (4%)	34	4
1	176-A	136/136 (100%)	131 (96%)	5 (4%)	34	4
1	177-A	60/136 (44%)	54 (90%)	6 (10%)	7	0
All	All	23996/24072 (100%)	22136 (92%)	1860 (8%)	12	1

5 of 1860 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	85-A	59	ASN
1	166-A	106	LYS
1	105-A	18	ASN
1	164-A	118	GLU
1	149-A	59	ASN

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 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	228-A	201	-	34,34,34	1.18	4 (11%)	44,47,47	2.07	9 (20%)
3	NAP	202-A	202	-	45,52,52	1.67	8 (17%)	56,80,80	1.52	10 (17%)
2	FOL	197-A	201	-	34,34,34	1.13	4 (11%)	44,47,47	1.67	8 (18%)
2	FOL	233-A	201	-	34,34,34	1.14	2 (5%)	44,47,47	2.12	12 (27%)
2	FOL	199-A	201	-	34,34,34	1.31	4 (11%)	44,47,47	2.37	15 (34%)
2	FOL	150-A	201	-	34,34,34	1.11	3 (8%)	44,47,47	2.48	10 (22%)
2	FOL	51-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	1.78	8 (18%)
2	FOL	141-A	201	-	34,34,34	1.04	2 (5%)	44,47,47	1.95	8 (18%)
3	NAP	55-A	202	-	45,52,52	1.99	7 (15%)	56,80,80	1.70	10 (17%)
3	NAP	213-A	202	-	45,52,52	2.06	6 (13%)	56,80,80	1.88	11 (19%)
2	FOL	59-A	201	-	34,34,34	1.09	3 (8%)	44,47,47	1.85	10 (22%)
2	FOL	206-A	201	-	34,34,34	1.04	3 (8%)	44,47,47	1.97	12 (27%)
3	NAP	93-A	202	-	45,52,52	1.67	6 (13%)	56,80,80	1.54	12 (21%)
3	NAP	10-A	202	-	45,52,52	1.71	8 (17%)	56,80,80	1.54	13 (23%)
2	FOL	230-A	201	-	34,34,34	1.03	2 (5%)	44,47,47	2.04	11 (25%)
3	NAP	45-A	202	-	45,52,52	2.08	7 (15%)	56,80,80	1.82	13 (23%)
3	NAP	125-A	202	-	45,52,52	1.68	7 (15%)	56,80,80	1.48	7 (12%)
3	NAP	32-A	202	-	45,52,52	1.68	7 (15%)	56,80,80	1.50	9 (16%)
2	FOL	50-A	201	-	34,34,34	1.15	3 (8%)	44,47,47	2.38	15 (34%)
2	FOL	120-A	201	-	34,34,34	1.09	2 (5%)	44,47,47	2.01	11 (25%)
3	NAP	24-A	202	-	45,52,52	1.67	7 (15%)	56,80,80	1.50	8 (14%)
3	NAP	52-A	202	-	45,52,52	1.69	7 (15%)	56,80,80	1.48	9 (16%)
2	FOL	164-A	201	-	34,34,34	1.09	3 (8%)	44,47,47	2.20	14 (31%)
3	NAP	58-A	202	-	45,52,52	1.70	7 (15%)	56,80,80	1.55	10 (17%)
2	FOL	68-A	201	-	34,34,34	1.13	4 (11%)	44,47,47	2.23	9 (20%)
3	NAP	153-A	202	-	45,52,52	1.75	7 (15%)	56,80,80	1.46	8 (14%)
3	NAP	184-A	202	-	45,52,52	1.66	6 (13%)	56,80,80	1.48	9 (16%)
3	NAP	70-A	202	-	45,52,52	1.64	6 (13%)	56,80,80	1.54	9 (16%)
3	NAP	95-A	202	-	45,52,52	1.77	7 (15%)	56,80,80	1.74	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	98-A	201	-	34,34,34	1.11	3 (8%)	44,47,47	2.33	14 (31%)
3	NAP	126-A	202	-	45,52,52	1.66	7 (15%)	56,80,80	1.48	9 (16%)
2	FOL	239-A	201	-	34,34,34	1.11	2 (5%)	44,47,47	2.33	12 (27%)
2	FOL	235-A	201	-	34,34,34	1.05	2 (5%)	44,47,47	2.05	11 (25%)
3	NAP	172-A	202	-	45,52,52	1.67	8 (17%)	56,80,80	1.52	7 (12%)
3	NAP	142-A	202	-	45,52,52	1.92	7 (15%)	56,80,80	2.07	11 (19%)
3	NAP	74-A	202	-	45,52,52	2.14	6 (13%)	56,80,80	1.87	12 (21%)
2	FOL	3-A	201	-	34,34,34	1.09	2 (5%)	44,47,47	2.00	10 (22%)
3	NAP	20-A	202	-	45,52,52	1.66	7 (15%)	56,80,80	1.50	9 (16%)
3	NAP	135-A	202	-	45,52,52	1.70	7 (15%)	56,80,80	1.65	9 (16%)
2	FOL	156-A	201	-	34,34,34	1.06	3 (8%)	44,47,47	2.56	17 (38%)
2	FOL	38-A	201	-	34,34,34	1.24	4 (11%)	44,47,47	2.31	13 (29%)
2	FOL	214-A	201	-	34,34,34	1.22	4 (11%)	44,47,47	2.05	10 (22%)
3	NAP	117-A	202	-	45,52,52	1.74	7 (15%)	56,80,80	1.55	10 (17%)
2	FOL	114-A	201	-	34,34,34	1.05	3 (8%)	44,47,47	1.85	10 (22%)
2	FOL	248-A	201	-	34,34,34	0.98	2 (5%)	44,47,47	1.94	12 (27%)
3	NAP	247-A	202	-	45,52,52	1.62	8 (17%)	56,80,80	2.08	10 (17%)
3	NAP	106-A	202	-	45,52,52	1.64	6 (13%)	56,80,80	1.52	10 (17%)
3	NAP	193-A	202	-	45,52,52	1.71	7 (15%)	56,80,80	1.54	11 (19%)
2	FOL	122-A	201	-	34,34,34	0.95	2 (5%)	44,47,47	1.94	11 (25%)
2	FOL	210-A	201	-	34,34,34	1.19	3 (8%)	44,47,47	2.23	12 (27%)
2	FOL	226-A	201	-	34,34,34	1.18	3 (8%)	44,47,47	1.75	7 (15%)
3	NAP	175-A	202	-	45,52,52	1.66	7 (15%)	56,80,80	1.55	9 (16%)
2	FOL	188-A	201	-	34,34,34	1.21	5 (14%)	44,47,47	1.97	11 (25%)
3	NAP	130-A	202	-	45,52,52	1.66	6 (13%)	56,80,80	1.44	7 (12%)
2	FOL	19-A	201	-	34,34,34	1.38	3 (8%)	44,47,47	2.31	15 (34%)
2	FOL	107-A	201	-	34,34,34	1.17	4 (11%)	44,47,47	2.06	11 (25%)
3	NAP	192-A	202	-	45,52,52	1.92	7 (15%)	56,80,80	1.91	11 (19%)
3	NAP	73-A	202	-	45,52,52	1.81	5 (11%)	56,80,80	1.73	8 (14%)
3	NAP	51-A	202	-	45,52,52	1.71	8 (17%)	56,80,80	1.66	9 (16%)
3	NAP	53-A	202	-	45,52,52	1.69	7 (15%)	56,80,80	1.49	8 (14%)
3	NAP	42-A	202	-	45,52,52	1.70	7 (15%)	56,80,80	1.43	7 (12%)
2	FOL	34-A	201	-	34,34,34	1.34	4 (11%)	44,47,47	2.00	14 (31%)
3	NAP	103-A	202	-	45,52,52	1.88	7 (15%)	56,80,80	1.55	6 (10%)
3	NAP	191-A	202	-	45,52,52	2.89	8 (17%)	56,80,80	1.92	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	218-A	202	-	45,52,52	1.66	6 (13%)	56,80,80	1.52	9 (16%)
2	FOL	165-A	201	-	34,34,34	1.01	3 (8%)	44,47,47	2.23	9 (20%)
3	NAP	100-A	202	-	45,52,52	1.67	6 (13%)	56,80,80	1.54	9 (16%)
3	NAP	14-A	202	-	45,52,52	1.71	9 (20%)	56,80,80	1.49	8 (14%)
2	FOL	37-A	201	-	34,34,34	1.26	6 (17%)	44,47,47	2.30	13 (29%)
2	FOL	88-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	2.10	12 (27%)
3	NAP	235-A	202	-	45,52,52	1.93	7 (15%)	56,80,80	1.92	11 (19%)
3	NAP	129-A	202	-	45,52,52	1.66	8 (17%)	56,80,80	1.47	9 (16%)
3	NAP	4-A	202	-	45,52,52	1.80	6 (13%)	56,80,80	2.53	11 (19%)
2	FOL	149-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	2.09	11 (25%)
3	NAP	63-A	202	-	45,52,52	2.40	7 (15%)	56,80,80	1.90	10 (17%)
2	FOL	232-A	201	-	34,34,34	1.32	5 (14%)	44,47,47	2.07	13 (29%)
2	FOL	152-A	201	-	34,34,34	1.10	2 (5%)	44,47,47	2.07	10 (22%)
2	FOL	11-A	201	-	34,34,34	1.18	3 (8%)	44,47,47	2.09	11 (25%)
3	NAP	33-A	202	-	45,52,52	1.65	6 (13%)	56,80,80	1.51	11 (19%)
3	NAP	181-A	202	-	45,52,52	1.68	6 (13%)	56,80,80	1.54	9 (16%)
3	NAP	39-A	202	-	45,52,52	1.65	6 (13%)	56,80,80	1.45	7 (12%)
2	FOL	198-A	201	-	34,34,34	1.22	4 (11%)	44,47,47	1.89	9 (20%)
2	FOL	30-A	201	-	34,34,34	1.14	2 (5%)	44,47,47	2.28	16 (36%)
2	FOL	83-A	201	-	34,34,34	1.28	3 (8%)	44,47,47	1.99	13 (29%)
3	NAP	68-A	202	-	45,52,52	1.65	7 (15%)	56,80,80	1.58	12 (21%)
2	FOL	106-A	201	-	34,34,34	1.31	3 (8%)	44,47,47	2.15	12 (27%)
2	FOL	1-A	201	-	34,34,34	0.97	1 (2%)	44,47,47	2.07	13 (29%)
3	NAP	177-A	202	-	45,52,52	1.69	7 (15%)	56,80,80	1.49	10 (17%)
3	NAP	168-A	202	-	45,52,52	1.68	7 (15%)	56,80,80	1.49	8 (14%)
2	FOL	200-A	201	-	34,34,34	1.11	3 (8%)	44,47,47	2.29	9 (20%)
2	FOL	245-A	201	-	34,34,34	1.05	2 (5%)	44,47,47	2.09	12 (27%)
3	NAP	225-A	202	-	45,52,52	1.67	7 (15%)	56,80,80	1.48	11 (19%)
2	FOL	13-A	201	-	34,34,34	1.25	3 (8%)	44,47,47	1.82	6 (13%)
3	NAP	141-A	202	-	45,52,52	2.19	9 (20%)	56,80,80	1.92	13 (23%)
2	FOL	12-A	201	-	34,34,34	1.26	3 (8%)	44,47,47	2.21	11 (25%)
2	FOL	182-A	201	-	34,34,34	0.98	2 (5%)	44,47,47	1.97	8 (18%)
2	FOL	108-A	201	-	34,34,34	1.23	3 (8%)	44,47,47	1.92	10 (22%)
2	FOL	162-A	201	-	34,34,34	0.92	2 (5%)	44,47,47	1.93	9 (20%)
2	FOL	65-A	201	-	34,34,34	1.19	3 (8%)	44,47,47	2.25	16 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	31-A	202	-	45,52,52	1.70	7 (15%)	56,80,80	1.50	9 (16%)
3	NAP	43-A	202	-	45,52,52	1.67	6 (13%)	56,80,80	1.53	10 (17%)
3	NAP	97-A	202	-	45,52,52	1.69	8 (17%)	56,80,80	1.46	8 (14%)
3	NAP	121-A	202	-	45,52,52	1.81	8 (17%)	56,80,80	1.44	5 (8%)
3	NAP	46-A	202	-	45,52,52	1.73	6 (13%)	56,80,80	1.47	9 (16%)
3	NAP	206-A	202	-	45,52,52	1.71	8 (17%)	56,80,80	1.44	6 (10%)
3	NAP	227-A	202	-	45,52,52	1.65	7 (15%)	56,80,80	1.44	8 (14%)
2	FOL	187-A	201	-	34,34,34	1.26	3 (8%)	44,47,47	2.16	9 (20%)
2	FOL	249-A	201	-	34,34,34	1.19	3 (8%)	44,47,47	1.92	9 (20%)
2	FOL	33-A	201	-	34,34,34	1.09	3 (8%)	44,47,47	2.10	12 (27%)
2	FOL	157-A	201	-	34,34,34	1.12	3 (8%)	44,47,47	2.27	13 (29%)
2	FOL	169-A	201	-	34,34,34	0.94	2 (5%)	44,47,47	1.90	10 (22%)
3	NAP	155-A	202	-	45,52,52	1.72	7 (15%)	56,80,80	1.53	10 (17%)
2	FOL	119-A	201	-	34,34,34	1.21	3 (8%)	44,47,47	1.71	7 (15%)
2	FOL	178-A	201	-	34,34,34	1.14	2 (5%)	44,47,47	1.77	6 (13%)
3	NAP	216-A	202	-	45,52,52	1.69	7 (15%)	56,80,80	1.58	10 (17%)
3	NAP	211-A	202	-	45,52,52	1.70	7 (15%)	56,80,80	1.47	6 (10%)
2	FOL	246-A	201	-	34,34,34	0.93	2 (5%)	44,47,47	1.92	9 (20%)
3	NAP	197-A	202	-	45,52,52	1.71	6 (13%)	56,80,80	1.45	8 (14%)
3	NAP	124-A	202	-	45,52,52	1.72	8 (17%)	56,80,80	1.47	8 (14%)
2	FOL	15-A	201	-	34,34,34	0.97	2 (5%)	44,47,47	2.13	8 (18%)
2	FOL	116-A	201	-	34,34,34	0.94	2 (5%)	44,47,47	1.92	12 (27%)
3	NAP	199-A	202	-	45,52,52	1.67	7 (15%)	56,80,80	1.45	7 (12%)
2	FOL	81-A	201	-	34,34,34	1.04	2 (5%)	44,47,47	1.94	9 (20%)
2	FOL	238-A	201	-	34,34,34	1.28	4 (11%)	44,47,47	1.82	10 (22%)
3	NAP	165-A	202	-	45,52,52	1.68	6 (13%)	56,80,80	2.46	10 (17%)
3	NAP	101-A	202	-	45,52,52	1.71	6 (13%)	56,80,80	1.64	11 (19%)
2	FOL	84-A	201	-	34,34,34	1.07	3 (8%)	44,47,47	2.63	16 (36%)
2	FOL	52-A	201	-	34,34,34	1.02	2 (5%)	44,47,47	2.05	13 (29%)
2	FOL	102-A	201	-	34,34,34	1.08	2 (5%)	44,47,47	1.87	9 (20%)
3	NAP	59-A	202	-	45,52,52	1.79	7 (15%)	56,80,80	1.62	7 (12%)
2	FOL	131-A	201	-	34,34,34	1.05	3 (8%)	44,47,47	2.15	13 (29%)
2	FOL	184-A	201	-	34,34,34	1.29	4 (11%)	44,47,47	2.32	12 (27%)
2	FOL	8-A	201	-	34,34,34	1.19	2 (5%)	44,47,47	1.91	10 (22%)
2	FOL	195-A	201	-	34,34,34	1.16	2 (5%)	44,47,47	2.24	15 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	66-A	201	-	34,34,34	1.03	2 (5%)	44,47,47	2.02	13 (29%)
2	FOL	170-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	2.27	9 (20%)
3	NAP	3-A	202	-	45,52,52	2.01	9 (20%)	56,80,80	2.00	13 (23%)
3	NAP	35-A	202	-	45,52,52	1.68	7 (15%)	56,80,80	1.51	11 (19%)
2	FOL	90-A	201	-	34,34,34	0.99	2 (5%)	44,47,47	1.91	10 (22%)
2	FOL	72-A	201	-	34,34,34	1.08	2 (5%)	44,47,47	1.90	6 (13%)
3	NAP	176-A	202	-	45,52,52	1.63	7 (15%)	56,80,80	1.48	8 (14%)
2	FOL	6-A	201	-	34,34,34	1.13	1 (2%)	44,47,47	2.41	12 (27%)
2	FOL	186-A	201	-	34,34,34	1.15	4 (11%)	44,47,47	2.01	12 (27%)
3	NAP	221-A	202	-	45,52,52	1.64	6 (13%)	56,80,80	1.46	8 (14%)
2	FOL	117-A	201	-	34,34,34	1.05	3 (8%)	44,47,47	2.13	11 (25%)
2	FOL	145-A	201	-	34,34,34	1.07	4 (11%)	44,47,47	2.05	12 (27%)
2	FOL	134-A	201	-	34,34,34	1.08	3 (8%)	44,47,47	1.98	10 (22%)
3	NAP	154-A	202	-	45,52,52	1.67	6 (13%)	56,80,80	1.76	10 (17%)
3	NAP	69-A	202	-	45,52,52	1.71	7 (15%)	56,80,80	1.66	10 (17%)
3	NAP	182-A	202	-	45,52,52	1.67	7 (15%)	56,80,80	1.46	9 (16%)
2	FOL	18-A	201	-	34,34,34	1.08	4 (11%)	44,47,47	2.61	16 (36%)
3	NAP	162-A	202	-	45,52,52	1.87	6 (13%)	56,80,80	2.53	10 (17%)
2	FOL	237-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	2.05	10 (22%)
2	FOL	17-A	201	-	34,34,34	1.04	2 (5%)	44,47,47	2.00	11 (25%)
2	FOL	7-A	201	-	34,34,34	1.04	2 (5%)	44,47,47	1.79	8 (18%)
3	NAP	214-A	202	-	45,52,52	1.63	8 (17%)	56,80,80	1.51	6 (10%)
3	NAP	169-A	202	-	45,52,52	1.71	8 (17%)	56,80,80	1.51	9 (16%)
3	NAP	57-A	202	-	45,52,52	1.68	7 (15%)	56,80,80	1.47	8 (14%)
3	NAP	164-A	202	-	45,52,52	2.90	9 (20%)	56,80,80	2.69	13 (23%)
2	FOL	144-A	201	-	34,34,34	1.26	3 (8%)	44,47,47	2.18	19 (43%)
2	FOL	148-A	201	-	34,34,34	0.99	3 (8%)	44,47,47	2.06	15 (34%)
2	FOL	96-A	201	-	34,34,34	1.08	2 (5%)	44,47,47	1.92	9 (20%)
3	NAP	29-A	202	-	45,52,52	1.96	6 (13%)	56,80,80	2.03	11 (19%)
2	FOL	211-A	201	-	34,34,34	1.07	2 (5%)	44,47,47	1.90	11 (25%)
3	NAP	104-A	202	-	45,52,52	1.67	8 (17%)	56,80,80	1.52	8 (14%)
2	FOL	41-A	201	-	34,34,34	1.09	2 (5%)	44,47,47	1.98	11 (25%)
2	FOL	56-A	201	-	34,34,34	1.40	6 (17%)	44,47,47	2.72	18 (40%)
2	FOL	64-A	201	-	34,34,34	1.31	3 (8%)	44,47,47	2.08	13 (29%)
3	NAP	30-A	202	-	45,52,52	1.92	6 (13%)	56,80,80	1.94	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	119-A	202	-	45,52,52	2.06	7 (15%)	56,80,80	1.96	11 (19%)
3	NAP	22-A	202	-	45,52,52	1.67	7 (15%)	56,80,80	1.44	7 (12%)
2	FOL	71-A	201	-	34,34,34	1.26	4 (11%)	44,47,47	2.24	17 (38%)
3	NAP	185-A	202	-	45,52,52	1.68	5 (11%)	56,80,80	1.48	9 (16%)
2	FOL	14-A	201	-	34,34,34	0.96	2 (5%)	44,47,47	2.09	9 (20%)
3	NAP	203-A	202	-	45,52,52	1.65	5 (11%)	56,80,80	1.44	8 (14%)
2	FOL	240-A	201	-	34,34,34	1.12	3 (8%)	44,47,47	1.78	9 (20%)
3	NAP	217-A	202	-	45,52,52	1.67	6 (13%)	56,80,80	1.48	9 (16%)
3	NAP	13-A	202	-	45,52,52	1.68	6 (13%)	56,80,80	1.50	8 (14%)
2	FOL	196-A	201	-	34,34,34	1.17	5 (14%)	44,47,47	1.93	7 (15%)
2	FOL	167-A	201	-	34,34,34	0.99	2 (5%)	44,47,47	1.94	11 (25%)
2	FOL	128-A	201	-	34,34,34	1.03	3 (8%)	44,47,47	2.33	14 (31%)
2	FOL	39-A	201	-	34,34,34	1.37	6 (17%)	44,47,47	2.48	15 (34%)
3	NAP	37-A	202	-	45,52,52	1.69	7 (15%)	56,80,80	1.50	10 (17%)
3	NAP	156-A	202	-	45,52,52	1.71	8 (17%)	56,80,80	1.49	8 (14%)
3	NAP	65-A	202	-	45,52,52	1.75	8 (17%)	56,80,80	1.60	7 (12%)
2	FOL	172-A	201	-	34,34,34	1.16	2 (5%)	44,47,47	1.89	11 (25%)
3	NAP	159-A	202	-	45,52,52	1.84	8 (17%)	56,80,80	2.03	12 (21%)
2	FOL	221-A	201	-	34,34,34	2.03	10 (29%)	44,47,47	4.43	26 (59%)
3	NAP	137-A	202	-	45,52,52	1.68	6 (13%)	56,80,80	1.47	9 (16%)
3	NAP	158-A	202	-	45,52,52	1.71	6 (13%)	56,80,80	1.47	7 (12%)
3	NAP	195-A	202	-	45,52,52	1.68	6 (13%)	56,80,80	1.49	10 (17%)
2	FOL	177-A	201	-	34,34,34	1.38	5 (14%)	44,47,47	2.76	15 (34%)
3	NAP	49-A	202	-	45,52,52	1.67	7 (15%)	56,80,80	1.51	7 (12%)
3	NAP	83-A	202	-	45,52,52	1.66	7 (15%)	56,80,80	1.48	7 (12%)
3	NAP	111-A	202	-	45,52,52	1.68	7 (15%)	56,80,80	1.53	10 (17%)
2	FOL	20-A	201	-	34,34,34	1.00	3 (8%)	44,47,47	2.23	12 (27%)
2	FOL	49-A	201	-	34,34,34	1.26	2 (5%)	44,47,47	1.88	9 (20%)
3	NAP	26-A	202	-	45,52,52	1.67	8 (17%)	56,80,80	1.56	10 (17%)
2	FOL	27-A	201	-	34,34,34	0.99	2 (5%)	44,47,47	2.14	10 (22%)
3	NAP	28-A	202	-	45,52,52	1.67	6 (13%)	56,80,80	1.49	8 (14%)
3	NAP	161-A	202	-	45,52,52	1.72	8 (17%)	56,80,80	2.37	10 (17%)
3	NAP	44-A	202	-	45,52,52	1.61	5 (11%)	56,80,80	1.49	9 (16%)
3	NAP	144-A	202	-	45,52,52	1.83	7 (15%)	56,80,80	1.41	7 (12%)
3	NAP	210-A	202	-	45,52,52	1.69	6 (13%)	56,80,80	1.57	9 (16%)

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	1.22	3 (8%)	44,47,47	1.86	10 (22%)
2	FOL	207-A	201	-	34,34,34	1.18	3 (8%)	44,47,47	2.17	16 (36%)
3	NAP	1-A	202	-	45,52,52	1.95	6 (13%)	56,80,80	2.99	13 (23%)
2	FOL	250-A	201	-	34,34,34	1.20	2 (5%)	44,47,47	2.14	15 (34%)
2	FOL	55-A	201	-	34,34,34	1.08	3 (8%)	44,47,47	2.37	16 (36%)
2	FOL	36-A	201	-	34,34,34	1.05	3 (8%)	44,47,47	1.94	12 (27%)
2	FOL	31-A	201	-	34,34,34	1.19	3 (8%)	44,47,47	1.98	8 (18%)
2	FOL	135-A	201	-	34,34,34	1.25	5 (14%)	44,47,47	1.77	6 (13%)
2	FOL	174-A	201	-	34,34,34	1.02	3 (8%)	44,47,47	2.11	17 (38%)
2	FOL	111-A	201	-	34,34,34	1.03	3 (8%)	44,47,47	1.99	9 (20%)
2	FOL	103-A	201	-	34,34,34	0.94	2 (5%)	44,47,47	2.50	18 (40%)
3	NAP	178-A	202	-	45,52,52	1.96	6 (13%)	56,80,80	1.67	6 (10%)
2	FOL	93-A	201	-	34,34,34	1.15	3 (8%)	44,47,47	2.04	12 (27%)
2	FOL	57-A	201	-	34,34,34	1.19	5 (14%)	44,47,47	2.38	11 (25%)
3	NAP	198-A	202	-	45,52,52	1.68	7 (15%)	56,80,80	1.57	8 (14%)
3	NAP	151-A	202	-	45,52,52	1.72	8 (17%)	56,80,80	1.47	10 (17%)
2	FOL	10-A	201	-	34,34,34	1.03	2 (5%)	44,47,47	2.02	12 (27%)
3	NAP	236-A	202	-	45,52,52	1.77	7 (15%)	56,80,80	1.68	6 (10%)
3	NAP	233-A	202	-	45,52,52	1.75	7 (15%)	56,80,80	1.46	9 (16%)
3	NAP	23-A	202	-	45,52,52	1.70	7 (15%)	56,80,80	1.44	7 (12%)
3	NAP	237-A	202	-	45,52,52	2.97	8 (17%)	56,80,80	2.08	10 (17%)
3	NAP	7-A	202	-	45,52,52	1.73	8 (17%)	56,80,80	1.47	8 (14%)
2	FOL	160-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	1.89	9 (20%)
2	FOL	190-A	201	-	34,34,34	1.12	3 (8%)	44,47,47	1.99	11 (25%)
2	FOL	60-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	2.07	11 (25%)
2	FOL	158-A	201	-	34,34,34	1.04	2 (5%)	44,47,47	2.17	11 (25%)
2	FOL	155-A	201	-	34,34,34	1.15	3 (8%)	44,47,47	2.07	11 (25%)
2	FOL	21-A	201	-	34,34,34	0.95	2 (5%)	44,47,47	1.94	10 (22%)
2	FOL	168-A	201	-	34,34,34	1.19	2 (5%)	44,47,47	1.76	6 (13%)
3	NAP	149-A	202	-	45,52,52	1.72	8 (17%)	56,80,80	1.46	9 (16%)
2	FOL	73-A	201	-	34,34,34	1.08	3 (8%)	44,47,47	2.08	12 (27%)
2	FOL	85-A	201	-	34,34,34	1.13	2 (5%)	44,47,47	1.94	10 (22%)
3	NAP	189-A	202	-	45,52,52	1.62	7 (15%)	56,80,80	1.51	8 (14%)
3	NAP	157-A	202	-	45,52,52	1.76	7 (15%)	56,80,80	1.42	8 (14%)
3	NAP	120-A	202	-	45,52,52	3.02	9 (20%)	56,80,80	2.36	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	220-A	202	-	45,52,52	1.62	5 (11%)	56,80,80	1.50	8 (14%)
2	FOL	97-A	201	-	34,34,34	0.90	1 (2%)	44,47,47	1.81	7 (15%)
3	NAP	208-A	202	-	45,52,52	1.77	7 (15%)	56,80,80	1.49	9 (16%)
3	NAP	77-A	202	-	45,52,52	1.69	5 (11%)	56,80,80	1.53	9 (16%)
2	FOL	2-A	201	-	34,34,34	1.16	2 (5%)	44,47,47	2.03	12 (27%)
2	FOL	91-A	201	-	34,34,34	1.23	4 (11%)	44,47,47	1.87	8 (18%)
3	NAP	116-A	202	-	45,52,52	1.70	7 (15%)	56,80,80	1.58	8 (14%)
3	NAP	9-A	202	-	45,52,52	1.73	8 (17%)	56,80,80	1.50	9 (16%)
2	FOL	42-A	201	-	34,34,34	1.24	4 (11%)	44,47,47	2.32	14 (31%)
3	NAP	81-A	202	-	45,52,52	1.68	7 (15%)	56,80,80	1.53	9 (16%)
2	FOL	89-A	201	-	34,34,34	0.97	2 (5%)	44,47,47	1.85	10 (22%)
2	FOL	112-A	201	-	34,34,34	1.00	2 (5%)	44,47,47	2.16	10 (22%)
3	NAP	200-A	202	-	45,52,52	1.69	7 (15%)	56,80,80	1.49	8 (14%)
3	NAP	148-A	202	-	45,52,52	1.75	6 (13%)	56,80,80	1.56	11 (19%)
3	NAP	102-A	202	-	45,52,52	1.62	6 (13%)	56,80,80	1.49	8 (14%)
2	FOL	161-A	201	-	34,34,34	1.06	2 (5%)	44,47,47	1.76	6 (13%)
3	NAP	8-A	202	-	45,52,52	1.75	7 (15%)	56,80,80	1.47	9 (16%)
3	NAP	94-A	202	-	45,52,52	1.70	8 (17%)	56,80,80	1.41	6 (10%)
2	FOL	110-A	201	-	34,34,34	1.14	2 (5%)	44,47,47	2.01	9 (20%)
3	NAP	234-A	202	-	45,52,52	1.68	7 (15%)	56,80,80	1.50	10 (17%)
2	FOL	243-A	201	-	34,34,34	1.06	3 (8%)	44,47,47	2.24	11 (25%)
2	FOL	139-A	201	-	34,34,34	1.06	2 (5%)	44,47,47	1.99	15 (34%)
2	FOL	130-A	201	-	34,34,34	1.08	3 (8%)	44,47,47	2.25	14 (31%)
2	FOL	5-A	201	-	34,34,34	1.03	3 (8%)	44,47,47	2.24	13 (29%)
2	FOL	151-A	201	-	34,34,34	0.97	2 (5%)	44,47,47	2.06	9 (20%)
2	FOL	242-A	201	-	34,34,34	1.01	3 (8%)	44,47,47	2.02	11 (25%)
3	NAP	90-A	202	-	45,52,52	1.67	7 (15%)	56,80,80	1.53	12 (21%)
3	NAP	15-A	202	-	45,52,52	1.68	6 (13%)	56,80,80	1.46	7 (12%)
3	NAP	109-A	202	-	45,52,52	1.90	7 (15%)	56,80,80	1.63	8 (14%)
2	FOL	183-A	201	-	34,34,34	1.18	2 (5%)	44,47,47	1.87	7 (15%)
3	NAP	207-A	202	-	45,52,52	1.70	7 (15%)	56,80,80	1.48	7 (12%)
3	NAP	238-A	202	-	45,52,52	1.95	7 (15%)	56,80,80	1.89	8 (14%)
3	NAP	240-A	202	-	45,52,52	1.63	9 (20%)	56,80,80	1.54	10 (17%)
3	NAP	145-A	202	-	45,52,52	1.79	8 (17%)	56,80,80	1.48	9 (16%)
2	FOL	86-A	201	-	34,34,34	0.95	2 (5%)	44,47,47	1.90	11 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	80-A	201	-	34,34,34	1.02	2 (5%)	44,47,47	2.20	9 (20%)
3	NAP	166-A	202	-	45,52,52	1.69	7 (15%)	56,80,80	1.58	9 (16%)
2	FOL	63-A	201	-	34,34,34	1.01	2 (5%)	44,47,47	1.98	11 (25%)
2	FOL	201-A	201	-	34,34,34	1.03	2 (5%)	44,47,47	1.81	11 (25%)
2	FOL	223-A	201	-	34,34,34	1.43	5 (14%)	44,47,47	2.39	10 (22%)
3	NAP	17-A	202	-	45,52,52	1.89	9 (20%)	56,80,80	1.50	7 (12%)
3	NAP	123-A	202	-	45,52,52	1.75	7 (15%)	56,80,80	1.56	8 (14%)
3	NAP	196-A	202	-	45,52,52	1.65	7 (15%)	56,80,80	1.47	7 (12%)
3	NAP	241-A	202	-	45,52,52	1.62	7 (15%)	56,80,80	1.51	7 (12%)
3	NAP	160-A	202	-	45,52,52	1.70	7 (15%)	56,80,80	2.42	11 (19%)
3	NAP	92-A	202	-	45,52,52	1.67	7 (15%)	56,80,80	1.48	9 (16%)
3	NAP	96-A	202	-	45,52,52	1.67	7 (15%)	56,80,80	1.79	8 (14%)
3	NAP	131-A	202	-	45,52,52	1.70	7 (15%)	56,80,80	1.38	8 (14%)
2	FOL	194-A	201	-	34,34,34	1.31	3 (8%)	44,47,47	1.85	8 (18%)
3	NAP	61-A	202	-	45,52,52	1.84	7 (15%)	56,80,80	1.52	7 (12%)
3	NAP	56-A	202	-	45,52,52	1.67	6 (13%)	56,80,80	1.47	7 (12%)
2	FOL	203-A	201	-	34,34,34	1.04	2 (5%)	44,47,47	2.11	16 (36%)
2	FOL	32-A	201	-	34,34,34	0.97	2 (5%)	44,47,47	1.94	11 (25%)
3	NAP	66-A	202	-	45,52,52	1.69	6 (13%)	56,80,80	1.51	10 (17%)
3	NAP	88-A	202	-	45,52,52	1.64	7 (15%)	56,80,80	1.47	8 (14%)
2	FOL	224-A	201	-	34,34,34	1.44	6 (17%)	44,47,47	1.92	6 (13%)
3	NAP	174-A	202	-	45,52,52	1.65	7 (15%)	56,80,80	1.57	8 (14%)
3	NAP	71-A	202	-	45,52,52	1.67	5 (11%)	56,80,80	1.57	9 (16%)
3	NAP	186-A	202	-	45,52,52	1.68	7 (15%)	56,80,80	1.51	8 (14%)
2	FOL	115-A	201	-	34,34,34	1.04	1 (2%)	44,47,47	2.11	13 (29%)
2	FOL	166-A	201	-	34,34,34	1.12	2 (5%)	44,47,47	1.99	10 (22%)
3	NAP	170-A	202	-	45,52,52	1.73	7 (15%)	56,80,80	1.44	7 (12%)
3	NAP	250-A	202	-	45,52,52	1.63	5 (11%)	56,80,80	1.55	11 (19%)
2	FOL	236-A	201	-	34,34,34	1.12	3 (8%)	44,47,47	1.88	9 (20%)
3	NAP	25-A	202	-	45,52,52	1.71	8 (17%)	56,80,80	1.52	10 (17%)
2	FOL	118-A	201	-	34,34,34	0.99	1 (2%)	44,47,47	2.20	10 (22%)
3	NAP	64-A	202	-	45,52,52	1.76	8 (17%)	56,80,80	1.50	6 (10%)
2	FOL	26-A	201	-	34,34,34	0.98	2 (5%)	44,47,47	2.01	11 (25%)
2	FOL	105-A	201	-	34,34,34	1.02	2 (5%)	44,47,47	1.97	14 (31%)
2	FOL	191-A	201	-	34,34,34	1.13	2 (5%)	44,47,47	2.13	13 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	35-A	201	-	34,34,34	1.20	4 (11%)	44,47,47	2.83	17 (38%)
3	NAP	128-A	202	-	45,52,52	1.69	9 (20%)	56,80,80	1.44	9 (16%)
3	NAP	167-A	202	-	45,52,52	1.68	6 (13%)	56,80,80	1.53	9 (16%)
2	FOL	127-A	201	-	34,34,34	1.00	3 (8%)	44,47,47	2.02	12 (27%)
2	FOL	244-A	201	-	34,34,34	1.07	2 (5%)	44,47,47	2.11	11 (25%)
3	NAP	11-A	202	-	45,52,52	1.69	7 (15%)	56,80,80	1.49	9 (16%)
3	NAP	76-A	202	-	45,52,52	1.65	5 (11%)	56,80,80	1.51	9 (16%)
2	FOL	212-A	201	-	34,34,34	1.20	2 (5%)	44,47,47	2.21	10 (22%)
3	NAP	60-A	202	-	45,52,52	1.75	7 (15%)	56,80,80	1.54	8 (14%)
3	NAP	239-A	202	-	45,52,52	2.01	7 (15%)	56,80,80	2.12	9 (16%)
3	NAP	79-A	202	-	45,52,52	1.71	7 (15%)	56,80,80	1.44	7 (12%)
2	FOL	40-A	201	-	34,34,34	1.35	5 (14%)	44,47,47	2.61	17 (38%)
2	FOL	136-A	201	-	34,34,34	1.16	4 (11%)	44,47,47	2.31	13 (29%)
2	FOL	216-A	201	-	34,34,34	1.01	3 (8%)	44,47,47	2.04	13 (29%)
3	NAP	85-A	202	-	45,52,52	1.61	7 (15%)	56,80,80	1.79	8 (14%)
2	FOL	124-A	201	-	34,34,34	1.14	3 (8%)	44,47,47	2.27	10 (22%)
3	NAP	27-A	202	-	45,52,52	1.69	6 (13%)	56,80,80	1.51	9 (16%)
2	FOL	217-A	201	-	34,34,34	1.52	6 (17%)	44,47,47	3.09	25 (56%)
3	NAP	2-A	202	-	45,52,52	2.01	7 (15%)	56,80,80	3.18	11 (19%)
3	NAP	38-A	202	-	45,52,52	1.64	5 (11%)	56,80,80	1.49	8 (14%)
3	NAP	67-A	202	-	45,52,52	1.68	6 (13%)	56,80,80	1.63	9 (16%)
3	NAP	147-A	202	-	45,52,52	1.73	8 (17%)	56,80,80	1.47	9 (16%)
2	FOL	231-A	201	-	34,34,34	1.26	4 (11%)	44,47,47	2.32	12 (27%)
2	FOL	78-A	201	-	34,34,34	1.23	5 (14%)	44,47,47	2.13	14 (31%)
3	NAP	114-A	202	-	45,52,52	1.63	7 (15%)	56,80,80	1.45	7 (12%)
3	NAP	226-A	202	-	45,52,52	1.70	7 (15%)	56,80,80	1.42	7 (12%)
2	FOL	140-A	201	-	34,34,34	1.08	3 (8%)	44,47,47	2.23	13 (29%)
3	NAP	201-A	202	-	45,52,52	1.75	7 (15%)	56,80,80	1.50	6 (10%)
3	NAP	91-A	202	-	45,52,52	1.68	8 (17%)	56,80,80	1.61	10 (17%)
3	NAP	54-A	202	-	45,52,52	1.68	6 (13%)	56,80,80	1.47	8 (14%)
3	NAP	87-A	202	-	45,52,52	1.66	6 (13%)	56,80,80	1.50	8 (14%)
2	FOL	241-A	201	-	34,34,34	1.01	2 (5%)	44,47,47	2.35	13 (29%)
3	NAP	190-A	202	-	45,52,52	1.66	7 (15%)	56,80,80	1.54	7 (12%)
3	NAP	243-A	202	-	45,52,52	1.78	9 (20%)	56,80,80	2.05	9 (16%)
3	NAP	99-A	202	-	45,52,52	1.66	7 (15%)	56,80,80	1.48	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	50-A	202	-	45,52,52	1.68	6 (13%)	56,80,80	1.55	10 (17%)
3	NAP	84-A	202	-	45,52,52	1.63	7 (15%)	56,80,80	1.50	9 (16%)
2	FOL	138-A	201	-	34,34,34	1.01	2 (5%)	44,47,47	2.03	10 (22%)
2	FOL	220-A	201	-	34,34,34	1.60	7 (20%)	44,47,47	2.94	19 (43%)
3	NAP	215-A	202	-	45,52,52	1.63	6 (13%)	56,80,80	1.48	9 (16%)
2	FOL	100-A	201	-	34,34,34	1.18	4 (11%)	44,47,47	1.87	9 (20%)
3	NAP	48-A	202	-	45,52,52	1.68	7 (15%)	56,80,80	1.51	10 (17%)
3	NAP	108-A	202	-	45,52,52	1.76	8 (17%)	56,80,80	1.47	9 (16%)
2	FOL	202-A	201	-	34,34,34	1.38	2 (5%)	44,47,47	2.24	16 (36%)
3	NAP	163-A	202	-	45,52,52	2.05	6 (13%)	56,80,80	2.28	13 (23%)
3	NAP	183-A	202	-	45,52,52	1.65	7 (15%)	56,80,80	1.48	11 (19%)
2	FOL	229-A	201	-	34,34,34	1.40	4 (11%)	44,47,47	2.43	19 (43%)
2	FOL	171-A	201	-	34,34,34	1.08	2 (5%)	44,47,47	2.33	18 (40%)
3	NAP	152-A	202	-	45,52,52	1.72	8 (17%)	56,80,80	1.48	8 (14%)
2	FOL	82-A	201	-	34,34,34	1.18	4 (11%)	44,47,47	2.07	8 (18%)
3	NAP	224-A	202	-	45,52,52	1.67	7 (15%)	56,80,80	1.48	11 (19%)
3	NAP	244-A	202	-	45,52,52	1.65	7 (15%)	56,80,80	2.32	10 (17%)
2	FOL	104-A	201	-	34,34,34	0.98	2 (5%)	44,47,47	2.19	14 (31%)
2	FOL	185-A	201	-	34,34,34	1.09	2 (5%)	44,47,47	2.15	12 (27%)
2	FOL	222-A	201	-	34,34,34	1.46	6 (17%)	44,47,47	3.06	18 (40%)
2	FOL	69-A	201	-	34,34,34	1.20	2 (5%)	44,47,47	2.54	17 (38%)
2	FOL	47-A	201	-	34,34,34	0.96	2 (5%)	44,47,47	2.04	10 (22%)
3	NAP	209-A	202	-	45,52,52	1.73	7 (15%)	56,80,80	1.61	8 (14%)
2	FOL	94-A	201	-	34,34,34	1.15	2 (5%)	44,47,47	1.85	8 (18%)
3	NAP	89-A	202	-	45,52,52	1.70	8 (17%)	56,80,80	1.54	8 (14%)
3	NAP	105-A	202	-	45,52,52	1.67	6 (13%)	56,80,80	1.57	11 (19%)
3	NAP	143-A	202	-	45,52,52	3.01	9 (20%)	56,80,80	2.33	15 (26%)
2	FOL	132-A	201	-	34,34,34	1.10	2 (5%)	44,47,47	2.39	15 (34%)
3	NAP	112-A	202	-	45,52,52	1.69	6 (13%)	56,80,80	1.52	10 (17%)
2	FOL	179-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	2.10	13 (29%)
3	NAP	127-A	202	-	45,52,52	1.70	6 (13%)	56,80,80	1.50	7 (12%)
3	NAP	204-A	202	-	45,52,52	1.69	7 (15%)	56,80,80	1.45	7 (12%)
3	NAP	146-A	202	-	45,52,52	1.77	6 (13%)	56,80,80	1.45	9 (16%)
3	NAP	180-A	202	-	45,52,52	1.72	7 (15%)	56,80,80	1.47	8 (14%)
3	NAP	110-A	202	-	45,52,52	1.66	6 (13%)	56,80,80	1.51	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	159-A	201	-	34,34,34	1.02	3 (8%)	44,47,47	1.90	9 (20%)
2	FOL	62-A	201	-	34,34,34	1.09	3 (8%)	44,47,47	2.18	11 (25%)
2	FOL	189-A	201	-	34,34,34	1.06	3 (8%)	44,47,47	1.86	11 (25%)
3	NAP	40-A	202	-	45,52,52	1.66	7 (15%)	56,80,80	1.60	11 (19%)
3	NAP	139-A	202	-	45,52,52	1.64	4 (8%)	56,80,80	1.48	7 (12%)
2	FOL	153-A	201	-	34,34,34	1.02	2 (5%)	44,47,47	2.05	14 (31%)
2	FOL	208-A	201	-	34,34,34	1.36	2 (5%)	44,47,47	2.46	14 (31%)
2	FOL	163-A	201	-	34,34,34	1.17	3 (8%)	44,47,47	1.94	9 (20%)
3	NAP	228-A	202	-	45,52,52	1.66	7 (15%)	56,80,80	1.42	8 (14%)
2	FOL	215-A	201	-	34,34,34	1.09	2 (5%)	44,47,47	1.97	10 (22%)
3	NAP	5-A	202	-	45,52,52	1.79	8 (17%)	56,80,80	1.75	10 (17%)
3	NAP	188-A	202	-	45,52,52	1.66	5 (11%)	56,80,80	1.44	9 (16%)
2	FOL	76-A	201	-	34,34,34	1.21	3 (8%)	44,47,47	1.94	11 (25%)
3	NAP	150-A	202	-	45,52,52	1.73	9 (20%)	56,80,80	1.48	8 (14%)
2	FOL	180-A	201	-	34,34,34	1.25	5 (14%)	44,47,47	2.34	13 (29%)
3	NAP	113-A	202	-	45,52,52	1.63	6 (13%)	56,80,80	1.52	10 (17%)
2	FOL	125-A	201	-	34,34,34	1.14	3 (8%)	44,47,47	2.02	10 (22%)
2	FOL	24-A	201	-	34,34,34	1.02	2 (5%)	44,47,47	1.89	11 (25%)
3	NAP	118-A	202	-	45,52,52	1.92	7 (15%)	56,80,80	1.68	8 (14%)
3	NAP	80-A	202	-	45,52,52	1.69	8 (17%)	56,80,80	1.54	9 (16%)
2	FOL	22-A	201	-	34,34,34	0.99	3 (8%)	44,47,47	1.80	8 (18%)
2	FOL	70-A	201	-	34,34,34	1.07	2 (5%)	44,47,47	1.92	8 (18%)
2	FOL	92-A	201	-	34,34,34	0.98	2 (5%)	44,47,47	2.00	9 (20%)
2	FOL	101-A	201	-	34,34,34	1.18	2 (5%)	44,47,47	1.77	5 (11%)
2	FOL	126-A	201	-	34,34,34	1.05	2 (5%)	44,47,47	2.42	11 (25%)
2	FOL	137-A	201	-	34,34,34	1.09	2 (5%)	44,47,47	2.25	12 (27%)
3	NAP	16-A	202	-	45,52,52	1.68	6 (13%)	56,80,80	1.51	9 (16%)
3	NAP	187-A	202	-	45,52,52	1.62	7 (15%)	56,80,80	1.50	9 (16%)
3	NAP	223-A	202	-	45,52,52	1.66	7 (15%)	56,80,80	1.63	7 (12%)
2	FOL	146-A	201	-	34,34,34	1.07	3 (8%)	44,47,47	2.10	9 (20%)
2	FOL	204-A	201	-	34,34,34	1.08	3 (8%)	44,47,47	1.85	10 (22%)
3	NAP	98-A	202	-	45,52,52	1.67	7 (15%)	56,80,80	1.49	8 (14%)
2	FOL	213-A	201	-	34,34,34	1.03	2 (5%)	44,47,47	2.11	13 (29%)
2	FOL	28-A	201	-	34,34,34	1.00	2 (5%)	44,47,47	1.93	9 (20%)
3	NAP	134-A	202	-	45,52,52	1.67	6 (13%)	56,80,80	1.47	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	107-A	202	-	45,52,52	1.65	7 (15%)	56,80,80	1.56	7 (12%)
3	NAP	194-A	202	-	45,52,52	1.74	7 (15%)	56,80,80	1.51	10 (17%)
3	NAP	229-A	202	-	45,52,52	1.68	6 (13%)	56,80,80	1.47	7 (12%)
3	NAP	205-A	202	-	45,52,52	1.92	7 (15%)	56,80,80	1.55	7 (12%)
2	FOL	45-A	201	-	34,34,34	1.05	3 (8%)	44,47,47	2.21	11 (25%)
3	NAP	86-A	202	-	45,52,52	1.64	6 (13%)	56,80,80	1.48	8 (14%)
3	NAP	82-A	202	-	45,52,52	1.67	7 (15%)	56,80,80	1.49	7 (12%)
3	NAP	245-A	202	-	45,52,52	1.59	5 (11%)	56,80,80	2.47	11 (19%)
3	NAP	72-A	202	-	45,52,52	1.66	7 (15%)	56,80,80	1.62	8 (14%)
2	FOL	23-A	201	-	34,34,34	1.32	6 (17%)	44,47,47	2.11	14 (31%)
3	NAP	242-A	202	-	45,52,52	1.77	9 (20%)	56,80,80	2.68	13 (23%)
3	NAP	249-A	202	-	45,52,52	1.65	6 (13%)	56,80,80	1.56	10 (17%)
2	FOL	95-A	201	-	34,34,34	1.18	2 (5%)	44,47,47	1.92	7 (15%)
2	FOL	193-A	201	-	34,34,34	1.50	3 (8%)	44,47,47	2.29	16 (36%)
2	FOL	129-A	201	-	34,34,34	0.99	3 (8%)	44,47,47	1.99	9 (20%)
2	FOL	147-A	201	-	34,34,34	1.33	4 (11%)	44,47,47	2.04	10 (22%)
3	NAP	115-A	202	-	45,52,52	1.75	8 (17%)	56,80,80	1.58	8 (14%)
3	NAP	36-A	202	-	45,52,52	1.66	8 (17%)	56,80,80	1.52	9 (16%)
3	NAP	248-A	202	-	45,52,52	1.64	6 (13%)	56,80,80	2.35	11 (19%)
2	FOL	192-A	201	-	34,34,34	1.31	4 (11%)	44,47,47	2.33	21 (47%)
2	FOL	109-A	201	-	34,34,34	1.29	5 (14%)	44,47,47	2.21	9 (20%)
3	NAP	173-A	202	-	45,52,52	1.63	5 (11%)	56,80,80	1.51	7 (12%)
3	NAP	133-A	202	-	45,52,52	1.73	8 (17%)	56,80,80	1.60	12 (21%)
3	NAP	6-A	202	-	45,52,52	1.77	7 (15%)	56,80,80	2.26	7 (12%)
3	NAP	212-A	202	-	45,52,52	1.83	8 (17%)	56,80,80	1.58	6 (10%)
3	NAP	75-A	202	-	45,52,52	1.65	7 (15%)	56,80,80	1.83	12 (21%)
3	NAP	138-A	202	-	45,52,52	1.64	6 (13%)	56,80,80	1.58	10 (17%)
3	NAP	136-A	202	-	45,52,52	1.58	4 (8%)	56,80,80	1.66	10 (17%)
3	NAP	19-A	202	-	45,52,52	1.60	6 (13%)	56,80,80	1.51	10 (17%)
2	FOL	218-A	201	-	34,34,34	1.15	4 (11%)	44,47,47	2.40	15 (34%)
2	FOL	77-A	201	-	34,34,34	1.04	3 (8%)	44,47,47	2.15	15 (34%)
3	NAP	21-A	202	-	45,52,52	1.68	7 (15%)	56,80,80	1.45	7 (12%)
2	FOL	29-A	201	-	34,34,34	1.08	3 (8%)	44,47,47	2.00	11 (25%)
2	FOL	133-A	201	-	34,34,34	1.09	3 (8%)	44,47,47	2.00	10 (22%)
3	NAP	18-A	202	-	45,52,52	2.11	7 (15%)	56,80,80	1.88	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	246-A	202	-	45,52,52	1.65	8 (17%)	56,80,80	2.60	10 (17%)
2	FOL	173-A	201	-	34,34,34	0.99	2 (5%)	44,47,47	1.72	11 (25%)
3	NAP	34-A	202	-	45,52,52	1.66	7 (15%)	56,80,80	1.56	10 (17%)
2	FOL	205-A	201	-	34,34,34	1.08	2 (5%)	44,47,47	1.90	9 (20%)
3	NAP	47-A	202	-	45,52,52	1.66	6 (13%)	56,80,80	1.54	10 (17%)
2	FOL	181-A	201	-	34,34,34	1.07	2 (5%)	44,47,47	2.06	12 (27%)
2	FOL	75-A	201	-	34,34,34	1.08	2 (5%)	44,47,47	1.96	12 (27%)
2	FOL	58-A	201	-	34,34,34	1.15	4 (11%)	44,47,47	1.79	10 (22%)
2	FOL	16-A	201	-	34,34,34	1.31	2 (5%)	44,47,47	2.33	13 (29%)
3	NAP	219-A	202	-	45,52,52	1.67	7 (15%)	56,80,80	1.49	9 (16%)
3	NAP	122-A	202	-	45,52,52	1.77	8 (17%)	56,80,80	1.43	5 (8%)
3	NAP	231-A	202	-	45,52,52	1.67	6 (13%)	56,80,80	1.47	7 (12%)
3	NAP	232-A	202	-	45,52,52	1.67	7 (15%)	56,80,80	1.49	10 (17%)
3	NAP	140-A	202	-	45,52,52	1.67	6 (13%)	56,80,80	1.59	9 (16%)
2	FOL	61-A	201	-	34,34,34	1.18	3 (8%)	44,47,47	2.59	15 (34%)
2	FOL	234-A	201	-	34,34,34	1.24	2 (5%)	44,47,47	1.92	9 (20%)
2	FOL	48-A	201	-	34,34,34	0.92	2 (5%)	44,47,47	1.88	8 (18%)
3	NAP	41-A	202	-	45,52,52	1.70	7 (15%)	56,80,80	1.61	9 (16%)
2	FOL	175-A	201	-	34,34,34	1.19	4 (11%)	44,47,47	2.09	14 (31%)
2	FOL	142-A	201	-	34,34,34	1.05	3 (8%)	44,47,47	1.97	9 (20%)
2	FOL	225-A	201	-	34,34,34	1.02	3 (8%)	44,47,47	1.81	9 (20%)
3	NAP	62-A	202	-	45,52,52	1.94	6 (13%)	56,80,80	2.06	10 (17%)
3	NAP	132-A	202	-	45,52,52	3.00	8 (17%)	56,80,80	1.96	14 (25%)
2	FOL	67-A	201	-	34,34,34	0.96	2 (5%)	44,47,47	1.69	8 (18%)
2	FOL	25-A	201	-	34,34,34	1.24	3 (8%)	44,47,47	2.67	13 (29%)
2	FOL	4-A	201	-	34,34,34	0.98	2 (5%)	44,47,47	1.90	11 (25%)
2	FOL	53-A	201	-	34,34,34	1.08	2 (5%)	44,47,47	1.92	9 (20%)
3	NAP	230-A	202	-	45,52,52	1.64	7 (15%)	56,80,80	1.50	9 (16%)
2	FOL	43-A	201	-	34,34,34	1.01	2 (5%)	44,47,47	1.86	10 (22%)
2	FOL	121-A	201	-	34,34,34	1.14	3 (8%)	44,47,47	1.79	5 (11%)
3	NAP	171-A	202	-	45,52,52	1.67	6 (13%)	56,80,80	1.53	9 (16%)
2	FOL	44-A	201	-	34,34,34	1.00	1 (2%)	44,47,47	2.09	10 (22%)
2	FOL	9-A	201	-	34,34,34	1.08	3 (8%)	44,47,47	2.18	14 (31%)
2	FOL	46-A	201	-	34,34,34	1.13	2 (5%)	44,47,47	2.07	10 (22%)
3	NAP	78-A	202	-	45,52,52	1.66	7 (15%)	56,80,80	1.49	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	12-A	202	-	45,52,52	1.68	6 (13%)	56,80,80	1.50	8 (14%)
2	FOL	113-A	201	-	34,34,34	1.23	3 (8%)	44,47,47	2.13	16 (36%)
2	FOL	227-A	201	-	34,34,34	0.96	2 (5%)	44,47,47	2.18	12 (27%)
2	FOL	143-A	201	-	34,34,34	1.21	5 (14%)	44,47,47	2.21	15 (34%)
2	FOL	74-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	1.91	12 (27%)
2	FOL	123-A	201	-	34,34,34	0.98	2 (5%)	44,47,47	1.84	7 (15%)
2	FOL	176-A	201	-	34,34,34	1.37	5 (14%)	44,47,47	2.44	14 (31%)
2	FOL	247-A	201	-	34,34,34	1.07	2 (5%)	44,47,47	2.26	12 (27%)
3	NAP	222-A	202	-	45,52,52	1.79	7 (15%)	56,80,80	1.69	7 (12%)
2	FOL	54-A	201	-	34,34,34	1.15	3 (8%)	44,47,47	1.83	11 (25%)
2	FOL	87-A	201	-	34,34,34	1.03	3 (8%)	44,47,47	1.79	7 (15%)
2	FOL	219-A	201	-	34,34,34	1.37	4 (11%)	44,47,47	3.04	20 (45%)
3	NAP	179-A	202	-	45,52,52	2.14	7 (15%)	56,80,80	1.77	10 (17%)
2	FOL	99-A	201	-	34,34,34	0.99	2 (5%)	44,47,47	2.15	14 (31%)
2	FOL	79-A	201	-	34,34,34	1.17	4 (11%)	44,47,47	1.87	10 (22%)
2	FOL	154-A	201	-	34,34,34	1.09	2 (5%)	44,47,47	2.16	11 (25%)

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	228-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	202-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	197-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	233-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	199-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	150-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	51-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	141-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	55-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	213-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	59-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	206-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	93-A	202	-	-	3/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	10-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	230-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	45-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	125-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	32-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	50-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	120-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	24-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	52-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	164-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	58-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	68-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	153-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	184-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	70-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	95-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	98-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	126-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	239-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	235-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	172-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	142-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	74-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	3-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	20-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	135-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	156-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	38-A	201	-	-	8/22/22/22	0/3/3/3
2	FOL	214-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	117-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	114-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	248-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	247-A	202	-	-	5/31/67/67	0/5/5/5
3	NAP	106-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	193-A	202	-	-	3/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	122-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	210-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	226-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	175-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	188-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	130-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	19-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	107-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	192-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	73-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	51-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	53-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	42-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	34-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	103-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	191-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	218-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	165-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	100-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	14-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	37-A	201	-	-	9/22/22/22	0/3/3/3
2	FOL	88-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	235-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	129-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	4-A	202	-	-	5/31/67/67	0/5/5/5
2	FOL	149-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	63-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	232-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	152-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	11-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	33-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	181-A	202	-	-	2/31/67/67	0/5/5/5
3	NAP	39-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	198-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	30-A	201	-	-	6/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	83-A	201	-	-	7/22/22/22	0/3/3/3
3	NAP	68-A	202	-	-	5/31/67/67	0/5/5/5
2	FOL	106-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	1-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	177-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	168-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	200-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	225-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	13-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	141-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	12-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	182-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	108-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	162-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	65-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	31-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	43-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	97-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	121-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	46-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	206-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	227-A	202	-	-	2/31/67/67	0/5/5/5
2	FOL	187-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	249-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	33-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	157-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	169-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	155-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	119-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	178-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	216-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	211-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	246-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	197-A	202	-	-	4/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	124-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	15-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	116-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	199-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	81-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	238-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	165-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	101-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	84-A	201	-	-	8/22/22/22	0/3/3/3
2	FOL	52-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	102-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	59-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	131-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	184-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	8-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	195-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	66-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	170-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	3-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	35-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	90-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	72-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	176-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	6-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	186-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	221-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	117-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	145-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	134-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	154-A	202	-	-	2/31/67/67	0/5/5/5
3	NAP	69-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	182-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	18-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	162-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	237-A	201	-	-	6/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	17-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	7-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	214-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	169-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	57-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	164-A	202	-	-	5/31/67/67	0/5/5/5
2	FOL	144-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	148-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	96-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	29-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	211-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	104-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	41-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	56-A	201	-	-	8/22/22/22	0/3/3/3
2	FOL	64-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	30-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	119-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	22-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	71-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	185-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	14-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	203-A	202	-	-	5/31/67/67	0/5/5/5
2	FOL	240-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	217-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	13-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	196-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	167-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	128-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	39-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	37-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	156-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	65-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	172-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	159-A	202	-	-	6/31/67/67	0/5/5/5
2	FOL	221-A	201	-	-	12/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	137-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	158-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	195-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	177-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	49-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	83-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	111-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	20-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	49-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	26-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	27-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	28-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	161-A	202	-	-	5/31/67/67	0/5/5/5
3	NAP	44-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	144-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	210-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	209-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	207-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	1-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	250-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	55-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	36-A	201	-	-	8/22/22/22	0/3/3/3
2	FOL	31-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	135-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	174-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	111-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	103-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	178-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	93-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	57-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	198-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	151-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	10-A	201	-	-	8/22/22/22	0/3/3/3
3	NAP	236-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	233-A	202	-	-	4/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	23-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	237-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	7-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	160-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	190-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	60-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	158-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	155-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	21-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	168-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	149-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	73-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	85-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	189-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	157-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	120-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	220-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	97-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	208-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	77-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	2-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	91-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	116-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	9-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	42-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	81-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	89-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	112-A	201	-	-	7/22/22/22	0/3/3/3
3	NAP	200-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	148-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	102-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	161-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	8-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	94-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	110-A	201	-	-	3/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	234-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	243-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	139-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	130-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	5-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	151-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	242-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	90-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	15-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	109-A	202	-	-	2/31/67/67	0/5/5/5
2	FOL	183-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	207-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	238-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	240-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	145-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	86-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	80-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	166-A	202	-	-	2/31/67/67	0/5/5/5
2	FOL	63-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	201-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	223-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	17-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	123-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	196-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	241-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	160-A	202	-	-	5/31/67/67	0/5/5/5
3	NAP	92-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	96-A	202	-	-	2/31/67/67	0/5/5/5
3	NAP	131-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	194-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	61-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	56-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	203-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	32-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	66-A	202	-	-	3/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	88-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	224-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	174-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	71-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	186-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	115-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	166-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	170-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	250-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	236-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	25-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	118-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	64-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	26-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	105-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	191-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	35-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	128-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	167-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	127-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	244-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	11-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	76-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	212-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	60-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	239-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	79-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	40-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	136-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	216-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	85-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	124-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	27-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	217-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	2-A	202	-	-	4/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	38-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	67-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	147-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	231-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	78-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	114-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	226-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	140-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	201-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	91-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	54-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	87-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	241-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	190-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	243-A	202	-	-	6/31/67/67	0/5/5/5
3	NAP	99-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	50-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	84-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	138-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	220-A	201	-	-	7/22/22/22	0/3/3/3
3	NAP	215-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	100-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	48-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	108-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	202-A	201	-	-	7/22/22/22	0/3/3/3
3	NAP	163-A	202	-	-	5/31/67/67	0/5/5/5
3	NAP	183-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	229-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	171-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	152-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	82-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	224-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	244-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	104-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	185-A	201	-	-	4/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	222-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	69-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	47-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	209-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	94-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	89-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	105-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	143-A	202	-	-	5/31/67/67	0/5/5/5
2	FOL	132-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	112-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	179-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	127-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	204-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	146-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	180-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	110-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	159-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	62-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	189-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	40-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	139-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	153-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	208-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	163-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	228-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	215-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	5-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	188-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	76-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	150-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	180-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	113-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	125-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	24-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	118-A	202	-	-	4/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	80-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	22-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	70-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	92-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	101-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	126-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	137-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	16-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	187-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	223-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	146-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	204-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	98-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	213-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	28-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	134-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	107-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	194-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	229-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	205-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	45-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	86-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	82-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	245-A	202	-	-	6/31/67/67	0/5/5/5
3	NAP	72-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	23-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	242-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	249-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	95-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	193-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	129-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	147-A	201	-	-	1/22/22/22	0/3/3/3
3	NAP	115-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	36-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	248-A	202	-	-	4/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	192-A	201	-	-	8/22/22/22	0/3/3/3
2	FOL	109-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	173-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	133-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	6-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	212-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	75-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	138-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	136-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	19-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	218-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	77-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	21-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	29-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	133-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	18-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	246-A	202	-	-	6/31/67/67	0/5/5/5
2	FOL	173-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	34-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	205-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	47-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	181-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	75-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	58-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	16-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	219-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	122-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	231-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	232-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	140-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	61-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	234-A	201	-	-	9/22/22/22	0/3/3/3
2	FOL	48-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	41-A	202	-	-	3/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	175-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	142-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	225-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	62-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	132-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	67-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	25-A	201	-	-	8/22/22/22	0/3/3/3
2	FOL	4-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	53-A	201	-	-	0/22/22/22	0/3/3/3
3	NAP	230-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	43-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	121-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	171-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	44-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	9-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	46-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	78-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	12-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	113-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	227-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	143-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	74-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	123-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	176-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	247-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	222-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	54-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	87-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	219-A	201	-	-	10/22/22/22	0/3/3/3
3	NAP	179-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	99-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	79-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	154-A	201	-	-	0/22/22/22	0/3/3/3

The worst 5 of 2442 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	132-A	202	NAP	O3B-C3B	-17.37	1.02	1.43
3	143-A	202	NAP	O3B-C3B	-17.05	1.02	1.43
3	237-A	202	NAP	O3B-C3B	-17.02	1.02	1.43
3	120-A	202	NAP	O3B-C3B	-16.80	1.03	1.43
3	191-A	202	NAP	O3B-C3B	-16.64	1.03	1.43

The worst 5 of 5123 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2-A	202	NAP	O2N-PN-O5D	-12.28	50.73	107.75
3	245-A	202	NAP	O2N-PN-O1N	12.21	172.62	112.24
3	161-A	202	NAP	O2N-PN-O1N	11.88	170.98	112.24
3	246-A	202	NAP	O2N-PN-O1N	11.67	169.91	112.24
3	160-A	202	NAP	O2N-PN-O1N	11.39	168.54	112.24

There are no chirality outliers.

5 of 1628 torsion outliers are listed below:

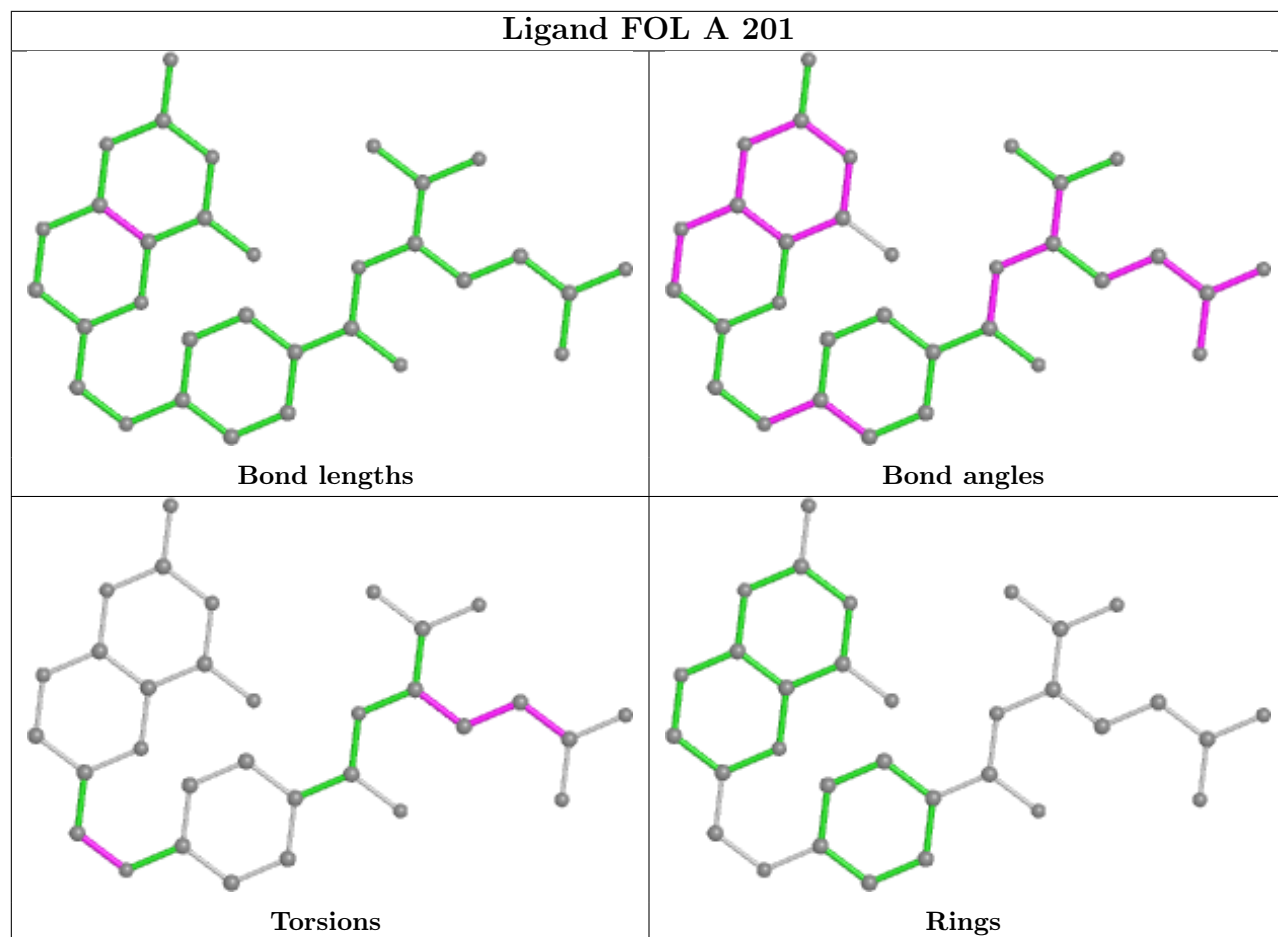
Mol	Chain	Res	Type	Atoms
2	6-A	201	FOL	C6-C9-N10-C14
2	13-A	201	FOL	N-CA-CB-CG
2	16-A	201	FOL	CT-CA-CB-CG
2	17-A	201	FOL	N-CA-CB-CG
2	17-A	201	FOL	CT-CA-CB-CG

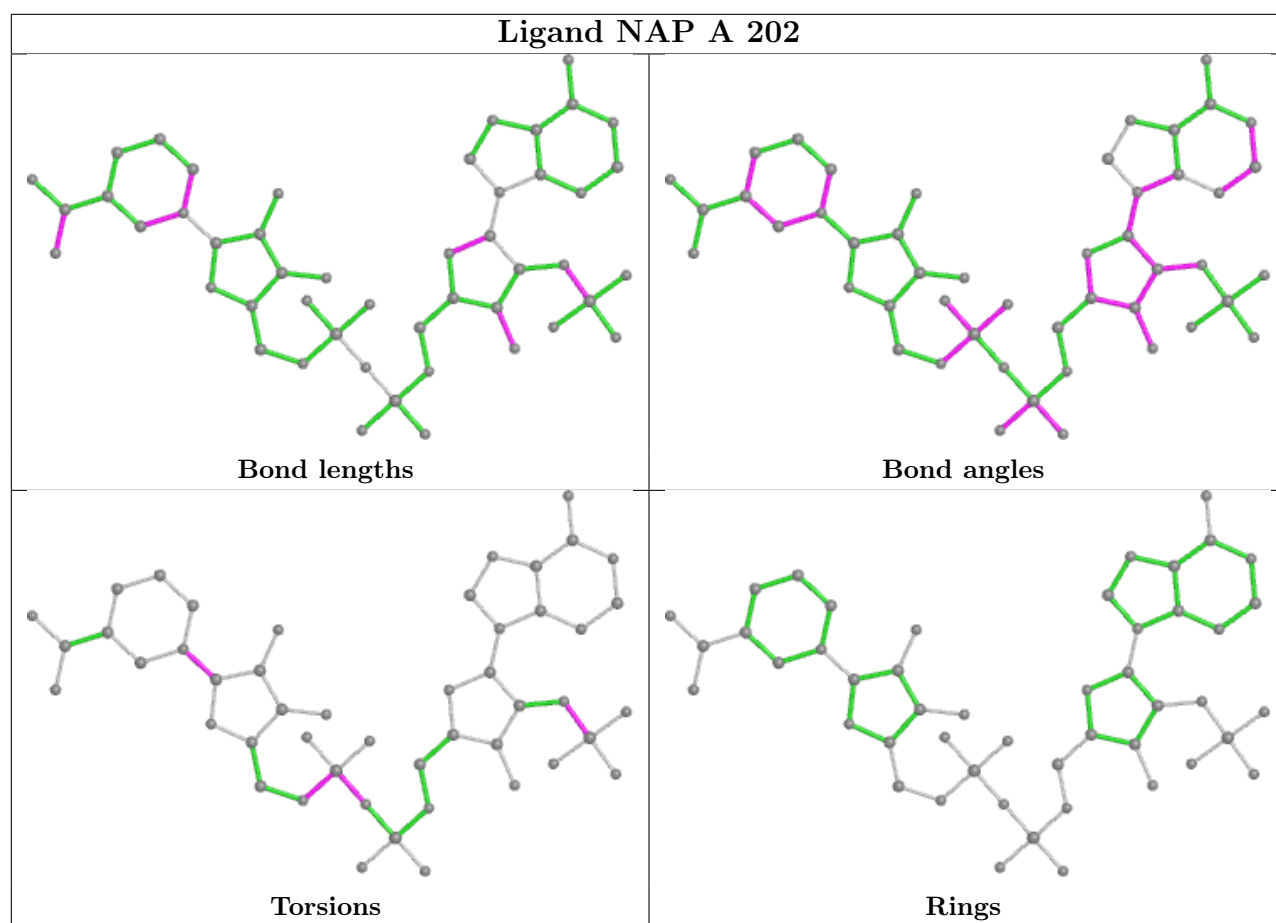
There are no ring outliers.

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.

Ligand FOL A 201





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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