



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2016 – 04:28 AM EDT

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

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : **FAILED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

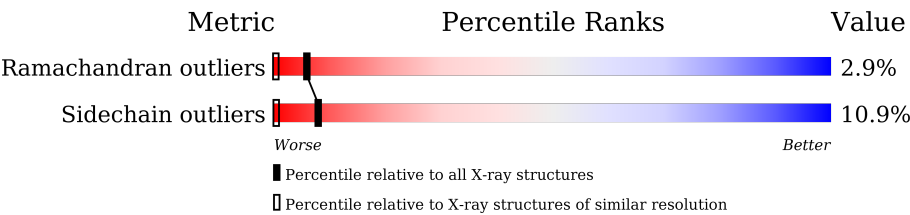
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	100387	2280 (1.40-1.32)
Sidechain outliers	100360	2279 (1.40-1.32)











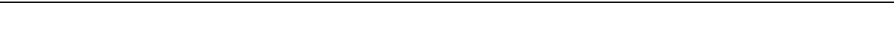

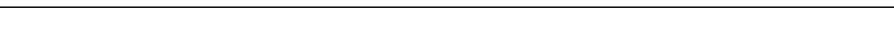
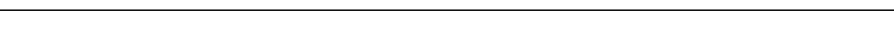











The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	1-A	159	<div><div></div><div>87%11% .</div></div>
1	10-A	159	<div><div></div><div>89%8% ..</div></div>
1	100-A	159	<div><div></div><div>87%11% .</div></div>
1	101-A	159	<div><div></div><div>92%6% .</div></div>
1	102-A	159	<div><div></div><div>90%9% ..</div></div>
1	103-A	159	<div><div></div><div>87%10% .</div></div>
1	104-A	159	<div><div></div><div>89%9% .</div></div>
1	105-A	159	<div><div></div><div>87%9% ..</div></div>
1	106-A	159	<div><div></div><div>82%16% .</div></div>


























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Mol	Chain	Length	Quality of chain
1	107-A	159	 83% 13% .
1	108-A	159	 84% 14% ..
1	109-A	159	 84% 14% ..
1	11-A	159	 87% 9% ..
1	110-A	159	 85% 12% .
1	111-A	159	 85% 13% ..
1	112-A	159	 85% 13% ..
1	113-A	159	 81% 14% . .
1	114-A	159	 82% 12% 5% .
1	115-A	159	 80% 15% . .
1	116-A	159	 83% 13% . .
1	117-A	159	 83% 13% . .
1	118-A	159	 84% 13% . .
1	119-A	159	 87% 12% .
1	12-A	159	 86% 11% .
1	120-A	159	 91% 8% .
1	121-A	159	 86% 13% .
1	122-A	159	 86% 11% .
1	123-A	159	 87% 11% .
1	124-A	159	 87% 13% .
1	125-A	159	 87% 12% .
1	126-A	159	 90% 9% .
1	127-A	159	 90% 9% .
1	128-A	159	 88% 11% .
1	129-A	159	 92% 7% .

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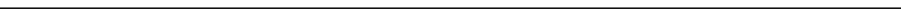











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Mol	Chain	Length	Quality of chain
1	13-A	159	 91% 8% .
1	130-A	159	 92% 6% .
1	131-A	159	 86% 13% .
1	132-A	159	 89% 8% ..
1	133-A	159	 90% 8% ..
1	134-A	159	 89% 9% .
1	135-A	159	 92% 7% ..
1	136-A	159	 86% 11% ..
1	137-A	159	 87% 8% ..
1	138-A	159	 85% 11% ..
1	139-A	159	 87% 11% ..
1	14-A	159	 87% 11% ..
1	140-A	159	 88% 9% ..
1	141-A	159	 86% 11% ..
1	142-A	159	 84% 13% ..
1	143-A	159	 87% 9% ..
1	144-A	159	 80% 15% . .
1	145-A	159	 84% 13% ..
1	146-A	159	 84% 13% ..
1	147-A	159	 87% 11% ..
1	148-A	159	 86% 11% ..
1	149-A	159	 87% 11% .
1	15-A	159	 87% 11% .
1	150-A	159	 84% 14% .
1	151-A	159	 85% 13% .

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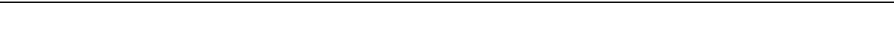

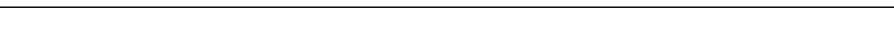
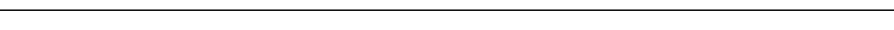













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Mol	Chain	Length	Quality of chain
1	152-A	159	 90% 9% .
1	153-A	159	 87% 9% . .
1	154-A	159	 88% 8% .
1	155-A	159	 86% 11% .
1	156-A	159	 81% 17% .
1	157-A	159	 77% 20% .
1	158-A	159	 86% 10% . .
1	159-A	159	 84% 9% 6% .
1	16-A	159	 86% 12% . .
1	160-A	159	 86% 12% . .
1	161-A	159	 86% 10% . .
1	162-A	159	 86% 10% . .
1	163-A	159	 86% 12% .
1	164-A	159	 86% 9% . .
1	165-A	159	 87% 11% . .
1	166-A	159	 88% 10% . .
1	167-A	159	 82% 13% . .
1	17-A	159	 87% 11% . .
1	18-A	159	 90% 9% .
1	19-A	159	 89% 10% . .
1	2-A	159	 89% 9% .
1	20-A	159	 86% 13% .
1	21-A	159	 88% 11% .
1	22-A	159	 89% 9% .
1	23-A	159	 88% 9% .











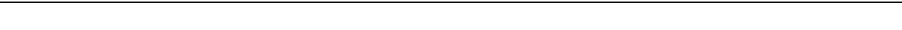

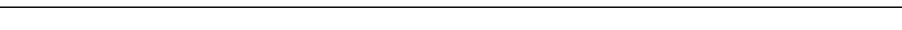
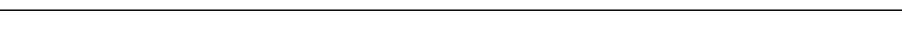











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Mol	Chain	Length	Quality of chain
1	24-A	159	 87% 11% .
1	25-A	159	 84% 14% .
1	26-A	159	 87% 12% ..
1	27-A	159	 85% 13% .
1	28-A	159	 84% 11% . .
1	29-A	159	 81% 16% . .
1	3-A	159	 88% 10% ..
1	30-A	159	 81% 14% 5%
1	31-A	159	 83% 11% 6%
1	32-A	159	 79% 16% . .
1	33-A	159	 83% 9% 6% .
1	34-A	159	 79% 17% .
1	35-A	159	 84% 12% . .
1	36-A	159	 83% 13% . .
1	37-A	159	 82% 15% .
1	38-A	159	 82% 15% .
1	39-A	159	 81% 16% .
1	4-A	159	 84% 14% ..
1	40-A	159	 84% 12% . .
1	41-A	159	 84% 13% . .
1	42-A	159	 86% 11% ..
1	43-A	159	 87% 11% ..
1	44-A	159	 87% 11% .
1	45-A	159	 84% 13% .
1	46-A	159	 86% 13% .


























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Mol	Chain	Length	Quality of chain
1	47-A	159	 86% 11% ..
1	48-A	159	 90% 7% ..
1	49-A	159	 87% 10% ..
1	5-A	159	 91% 6% ..
1	50-A	159	 84% 12% ..
1	51-A	159	 86% 11% ..
1	52-A	159	 85% 12% ..
1	53-A	159	 86% 9% ..
1	54-A	159	 87% 12% .
1	55-A	159	 87% 12% .
1	56-A	159	 87% 9% .
1	57-A	159	 87% 10% ..
1	58-A	159	 89% 10% .
1	59-A	159	 92% 6% .
1	6-A	159	 84% 13% .
1	60-A	159	 85% 12% .
1	61-A	159	 86% 11% ..
1	62-A	159	 85% 14% .
1	63-A	159	 89% 11%
1	64-A	159	 91% 8% .
1	65-A	159	 87% 12% .
1	66-A	159	 87% 9% ..
1	67-A	159	 89% 8% .
1	68-A	159	 89% 8% ..
1	69-A	159	 87% 9% ..

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Mol	Chain	Length	Quality of chain
1	7-A	159	 82% 15% ..
1	70-A	159	 87% 10% ..
1	71-A	159	 87% 9% .
1	72-A	159	 84% 13% ..
1	73-A	159	 87% 9% ..
1	74-A	159	 86% 11% ..
1	75-A	159	 88% 10% .
1	76-A	159	 85% 14% .
1	77-A	159	 90% 9% .
1	78-A	159	 84% 14% .
1	79-A	159	 87% 10% ..
1	8-A	159	 84% 12% ..
1	80-A	159	 84% 12% ..
1	81-A	159	 88% 8% ..
1	82-A	159	 87% 10% ..
1	83-A	159	 87% 11% ..
1	84-A	159	 91% 8% .
1	85-A	159	 86% 12% .
1	86-A	159	 89% 9% ..
1	87-A	159	 91% 6% .
1	88-A	159	 87% 12% .
1	89-A	159	 87% 11% .
1	9-A	159	 87% 9% ..
1	90-A	159	 87% 10% .
1	91-A	159	 89% 9% .

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Mol	Chain	Length	Quality of chain
1	92-A	159	 88% 10% .
1	93-A	159	 89% 9% .
1	94-A	159	 84% 15% .
1	95-A	159	 84% 14% ..
1	96-A	159	 87% 10% .
1	97-A	159	 86% 11% .
1	98-A	159	 86% 13% .
1	99-A	159	 86% 14% .

## 2 Entry composition

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

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

- Molecule 1 is a protein called Dihydrofolate reductase.

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

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

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

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

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

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

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

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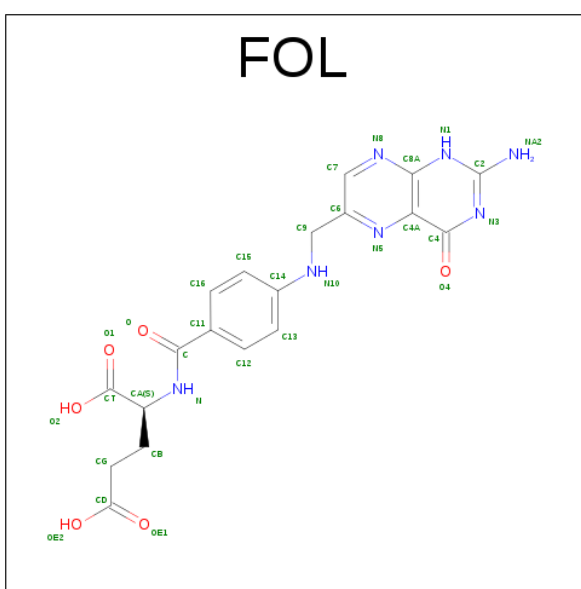
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	143-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	144-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	145-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	146-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239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

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

- Molecule 2 is FOLIC ACID (three-letter code: FOL) (formula: C<sub>19</sub>H<sub>19</sub>N<sub>7</sub>O<sub>6</sub>).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	8-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	9-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	10-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	11-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	12-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	13-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	14-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	15-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	16-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	17-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	18-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	19-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	20-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	21-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	22-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	23-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	24-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	25-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	26-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	27-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	28-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	29-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	30-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	31-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	32-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	33-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	34-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	35-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	36-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	37-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	38-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	39-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	40-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	41-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	42-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	43-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	44-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	45-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	46-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	47-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	48-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	49-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	50-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	51-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	52-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	53-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	54-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	55-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	56-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	57-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	58-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	59-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	60-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	61-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	62-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	63-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	64-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	65-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	66-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	67-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	68-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	69-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	70-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	71-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	72-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	73-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	74-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	75-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	76-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	77-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	78-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	79-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	80-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	81-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	82-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	83-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	84-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	85-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	86-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	87-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	88-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	89-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	90-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	91-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	113-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	114-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	115-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	116-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	117-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	118-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	119-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	120-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	121-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	122-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	123-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	124-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	125-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	126-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	127-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	128-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	129-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	130-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	131-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	132-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	133-A	1	Total 49	C 19	H 17	N 7	O 6	0	0

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	122-A	2	Total 2	Ca 2	0	0
3	110-A	2	Total 2	Ca 2	0	0
3	37-A	2	Total 2	Ca 2	0	0
3	80-A	2	Total 2	Ca 2	0	0
3	94-A	2	Total 2	Ca 2	0	0
3	167-A	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	162-A	2	Total 2	Ca 2	0	0
3	60-A	2	Total 2	Ca 2	0	0
3	148-A	2	Total 2	Ca 2	0	0
3	123-A	2	Total 2	Ca 2	0	0
3	44-A	2	Total 2	Ca 2	0	0
3	150-A	2	Total 2	Ca 2	0	0
3	128-A	2	Total 2	Ca 2	0	0
3	135-A	2	Total 2	Ca 2	0	0
3	50-A	2	Total 2	Ca 2	0	0
3	138-A	2	Total 2	Ca 2	0	0
3	104-A	2	Total 2	Ca 2	0	0
3	12-A	2	Total 2	Ca 2	0	0
3	114-A	2	Total 2	Ca 2	0	0
3	19-A	2	Total 2	Ca 2	0	0
3	165-A	2	Total 2	Ca 2	0	0
3	73-A	2	Total 2	Ca 2	0	0
3	1-A	2	Total 2	Ca 2	0	0
3	53-A	2	Total 2	Ca 2	0	0
3	143-A	2	Total 2	Ca 2	0	0
3	25-A	2	Total 2	Ca 2	0	0
3	131-A	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	32-A	2	Total 2	Ca 2	0	0
3	93-A	2	Total 2	Ca 2	0	0
3	77-A	2	Total 2	Ca 2	0	0
3	161-A	2	Total 2	Ca 2	0	0
3	58-A	2	Total 2	Ca 2	0	0
3	130-A	2	Total 2	Ca 2	0	0
3	57-A	2	Total 2	Ca 2	0	0
3	29-A	2	Total 2	Ca 2	0	0
3	101-A	2	Total 2	Ca 2	0	0
3	3-A	2	Total 2	Ca 2	0	0
3	11-A	2	Total 2	Ca 2	0	0
3	84-A	2	Total 2	Ca 2	0	0
3	98-A	2	Total 2	Ca 2	0	0
3	144-A	2	Total 2	Ca 2	0	0
3	127-A	2	Total 2	Ca 2	0	0
3	154-A	2	Total 2	Ca 2	0	0
3	108-A	2	Total 2	Ca 2	0	0
3	16-A	2	Total 2	Ca 2	0	0
3	65-A	2	Total 2	Ca 2	0	0
3	117-A	2	Total 2	Ca 2	0	0
3	41-A	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	5-A	2	Total 2	Ca 2	0	0
3	8-A	2	Total 2	Ca 2	0	0
3	21-A	2	Total 2	Ca 2	0	0
3	109-A	2	Total 2	Ca 2	0	0
3	102-A	2	Total 2	Ca 2	0	0
3	113-A	2	Total 2	Ca 2	0	0
3	36-A	2	Total 2	Ca 2	0	0
3	81-A	2	Total 2	Ca 2	0	0
3	160-A	2	Total 2	Ca 2	0	0
3	97-A	2	Total 2	Ca 2	0	0
3	61-A	2	Total 2	Ca 2	0	0
3	149-A	2	Total 2	Ca 2	0	0
3	48-A	2	Total 2	Ca 2	0	0
3	124-A	2	Total 2	Ca 2	0	0
3	45-A	2	Total 2	Ca 2	0	0
3	153-A	2	Total 2	Ca 2	0	0
3	129-A	2	Total 2	Ca 2	0	0
3	134-A	2	Total 2	Ca 2	0	0
3	35-A	2	Total 2	Ca 2	0	0
3	105-A	2	Total 2	Ca 2	0	0
3	7-A	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	15-A	2	Total 2	Ca 2	0	0
3	88-A	2	Total 2	Ca 2	0	0
3	18-A	2	Total 2	Ca 2	0	0
3	72-A	2	Total 2	Ca 2	0	0
3	159-A	2	Total 2	Ca 2	0	0
3	52-A	2	Total 2	Ca 2	0	0
3	140-A	2	Total 2	Ca 2	0	0
3	26-A	2	Total 2	Ca 2	0	0
3	120-A	2	Total 2	Ca 2	0	0
3	118-A	2	Total 2	Ca 2	0	0
3	89-A	2	Total 2	Ca 2	0	0
3	31-A	2	Total 2	Ca 2	0	0
3	82-A	2	Total 2	Ca 2	0	0
3	92-A	2	Total 2	Ca 2	0	0
3	76-A	2	Total 2	Ca 2	0	0
3	46-A	2	Total 2	Ca 2	0	0
3	137-A	2	Total 2	Ca 2	0	0
3	56-A	2	Total 2	Ca 2	0	0
3	106-A	2	Total 2	Ca 2	0	0
3	10-A	2	Total 2	Ca 2	0	0
3	85-A	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	145-A	2	Total 2	Ca 2	0	0
3	157-A	2	Total 2	Ca 2	0	0
3	39-A	2	Total 2	Ca 2	0	0
3	133-A	2	Total 2	Ca 2	0	0
3	91-A	2	Total 2	Ca 2	0	0
3	66-A	2	Total 2	Ca 2	0	0
3	79-A	2	Total 2	Ca 2	0	0
3	55-A	2	Total 2	Ca 2	0	0
3	22-A	2	Total 2	Ca 2	0	0
3	103-A	2	Total 2	Ca 2	0	0
3	112-A	2	Total 2	Ca 2	0	0
3	86-A	2	Total 2	Ca 2	0	0
3	96-A	2	Total 2	Ca 2	0	0
3	62-A	2	Total 2	Ca 2	0	0
3	146-A	2	Total 2	Ca 2	0	0
3	49-A	2	Total 2	Ca 2	0	0
3	125-A	2	Total 2	Ca 2	0	0
3	42-A	2	Total 2	Ca 2	0	0
3	152-A	2	Total 2	Ca 2	0	0
3	119-A	2	Total 2	Ca 2	0	0
3	34-A	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	14-A	2	Total 2	Ca 2	0	0
3	63-A	2	Total 2	Ca 2	0	0
3	68-A	2	Total 2	Ca 2	0	0
3	71-A	2	Total 2	Ca 2	0	0
3	158-A	2	Total 2	Ca 2	0	0
3	141-A	2	Total 2	Ca 2	0	0
3	27-A	2	Total 2	Ca 2	0	0
3	163-A	2	Total 2	Ca 2	0	0
3	121-A	2	Total 2	Ca 2	0	0
3	111-A	2	Total 2	Ca 2	0	0
3	30-A	2	Total 2	Ca 2	0	0
3	83-A	2	Total 2	Ca 2	0	0
3	95-A	2	Total 2	Ca 2	0	0
3	2-A	2	Total 2	Ca 2	0	0
3	9-A	2	Total 2	Ca 2	0	0
3	75-A	2	Total 2	Ca 2	0	0
3	47-A	2	Total 2	Ca 2	0	0
3	151-A	2	Total 2	Ca 2	0	0
3	136-A	2	Total 2	Ca 2	0	0
3	51-A	2	Total 2	Ca 2	0	0
3	139-A	2	Total 2	Ca 2	0	0

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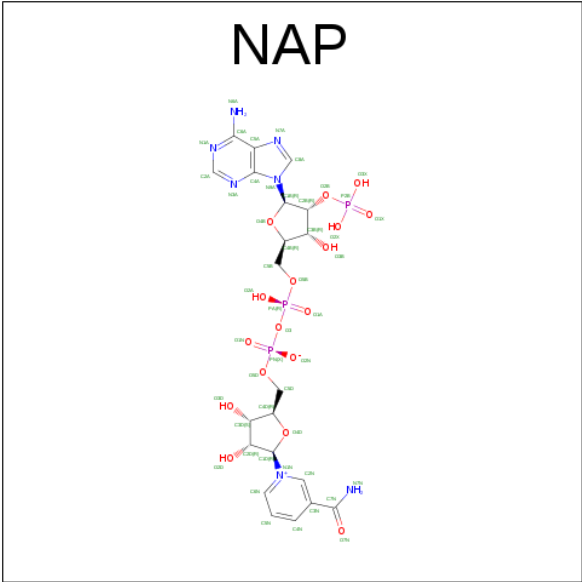
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	107-A	2	Total 2	Ca 2	0	0
3	13-A	2	Total 2	Ca 2	0	0
3	115-A	2	Total 2	Ca 2	0	0
3	74-A	2	Total 2	Ca 2	0	0
3	142-A	2	Total 2	Ca 2	0	0
3	24-A	2	Total 2	Ca 2	0	0
3	156-A	2	Total 2	Ca 2	0	0
3	4-A	2	Total 2	Ca 2	0	0
3	38-A	2	Total 2	Ca 2	0	0
3	132-A	2	Total 2	Ca 2	0	0
3	33-A	2	Total 2	Ca 2	0	0
3	116-A	2	Total 2	Ca 2	0	0
3	164-A	2	Total 2	Ca 2	0	0
3	90-A	2	Total 2	Ca 2	0	0
3	67-A	2	Total 2	Ca 2	0	0
3	166-A	2	Total 2	Ca 2	0	0
3	78-A	2	Total 2	Ca 2	0	0
3	59-A	2	Total 2	Ca 2	0	0
3	54-A	2	Total 2	Ca 2	0	0
3	23-A	2	Total 2	Ca 2	0	0
3	28-A	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	100-A	2	Total 2	Ca 2	0	0
3	87-A	2	Total 2	Ca 2	0	0
3	99-A	2	Total 2	Ca 2	0	0
3	6-A	2	Total 2	Ca 2	0	0
3	147-A	2	Total 2	Ca 2	0	0
3	126-A	2	Total 2	Ca 2	0	0
3	43-A	2	Total 2	Ca 2	0	0
3	155-A	2	Total 2	Ca 2	0	0
3	17-A	2	Total 2	Ca 2	0	0
3	64-A	2	Total 2	Ca 2	0	0
3	69-A	2	Total 2	Ca 2	0	0
3	70-A	2	Total 2	Ca 2	0	0
3	40-A	2	Total 2	Ca 2	0	0
3	20-A	2	Total 2	Ca 2	0	0

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

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

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

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

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

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

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Table 1. Summary of the protein structure data.

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

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

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

- Molecule 5 is water.

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

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

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

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

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

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

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

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

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

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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.

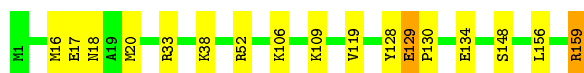
- Molecule 1: Dihydrofolate reductase

Chain 1-A:  87% 11% .




- Molecule 1: Dihydrofolate reductase

Chain 2-A:  89% 9% .




- Molecule 1: Dihydrofolate reductase

Chain 3-A:  88% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 4-A:  84% 14% ..




- Molecule 1: Dihydrofolate reductase

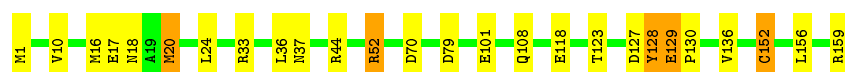
Chain 5-A:  91% 6% ..




- Molecule 1: Dihydrofolate reductase



Chain 6-A:  84% 13% .




- Molecule 1: Dihydrofolate reductase

Chain 7-A:  82% 15% . .




- Molecule 1: Dihydrofolate reductase

Chain 8-A:  84% 12% . .



- Molecule 1: Dihydrofolate reductase

Chain 9-A:  87% 9% . .



- Molecule 1: Dihydrofolate reductase

Chain 10-A:  89% 8% . .




- Molecule 1: Dihydrofolate reductase

Chain 11-A:  87% 9% . .



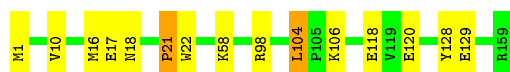
- Molecule 1: Dihydrofolate reductase

Chain 12-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 13-A:  91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 14-A: 87% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 15-A: 87% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 16-A: 86% 12% ..



- Molecule 1: Dihydrofolate reductase

Chain 17-A: 87% 11% ..



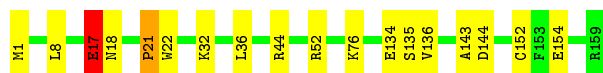
- Molecule 1: Dihydrofolate reductase

Chain 18-A: 90% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 19-A: 89% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 20-A: 86% 13% .



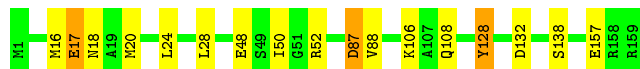
- Molecule 1: Dihydrofolate reductase

Chain 21-A:  88% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 22-A:  89% 9% .



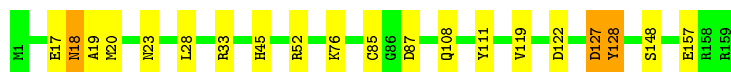
- Molecule 1: Dihydrofolate reductase

Chain 23-A:  88% 9% .



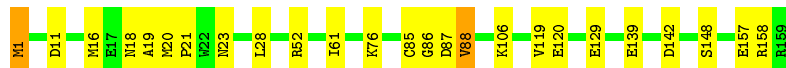
- Molecule 1: Dihydrofolate reductase

Chain 24-A:  87% 11% .




- Molecule 1: Dihydrofolate reductase

Chain 25-A:  84% 14% .




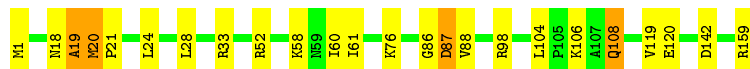
- Molecule 1: Dihydrofolate reductase

Chain 26-A:  87% 12% ..




- Molecule 1: Dihydrofolate reductase

Chain 27-A:  85% 13% .




- Molecule 1: Dihydrofolate reductase

Chain 28-A:  84% 11% . .




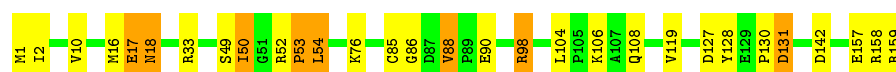
- Molecule 1: Dihydrofolate reductase

Chain 29-A:  81% 16% . .




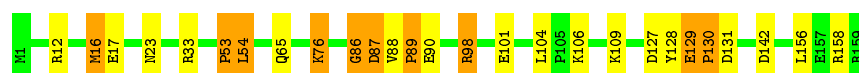
- Molecule 1: Dihydrofolate reductase

Chain 30-A:  81% 14% 5%




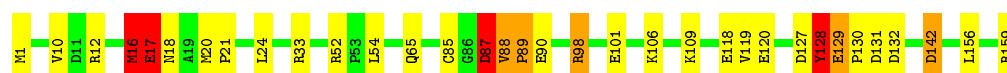
- Molecule 1: Dihydrofolate reductase

Chain 31-A:  83% 11% 6%



- Molecule 1: Dihydrofolate reductase

Chain 32-A:  79% 16% . .




- Molecule 1: Dihydrofolate reductase

Chain 33-A:  83% 9% 6% .




- Molecule 1: Dihydrofolate reductase

Chain 34-A:  79% 17% .



- Molecule 1: Dihydrofolate reductase

Chain 35-A:  84% 12% . .



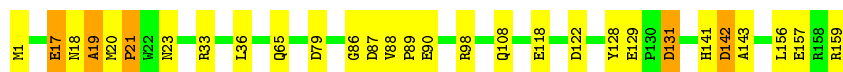
- Molecule 1: Dihydrofolate reductase

Chain 36-A: 83% 13% ..



- Molecule 1: Dihydrofolate reductase

Chain 37-A: 82% 15% .



- Molecule 1: Dihydrofolate reductase

Chain 38-A: 82% 15% .



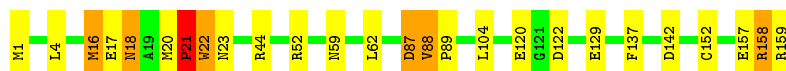
- Molecule 1: Dihydrofolate reductase

Chain 39-A: 81% 16% .



- Molecule 1: Dihydrofolate reductase

Chain 40-A: 84% 12% ..



- Molecule 1: Dihydrofolate reductase

Chain 41-A: 84% 13% ..




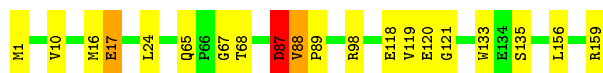
- Molecule 1: Dihydrofolate reductase

Chain 42-A: 86% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 43-A:  87% 11% ..




- Molecule 1: Dihydrofolate reductase

Chain 44-A:  87% 11% .




- Molecule 1: Dihydrofolate reductase

Chain 45-A:  84% 13% .




- Molecule 1: Dihydrofolate reductase

Chain 46-A:  86% 13% .



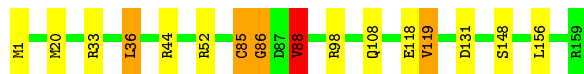
- Molecule 1: Dihydrofolate reductase

Chain 47-A:  86% 11% ..




- Molecule 1: Dihydrofolate reductase

Chain 48-A:  90% 7% ..




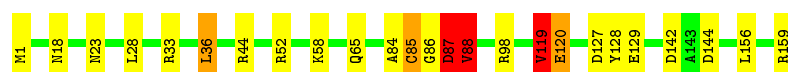
- Molecule 1: Dihydrofolate reductase

Chain 49-A:  87% 10% ..




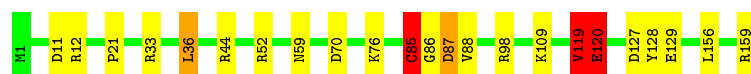
- Molecule 1: Dihydrofolate reductase

Chain 50-A:  84% 12% ..




- Molecule 1: Dihydrofolate reductase

Chain 51-A:  86% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 52-A:  85% 12% ..



- Molecule 1: Dihydrofolate reductase

Chain 53-A:  86% 9% ..



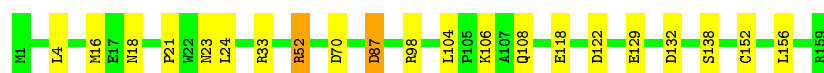
- Molecule 1: Dihydrofolate reductase

Chain 54-A:  87% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 55-A:  87% 12% .



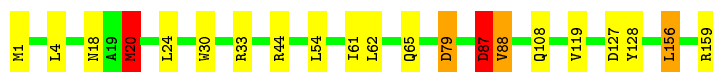
- Molecule 1: Dihydrofolate reductase

Chain 56-A:  87% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 57-A:  87% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 58-A: 89% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 59-A: 92% 6% .



- Molecule 1: Dihydrofolate reductase

Chain 60-A: 85% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 61-A: 86% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 62-A: 85% 14% .



- Molecule 1: Dihydrofolate reductase

Chain 63-A: 89% 11%



- Molecule 1: Dihydrofolate reductase

Chain 64-A: 91% 8% .





- Molecule 1: Dihydrofolate reductase

Chain 65-A:  87% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 66-A:  87% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 67-A:  89% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 68-A:  89% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 69-A:  87% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 70-A:  87% 10% ..




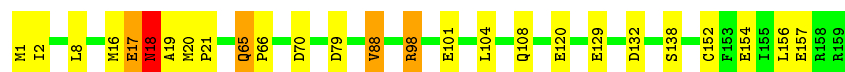
- Molecule 1: Dihydrofolate reductase

Chain 71-A:  87% 9% .




- Molecule 1: Dihydrofolate reductase

Chain 72-A:  84% 13% . .



- Molecule 1: Dihydrofolate reductase

Chain 73-A:  87% 9% . .



- Molecule 1: Dihydrofolate reductase

Chain 74-A:  86% 11% . .




- Molecule 1: Dihydrofolate reductase

Chain 75-A:  88% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 76-A:  85% 14% .




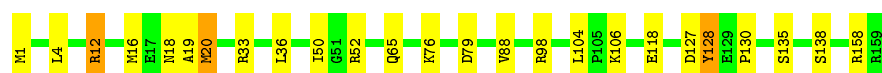
- Molecule 1: Dihydrofolate reductase

Chain 77-A:  90% 9% .




- Molecule 1: Dihydrofolate reductase

Chain 78-A:  84% 14% .



- Molecule 1: Dihydrofolate reductase

Chain 79-A:  87% 10% . .



- Molecule 1: Dihydrofolate reductase

Chain 80-A: 84% 12% ..



- Molecule 1: Dihydrofolate reductase

Chain 81-A: 88% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 82-A: 87% 10% ..



- Molecule 1: Dihydrofolate reductase

Chain 83-A: 87% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 84-A: 91% 8% .



- Molecule 1: Dihydrofolate reductase

Chain 85-A: 86% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 86-A: 89% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 87-A:  91% 6%



- Molecule 1: Dihydrofolate reductase

Chain 88-A:  87% 12%



- Molecule 1: Dihydrofolate reductase

Chain 89-A:  87% 11%



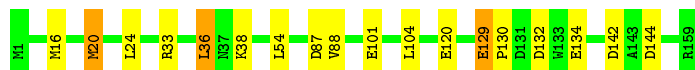
- Molecule 1: Dihydrofolate reductase

Chain 90-A:  87% 10%



- Molecule 1: Dihydrofolate reductase

Chain 91-A:  89% 9%



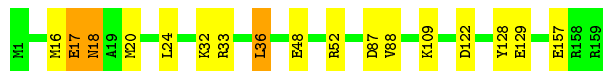
- Molecule 1: Dihydrofolate reductase

Chain 92-A:  88% 10%




- Molecule 1: Dihydrofolate reductase

Chain 93-A:  89% 9%



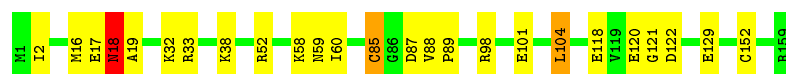
- Molecule 1: Dihydrofolate reductase

Chain 94-A:  84% 15% .



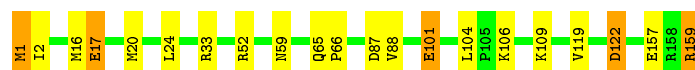
- Molecule 1: Dihydrofolate reductase

Chain 95-A:  84% 14% ..




- Molecule 1: Dihydrofolate reductase

Chain 96-A:  87% 10% .




- Molecule 1: Dihydrofolate reductase

Chain 97-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 98-A:  86% 13% .



- Molecule 1: Dihydrofolate reductase

Chain 99-A:  86% 14% .



- Molecule 1: Dihydrofolate reductase

Chain 100-A:  87% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 101-A:  92% 6% .



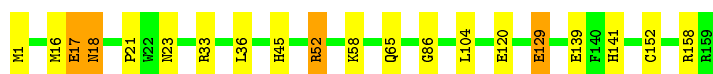
- Molecule 1: Dihydrofolate reductase

Chain 102-A: 90% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 103-A: 87% 10% .



- Molecule 1: Dihydrofolate reductase

Chain 104-A: 89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 105-A: 87% 9% ..



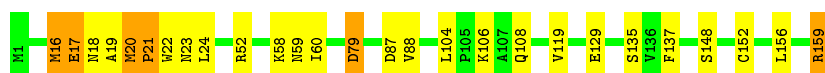
- Molecule 1: Dihydrofolate reductase

Chain 106-A: 82% 16% .



- Molecule 1: Dihydrofolate reductase

Chain 107-A: 83% 13% .

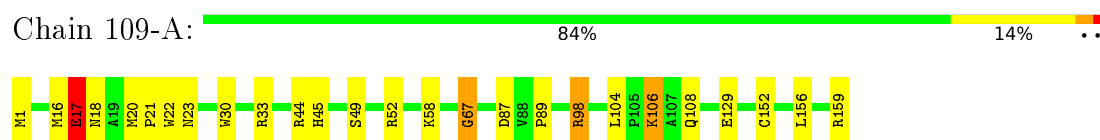


- Molecule 1: Dihydrofolate reductase

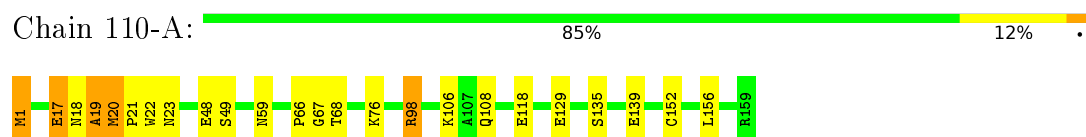
Chain 108-A: 84% 14% ..



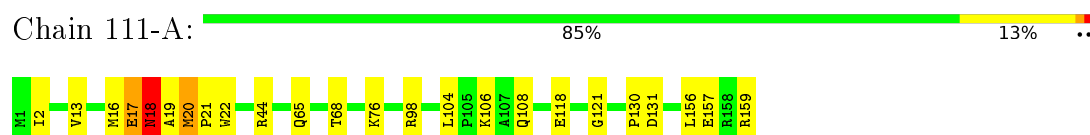
- Molecule 1: Dihydrofolate reductase



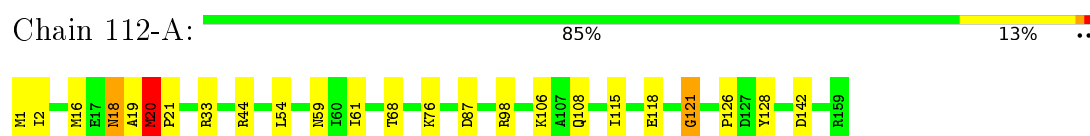
- Molecule 1: Dihydrofolate reductase



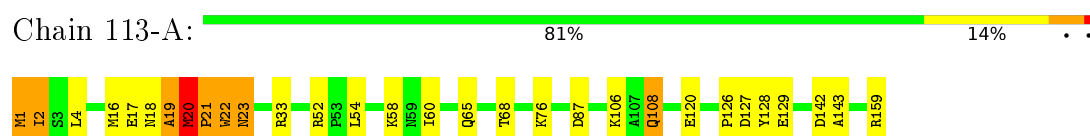
- Molecule 1: Dihydrofolate reductase



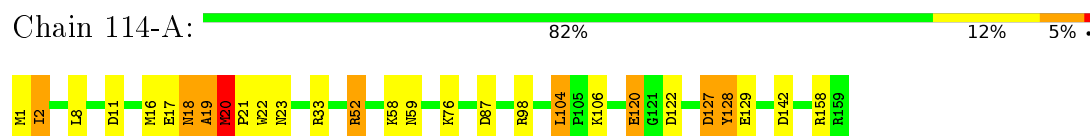
- Molecule 1: Dihydrofolate reductase



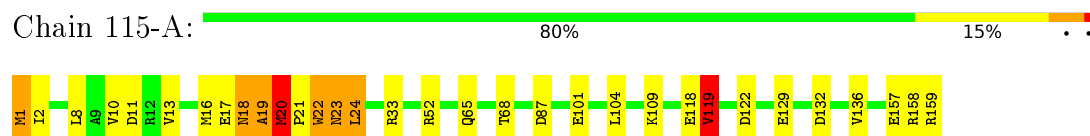
- Molecule 1: Dihydrofolate reductase




- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase




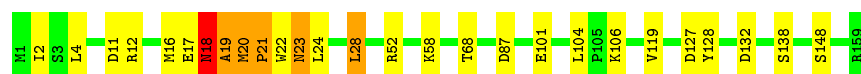
- Molecule 1: Dihydrofolate reductase

Chain 116-A:  83% 13% ..



- Molecule 1: Dihydrofolate reductase

Chain 117-A:  83% 13% ..



- Molecule 1: Dihydrofolate reductase

Chain 118-A:  84% 13% ..



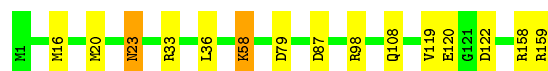
- Molecule 1: Dihydrofolate reductase

Chain 119-A:  87% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 120-A:  91% 8% .




- Molecule 1: Dihydrofolate reductase

Chain 121-A:  86% 13% .



- Molecule 1: Dihydrofolate reductase

Chain 122-A:  86% 11% .



- Molecule 1: Dihydrofolate reductase

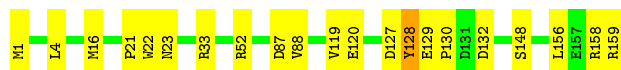
Chain 123-A:  87% 11% .





- Molecule 1: Dihydrofolate reductase

Chain 124-A: 87% 13% .



- Molecule 1: Dihydrofolate reductase

Chain 125-A: 87% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 126-A: 90% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 127-A: 90% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 128-A: 88% 11% .



- Molecule 1: Dihydrofolate reductase

Chain 129-A: 92% 7% .

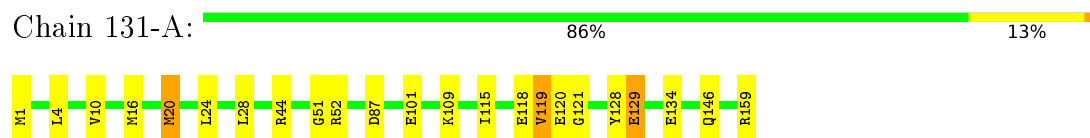


- Molecule 1: Dihydrofolate reductase

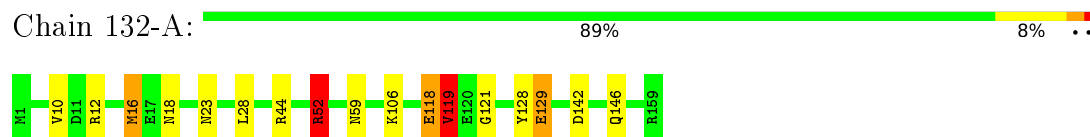
Chain 130-A: 92% 6% .



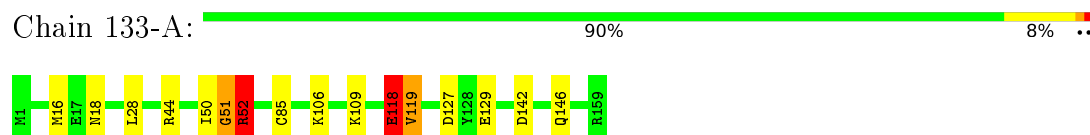
- Molecule 1: Dihydrofolate reductase



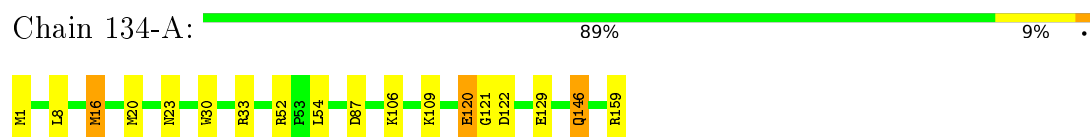
- Molecule 1: Dihydrofolate reductase



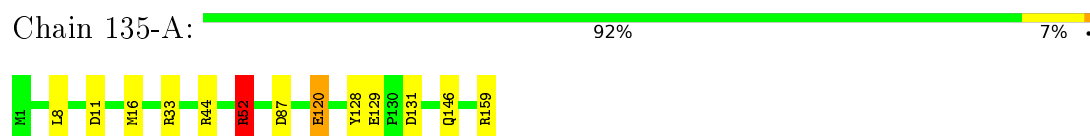
- Molecule 1: Dihydrofolate reductase



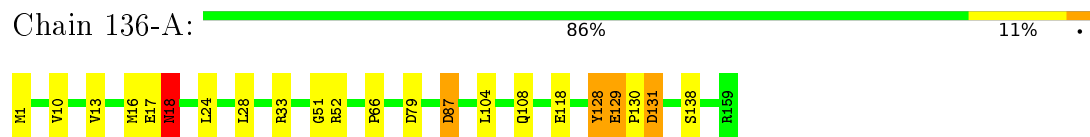
- Molecule 1: Dihydrofolate reductase



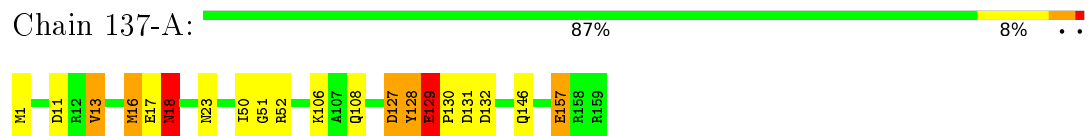
- Molecule 1: Dihydrofolate reductase




- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase

Chain 138-A:  85% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 139-A:  87% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 140-A:  88% 9% ..




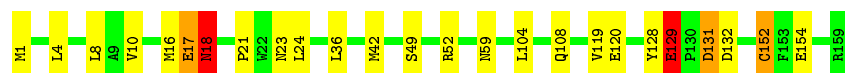
- Molecule 1: Dihydrofolate reductase

Chain 141-A:  86% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 142-A:  84% 13% ..




- Molecule 1: Dihydrofolate reductase

Chain 143-A:  87% 9% ..




- Molecule 1: Dihydrofolate reductase

Chain 144-A:  80% 15% ..



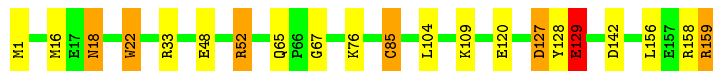
- Molecule 1: Dihydrofolate reductase

Chain 145-A:  84% 13% ..



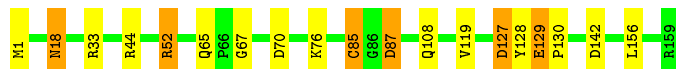
- Molecule 1: Dihydrofolate reductase

Chain 153-A:  87% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 154-A:  88% 8% .




- Molecule 1: Dihydrofolate reductase

Chain 155-A:  86% 11% .




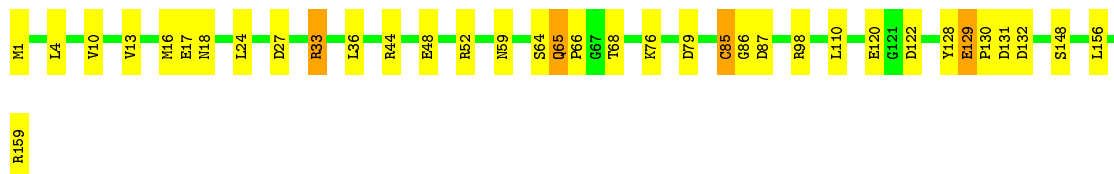
- Molecule 1: Dihydrofolate reductase

Chain 156-A:  81% 17% .



- Molecule 1: Dihydrofolate reductase

Chain 157-A:  77% 20% .



- Molecule 1: Dihydrofolate reductase

Chain 158-A:  86% 10% ..

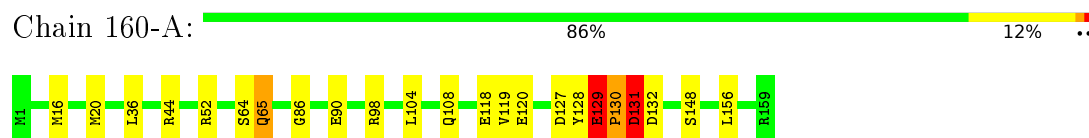


- Molecule 1: Dihydrofolate reductase

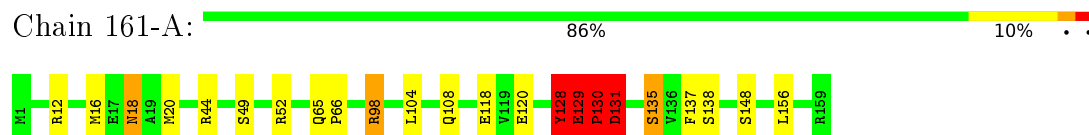
Chain 159-A:  84% 9% 6% .



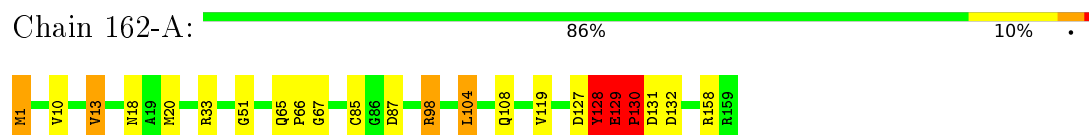
- Molecule 1: Dihydrofolate reductase



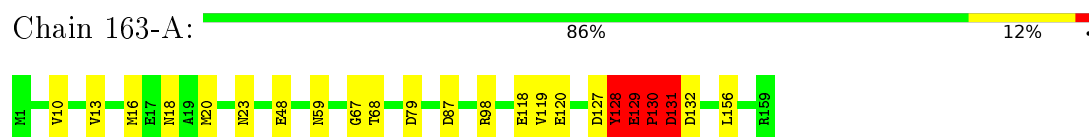
- Molecule 1: Dihydrofolate reductase



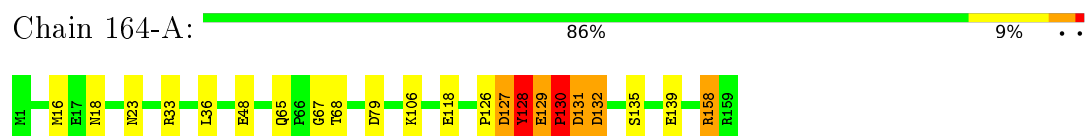
- Molecule 1: Dihydrofolate reductase



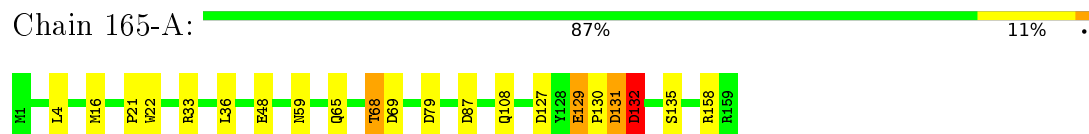
- Molecule 1: Dihydrofolate reductase



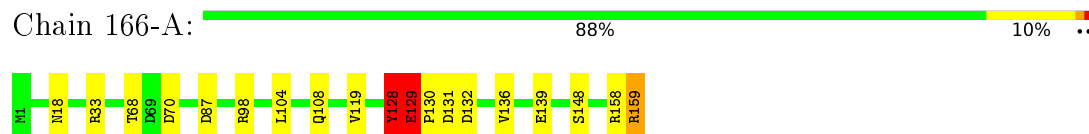
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



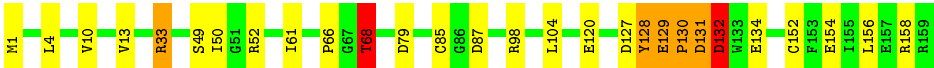
- Molecule 1: Dihydrofolate reductase

Chain 167-A: 

82%

13%

..



## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	34.32Å 45.51Å 98.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.34 – 1.35	Depositor
% Data completeness (in resolution range)	91.6 (41.34-1.35)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 1.35Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement: 1.8.4_1496)	Depositor
R, $R_{free}$	0.118 , 0.153	Depositor
Wilson B-factor (Å <sup>2</sup> )	11.3	Xtriage
Anisotropy	0.174	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	451154	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	9.0	wwPDB-VP

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

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, CA, 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	0.70	0/1302	0.91	3/1770 (0.2%)
1	2-A	0.71	0/1302	0.91	2/1770 (0.1%)
1	3-A	0.70	0/1302	1.01	4/1770 (0.2%)
1	4-A	0.76	2/1302 (0.2%)	0.97	5/1770 (0.3%)
1	5-A	0.73	0/1302	1.03	3/1770 (0.2%)
1	6-A	0.91	4/1302 (0.3%)	1.03	6/1770 (0.3%)
1	7-A	0.94	6/1302 (0.5%)	1.09	8/1770 (0.5%)
1	8-A	0.86	5/1302 (0.4%)	1.14	11/1770 (0.6%)
1	9-A	0.82	0/1302	1.00	6/1770 (0.3%)
1	10-A	0.66	0/1302	0.87	2/1770 (0.1%)
1	11-A	0.73	1/1302 (0.1%)	0.94	4/1770 (0.2%)
1	12-A	0.73	1/1302 (0.1%)	0.98	3/1770 (0.2%)
1	13-A	0.67	1/1302 (0.1%)	0.91	2/1770 (0.1%)
1	14-A	0.78	1/1302 (0.1%)	0.92	2/1770 (0.1%)
1	15-A	0.76	0/1302	0.94	1/1770 (0.1%)
1	16-A	0.72	0/1302	0.99	5/1770 (0.3%)
1	17-A	0.75	3/1302 (0.2%)	0.94	2/1770 (0.1%)
1	18-A	0.74	1/1302 (0.1%)	0.91	1/1770 (0.1%)
1	19-A	0.73	2/1302 (0.2%)	0.90	1/1770 (0.1%)
1	20-A	0.76	2/1302 (0.2%)	0.93	7/1770 (0.4%)
1	21-A	0.76	2/1302 (0.2%)	0.97	5/1770 (0.3%)
1	22-A	0.71	0/1302	0.99	4/1770 (0.2%)
1	23-A	0.75	0/1302	0.95	4/1770 (0.2%)
1	24-A	0.71	0/1302	0.95	3/1770 (0.2%)
1	25-A	0.72	0/1302	0.93	2/1770 (0.1%)
1	26-A	0.78	0/1302	0.95	4/1770 (0.2%)
1	27-A	0.78	0/1302	0.98	5/1770 (0.3%)
1	28-A	0.80	1/1302 (0.1%)	1.04	5/1770 (0.3%)
1	29-A	0.86	4/1302 (0.3%)	1.01	4/1770 (0.2%)
1	30-A	0.85	1/1302 (0.1%)	1.18	8/1770 (0.5%)
1	31-A	0.91	3/1302 (0.2%)	1.17	9/1770 (0.5%)
1	32-A	0.99	4/1302 (0.3%)	1.15	13/1770 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	33-A	0.91	2/1302 (0.2%)	1.15	10/1770 (0.6%)
1	34-A	0.95	5/1302 (0.4%)	1.09	10/1770 (0.6%)
1	35-A	0.88	3/1302 (0.2%)	1.08	7/1770 (0.4%)
1	36-A	0.86	3/1302 (0.2%)	1.08	8/1770 (0.5%)
1	37-A	0.82	2/1302 (0.2%)	1.06	6/1770 (0.3%)
1	38-A	0.81	1/1302 (0.1%)	1.02	9/1770 (0.5%)
1	39-A	0.79	3/1302 (0.2%)	1.09	10/1770 (0.6%)
1	40-A	0.81	1/1302 (0.1%)	1.07	10/1770 (0.6%)
1	41-A	0.71	0/1302	1.09	7/1770 (0.4%)
1	42-A	0.73	0/1302	1.04	10/1770 (0.6%)
1	43-A	0.74	1/1302 (0.1%)	1.03	8/1770 (0.5%)
1	44-A	0.74	1/1302 (0.1%)	0.94	3/1770 (0.2%)
1	45-A	0.71	1/1302 (0.1%)	0.94	4/1770 (0.2%)
1	46-A	0.76	2/1302 (0.2%)	1.00	4/1770 (0.2%)
1	47-A	0.76	1/1302 (0.1%)	1.03	7/1770 (0.4%)
1	48-A	0.71	0/1302	0.96	4/1770 (0.2%)
1	49-A	0.77	3/1302 (0.2%)	0.96	6/1770 (0.3%)
1	50-A	0.76	1/1302 (0.1%)	1.06	5/1770 (0.3%)
1	51-A	0.79	3/1302 (0.2%)	1.01	4/1770 (0.2%)
1	52-A	0.79	3/1302 (0.2%)	1.10	8/1770 (0.5%)
1	53-A	0.74	1/1302 (0.1%)	1.04	8/1770 (0.5%)
1	54-A	0.71	1/1302 (0.1%)	0.92	2/1770 (0.1%)
1	55-A	0.74	1/1302 (0.1%)	0.96	3/1770 (0.2%)
1	56-A	0.90	5/1302 (0.4%)	1.09	7/1770 (0.4%)
1	57-A	0.80	2/1302 (0.2%)	1.11	12/1770 (0.7%)
1	58-A	0.93	1/1302 (0.1%)	1.09	10/1770 (0.6%)
1	59-A	0.86	2/1302 (0.2%)	0.99	5/1770 (0.3%)
1	60-A	0.73	1/1302 (0.1%)	0.94	6/1770 (0.3%)
1	61-A	0.70	1/1302 (0.1%)	0.94	5/1770 (0.3%)
1	62-A	0.71	0/1302	0.93	3/1770 (0.2%)
1	63-A	0.73	0/1302	1.00	4/1770 (0.2%)
1	64-A	0.67	0/1302	0.88	1/1770 (0.1%)
1	65-A	0.68	0/1302	1.05	10/1770 (0.6%)
1	66-A	0.74	1/1302 (0.1%)	1.01	6/1770 (0.3%)
1	67-A	0.78	1/1302 (0.1%)	0.95	3/1770 (0.2%)
1	68-A	0.77	1/1302 (0.1%)	1.10	12/1770 (0.7%)
1	69-A	0.81	1/1302 (0.1%)	1.04	10/1770 (0.6%)
1	70-A	1.04	4/1302 (0.3%)	1.00	5/1770 (0.3%)
1	71-A	0.95	4/1302 (0.3%)	1.01	7/1770 (0.4%)
1	72-A	0.74	1/1302 (0.1%)	1.00	4/1770 (0.2%)
1	73-A	0.73	2/1302 (0.2%)	0.98	7/1770 (0.4%)
1	74-A	0.79	2/1302 (0.2%)	1.00	5/1770 (0.3%)
1	75-A	0.79	3/1302 (0.2%)	0.96	3/1770 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	76-A	0.73	0/1302	0.96	5/1770 (0.3%)
1	77-A	0.72	0/1302	0.88	4/1770 (0.2%)
1	78-A	0.72	1/1302 (0.1%)	0.97	4/1770 (0.2%)
1	79-A	0.72	0/1302	1.05	9/1770 (0.5%)
1	80-A	0.79	3/1302 (0.2%)	1.05	7/1770 (0.4%)
1	81-A	0.86	4/1302 (0.3%)	1.09	9/1770 (0.5%)
1	82-A	0.84	3/1302 (0.2%)	1.07	6/1770 (0.3%)
1	83-A	0.91	4/1302 (0.3%)	1.10	10/1770 (0.6%)
1	84-A	0.83	1/1302 (0.1%)	1.09	6/1770 (0.3%)
1	85-A	0.71	1/1302 (0.1%)	0.96	5/1770 (0.3%)
1	86-A	0.78	1/1302 (0.1%)	1.00	3/1770 (0.2%)
1	87-A	0.74	1/1302 (0.1%)	0.95	5/1770 (0.3%)
1	88-A	0.74	2/1302 (0.2%)	0.98	3/1770 (0.2%)
1	89-A	0.74	2/1302 (0.2%)	0.97	3/1770 (0.2%)
1	90-A	0.71	1/1302 (0.1%)	0.99	4/1770 (0.2%)
1	91-A	0.76	0/1302	1.04	4/1770 (0.2%)
1	92-A	0.77	2/1302 (0.2%)	1.03	4/1770 (0.2%)
1	93-A	0.74	0/1302	1.00	4/1770 (0.2%)
1	94-A	0.73	2/1302 (0.2%)	0.94	3/1770 (0.2%)
1	95-A	0.84	6/1302 (0.5%)	0.95	2/1770 (0.1%)
1	96-A	0.76	1/1302 (0.1%)	0.99	4/1770 (0.2%)
1	97-A	0.72	2/1302 (0.2%)	0.98	6/1770 (0.3%)
1	98-A	0.71	1/1302 (0.1%)	1.00	7/1770 (0.4%)
1	99-A	0.69	2/1302 (0.2%)	0.99	8/1770 (0.5%)
1	100-A	0.66	0/1302	0.95	5/1770 (0.3%)
1	101-A	0.76	1/1302 (0.1%)	0.90	3/1770 (0.2%)
1	102-A	0.73	1/1302 (0.1%)	0.90	2/1770 (0.1%)
1	103-A	0.71	0/1302	0.96	5/1770 (0.3%)
1	104-A	0.83	4/1302 (0.3%)	1.05	4/1770 (0.2%)
1	105-A	0.88	4/1302 (0.3%)	1.04	5/1770 (0.3%)
1	106-A	0.85	3/1302 (0.2%)	1.10	7/1770 (0.4%)
1	107-A	0.86	2/1302 (0.2%)	1.07	7/1770 (0.4%)
1	108-A	1.05	1/1302 (0.1%)	1.14	4/1770 (0.2%)
1	109-A	0.84	3/1302 (0.2%)	1.21	12/1770 (0.7%)
1	110-A	0.77	2/1302 (0.2%)	1.11	4/1770 (0.2%)
1	111-A	0.74	1/1302 (0.1%)	1.12	7/1770 (0.4%)
1	112-A	0.78	0/1302	1.02	4/1770 (0.2%)
1	113-A	0.80	2/1302 (0.2%)	1.08	6/1770 (0.3%)
1	114-A	0.78	1/1302 (0.1%)	1.08	10/1770 (0.6%)
1	115-A	0.81	3/1302 (0.2%)	1.08	11/1770 (0.6%)
1	116-A	0.87	5/1302 (0.4%)	1.02	5/1770 (0.3%)
1	117-A	0.82	2/1302 (0.2%)	1.05	8/1770 (0.5%)
1	118-A	0.80	2/1302 (0.2%)	0.98	3/1770 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	119-A	0.74	0/1302	0.90	3/1770 (0.2%)
1	120-A	0.74	1/1302 (0.1%)	0.99	7/1770 (0.4%)
1	121-A	0.79	1/1302 (0.1%)	1.01	5/1770 (0.3%)
1	122-A	0.76	2/1302 (0.2%)	1.04	6/1770 (0.3%)
1	123-A	0.72	0/1302	0.93	2/1770 (0.1%)
1	124-A	0.71	0/1302	0.93	0/1770
1	125-A	0.74	1/1302 (0.1%)	0.93	2/1770 (0.1%)
1	126-A	0.67	0/1302	0.91	4/1770 (0.2%)
1	127-A	0.71	2/1302 (0.2%)	0.97	4/1770 (0.2%)
1	128-A	0.74	1/1302 (0.1%)	0.89	1/1770 (0.1%)
1	129-A	0.78	2/1302 (0.2%)	0.87	3/1770 (0.2%)
1	130-A	0.68	0/1302	0.96	5/1770 (0.3%)
1	131-A	0.85	2/1302 (0.2%)	1.09	9/1770 (0.5%)
1	132-A	0.77	2/1302 (0.2%)	1.02	7/1770 (0.4%)
1	133-A	0.85	3/1302 (0.2%)	1.02	3/1770 (0.2%)
1	134-A	0.84	2/1302 (0.2%)	1.01	3/1770 (0.2%)
1	135-A	0.71	0/1302	0.91	3/1770 (0.2%)
1	136-A	0.71	1/1302 (0.1%)	0.99	7/1770 (0.4%)
1	137-A	0.71	1/1302 (0.1%)	0.99	7/1770 (0.4%)
1	138-A	0.75	3/1302 (0.2%)	1.01	5/1770 (0.3%)
1	139-A	0.75	0/1302	0.99	5/1770 (0.3%)
1	140-A	0.78	1/1302 (0.1%)	0.97	5/1770 (0.3%)
1	141-A	0.85	3/1302 (0.2%)	0.97	4/1770 (0.2%)
1	142-A	0.77	3/1302 (0.2%)	1.00	6/1770 (0.3%)
1	143-A	0.82	1/1302 (0.1%)	1.00	6/1770 (0.3%)
1	144-A	0.93	7/1302 (0.5%)	1.10	11/1770 (0.6%)
1	145-A	0.74	1/1302 (0.1%)	1.02	6/1770 (0.3%)
1	146-A	0.84	3/1302 (0.2%)	1.04	7/1770 (0.4%)
1	147-A	0.80	1/1302 (0.1%)	1.00	5/1770 (0.3%)
1	148-A	0.74	1/1302 (0.1%)	1.06	6/1770 (0.3%)
1	149-A	0.83	3/1302 (0.2%)	1.03	5/1770 (0.3%)
1	150-A	0.69	1/1302 (0.1%)	0.94	2/1770 (0.1%)
1	151-A	0.76	1/1302 (0.1%)	1.06	9/1770 (0.5%)
1	152-A	0.79	3/1302 (0.2%)	0.99	5/1770 (0.3%)
1	153-A	0.75	2/1302 (0.2%)	0.95	4/1770 (0.2%)
1	154-A	0.76	1/1302 (0.1%)	1.03	8/1770 (0.5%)
1	155-A	0.79	1/1302 (0.1%)	1.12	11/1770 (0.6%)
1	156-A	0.86	5/1302 (0.4%)	1.02	4/1770 (0.2%)
1	157-A	0.99	7/1302 (0.5%)	1.20	11/1770 (0.6%)
1	158-A	0.91	1/1302 (0.1%)	1.14	10/1770 (0.6%)
1	159-A	1.03	11/1302 (0.8%)	1.15	11/1770 (0.6%)
1	160-A	0.78	0/1302	1.02	6/1770 (0.3%)
1	161-A	0.80	1/1302 (0.1%)	1.04	6/1770 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	162-A	0.86	6/1302 (0.5%)	1.00	6/1770 (0.3%)
1	163-A	0.78	2/1302 (0.2%)	0.96	4/1770 (0.2%)
1	164-A	0.76	1/1302 (0.1%)	0.96	4/1770 (0.2%)
1	165-A	0.74	1/1302 (0.1%)	0.97	5/1770 (0.3%)
1	166-A	0.77	1/1302 (0.1%)	1.00	8/1770 (0.5%)
1	167-A	0.76	2/1302 (0.2%)	1.01	7/1770 (0.4%)
All	All	0.79	287/217434 (0.1%)	1.01	932/295590 (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	2-A	0	1
1	3-A	0	1
1	4-A	0	3
1	5-A	0	3
1	6-A	0	2
1	7-A	0	5
1	8-A	0	4
1	9-A	0	5
1	10-A	0	5
1	11-A	0	2
1	12-A	0	3
1	13-A	0	3
1	14-A	0	3
1	15-A	0	1
1	16-A	0	3
1	17-A	0	4
1	18-A	0	2
1	19-A	0	2
1	20-A	0	2
1	21-A	0	2
1	22-A	0	1
1	23-A	0	3
1	24-A	0	2
1	25-A	0	3
1	26-A	0	3
1	27-A	0	1
1	28-A	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	29-A	0	1
1	30-A	0	1
1	31-A	0	2
1	32-A	0	4
1	33-A	0	6
1	34-A	0	3
1	35-A	0	2
1	36-A	0	4
1	37-A	0	2
1	38-A	0	2
1	39-A	0	1
1	40-A	0	2
1	41-A	0	4
1	42-A	0	2
1	43-A	0	1
1	44-A	0	2
1	45-A	0	2
1	46-A	0	3
1	47-A	0	1
1	48-A	0	2
1	49-A	0	4
1	50-A	0	4
1	51-A	0	3
1	52-A	0	4
1	53-A	0	4
1	57-A	0	1
1	61-A	0	1
1	62-A	0	1
1	63-A	0	1
1	66-A	0	3
1	67-A	0	1
1	68-A	0	2
1	69-A	0	1
1	70-A	0	1
1	71-A	0	2
1	72-A	0	4
1	73-A	0	2
1	74-A	0	1
1	75-A	0	1
1	78-A	0	1
1	79-A	0	2
1	80-A	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	81-A	0	2
1	82-A	0	1
1	83-A	0	1
1	84-A	0	1
1	85-A	0	1
1	86-A	0	2
1	88-A	0	1
1	89-A	0	2
1	90-A	0	2
1	91-A	0	1
1	94-A	0	1
1	95-A	0	1
1	97-A	0	1
1	98-A	0	1
1	99-A	0	1
1	100-A	0	1
1	102-A	0	1
1	104-A	0	2
1	105-A	0	4
1	107-A	0	3
1	108-A	0	2
1	109-A	0	2
1	110-A	0	2
1	111-A	0	2
1	112-A	0	2
1	113-A	0	5
1	114-A	0	4
1	115-A	0	3
1	116-A	0	3
1	117-A	0	4
1	122-A	0	3
1	124-A	0	1
1	126-A	0	1
1	127-A	0	1
1	130-A	0	1
1	131-A	0	2
1	132-A	0	3
1	133-A	0	3
1	134-A	0	1
1	136-A	0	2
1	137-A	0	2
1	138-A	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	139-A	0	1
1	140-A	0	2
1	141-A	0	1
1	143-A	0	2
1	144-A	0	2
1	145-A	0	4
1	146-A	0	4
1	147-A	0	1
1	149-A	0	2
1	150-A	0	2
1	151-A	0	2
1	152-A	0	2
1	154-A	0	1
1	155-A	0	2
1	156-A	0	1
1	157-A	0	3
1	158-A	0	2
1	159-A	0	5
1	160-A	0	3
1	161-A	0	3
1	162-A	0	5
1	163-A	0	5
1	164-A	0	5
1	165-A	0	1
1	166-A	0	2
1	167-A	0	1
All	All	0	312

The worst 5 of 287 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	70-A	152	CYS	CB-SG	24.25	2.23	1.82
1	108-A	152	CYS	CB-SG	21.03	2.18	1.82
1	71-A	152	CYS	CB-SG	18.24	2.13	1.82
1	58-A	152	CYS	CB-SG	16.08	2.09	1.82
1	129-A	152	CYS	CB-SG	13.95	2.06	1.82

The worst 5 of 932 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	110-A	98	ARG	NE-CZ-NH1	16.84	128.72	120.30
1	84-A	36	LEU	CA-CB-CG	16.15	152.45	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	109-A	98	ARG	NE-CZ-NH2	-15.74	112.43	120.30
1	109-A	98	ARG	NE-CZ-NH1	15.70	128.15	120.30
1	68-A	20	MET	C-N-CD	-14.29	89.16	120.60

There are no chirality outliers.

5 of 312 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	128	TYR	Peptide
1	2-A	20	MET	Peptide
1	3-A	129	GLU	Peptide
1	4-A	127	ASP	Peptide
1	4-A	86	GLY	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	1223	1223	0	0
1	2-A	1268	1223	1223	0	0
1	3-A	1268	1223	1223	0	0
1	4-A	1268	1223	1223	0	0
1	5-A	1268	1223	1223	0	0
1	6-A	1268	1223	1223	0	0
1	7-A	1268	1223	1223	0	0
1	8-A	1268	1223	1223	0	0
1	9-A	1268	1223	1223	0	0
1	10-A	1268	1223	1223	0	0
1	11-A	1268	1223	1223	0	0
1	12-A	1268	1223	1222	0	0
1	13-A	1268	1223	1223	0	0
1	14-A	1268	1223	1223	0	0
1	15-A	1268	1223	1223	0	0
1	16-A	1268	1223	1223	0	0
1	17-A	1268	1223	1223	0	0
1	18-A	1268	1223	1223	0	0
1	19-A	1268	1223	1223	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	20-A	1268	1223	1223	0	0
1	21-A	1268	1223	1223	0	0
1	22-A	1268	1223	1223	0	0
1	23-A	1268	1223	1223	0	0
1	24-A	1268	1223	1223	0	0
1	25-A	1268	1223	1223	0	0
1	26-A	1268	1223	1223	0	0
1	27-A	1268	1223	1222	0	0
1	28-A	1268	1223	1223	0	0
1	29-A	1268	1223	1223	0	0
1	30-A	1268	1223	1222	0	0
1	31-A	1268	1223	1223	0	0
1	32-A	1268	1223	1223	0	0
1	33-A	1268	1223	1223	0	0
1	34-A	1268	1223	1223	0	0
1	35-A	1268	1223	1223	0	0
1	36-A	1268	1223	1223	0	0
1	37-A	1268	1223	1223	0	0
1	38-A	1268	1223	1223	0	0
1	39-A	1268	1223	1223	0	0
1	40-A	1268	1223	1223	0	0
1	41-A	1268	1223	1223	0	0
1	42-A	1268	1223	1223	0	0
1	43-A	1268	1223	1223	0	0
1	44-A	1268	1223	1223	0	0
1	45-A	1268	1223	1223	0	0
1	46-A	1268	1223	1223	0	0
1	47-A	1268	1223	1223	0	0
1	48-A	1268	1223	1223	0	0
1	49-A	1268	1223	1223	0	0
1	50-A	1268	1223	1223	0	0
1	51-A	1268	1223	1223	0	0
1	52-A	1268	1223	1223	0	0
1	53-A	1268	1223	1223	0	0
1	54-A	1268	1223	1223	0	0
1	55-A	1268	1223	1222	0	0
1	56-A	1268	1223	1223	0	0
1	57-A	1268	1223	1222	0	0
1	58-A	1268	1223	1223	0	0
1	59-A	1268	1223	1223	0	0
1	60-A	1268	1223	1223	0	0
1	61-A	1268	1223	1223	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	62-A	1268	1223	1223	0	0
1	63-A	1268	1223	1223	0	0
1	64-A	1268	1223	1223	0	0
1	65-A	1268	1223	1223	0	0
1	66-A	1268	1223	1223	0	0
1	67-A	1268	1223	1223	0	0
1	68-A	1268	1223	1223	0	0
1	69-A	1268	1223	1223	0	0
1	70-A	1268	1223	1223	0	0
1	71-A	1268	1223	1223	0	0
1	72-A	1268	1223	1223	0	0
1	73-A	1268	1223	1223	0	0
1	74-A	1268	1223	1223	0	0
1	75-A	1268	1223	1223	0	0
1	76-A	1268	1223	1222	0	0
1	77-A	1268	1223	1223	0	0
1	78-A	1268	1223	1223	0	0
1	79-A	1268	1223	1222	0	0
1	80-A	1268	1223	1223	0	0
1	81-A	1268	1223	1223	0	0
1	82-A	1268	1223	1223	0	0
1	83-A	1268	1223	1223	0	0
1	84-A	1268	1223	1223	0	0
1	85-A	1268	1223	1223	0	0
1	86-A	1268	1223	1222	0	0
1	87-A	1268	1223	1223	0	0
1	88-A	1268	1223	1223	0	0
1	89-A	1268	1223	1222	0	0
1	90-A	1268	1223	1223	0	0
1	91-A	1268	1223	1223	0	0
1	92-A	1268	1223	1223	0	0
1	93-A	1268	1223	1223	0	0
1	94-A	1268	1223	1223	0	0
1	95-A	1268	1223	1223	0	0
1	96-A	1268	1223	1223	0	0
1	97-A	1268	1223	1223	0	0
1	98-A	1268	1223	1223	0	0
1	99-A	1268	1223	1223	0	0
1	100-A	1268	1223	1223	0	0
1	101-A	1268	1223	1223	0	0
1	102-A	1268	1223	1223	0	0
1	103-A	1268	1223	1223	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	104-A	1268	1223	1223	0	0
1	105-A	1268	1223	1223	0	0
1	106-A	1268	1223	1223	0	0
1	107-A	1268	1223	1223	0	0
1	108-A	1268	1223	1223	0	0
1	109-A	1268	1223	1223	0	0
1	110-A	1268	1223	1223	0	0
1	111-A	1268	1223	1223	0	0
1	112-A	1268	1223	1223	0	0
1	113-A	1268	1223	1223	0	0
1	114-A	1268	1223	1223	0	0
1	115-A	1268	1223	1223	0	0
1	116-A	1268	1223	1223	0	0
1	117-A	1268	1223	1223	0	0
1	118-A	1268	1223	1223	0	0
1	119-A	1268	1223	1222	0	0
1	120-A	1268	1223	1222	0	0
1	121-A	1268	1223	1223	0	0
1	122-A	1268	1223	1223	0	0
1	123-A	1268	1223	1223	0	0
1	124-A	1268	1223	1223	0	0
1	125-A	1268	1223	1223	0	0
1	126-A	1268	1223	1223	0	0
1	127-A	1268	1223	1223	0	0
1	128-A	1268	1223	1223	0	0
1	129-A	1268	1223	1223	0	0
1	130-A	1268	1223	1223	0	0
1	131-A	1268	1223	1223	0	0
1	132-A	1268	1223	1223	0	0
1	133-A	1268	1223	1223	0	0
1	134-A	1268	1223	1223	0	0
1	135-A	1268	1223	1223	0	0
1	136-A	1268	1223	1223	0	0
1	137-A	1268	1223	1223	0	0
1	138-A	1268	1223	1223	0	0
1	139-A	1268	1223	1223	0	0
1	140-A	1268	1223	1223	0	0
1	141-A	1268	1223	1222	0	0
1	142-A	1268	1223	1223	0	0
1	143-A	1268	1223	1223	0	0
1	144-A	1268	1223	1223	0	0
1	145-A	1268	1223	1223	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	146-A	1268	1223	1223	0	0
1	147-A	1268	1223	1222	0	0
1	148-A	1268	1223	1223	0	0
1	149-A	1268	1223	1222	0	0
1	150-A	1268	1223	1223	0	0
1	151-A	1268	1223	1223	0	0
1	152-A	1268	1223	1223	0	0
1	153-A	1268	1223	1222	0	0
1	154-A	1268	1223	1222	0	0
1	155-A	1268	1223	1223	0	0
1	156-A	1268	1223	1223	0	0
1	157-A	1268	1223	1223	0	0
1	158-A	1268	1223	1223	0	0
1	159-A	1268	1223	1223	0	0
1	160-A	1268	1223	1223	0	0
1	161-A	1268	1223	1222	0	0
1	162-A	1268	1223	1222	0	0
1	163-A	1268	1223	1223	0	0
1	164-A	1268	1223	1223	0	0
1	165-A	1268	1223	1223	0	0
1	166-A	1268	1223	1223	0	0
1	167-A	1268	1223	1223	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	17	0	0
2	38-A	32	17	17	0	0
2	39-A	32	17	17	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
2	166-A	32	17	17	0	0
2	167-A	32	17	17	0	0
3	1-A	2	0	0	0	0
3	2-A	2	0	0	0	0
3	3-A	2	0	0	0	0
3	4-A	2	0	0	0	0
3	5-A	2	0	0	0	0
3	6-A	2	0	0	0	0
3	7-A	2	0	0	0	0
3	8-A	2	0	0	0	0
3	9-A	2	0	0	0	0
3	10-A	2	0	0	0	0
3	11-A	2	0	0	0	0
3	12-A	2	0	0	0	0
3	13-A	2	0	0	0	0
3	14-A	2	0	0	0	0
3	15-A	2	0	0	0	0
3	16-A	2	0	0	0	0
3	17-A	2	0	0	0	0
3	18-A	2	0	0	0	0
3	19-A	2	0	0	0	0
3	20-A	2	0	0	0	0
3	21-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	22-A	2	0	0	0	0
3	23-A	2	0	0	0	0
3	24-A	2	0	0	0	0
3	25-A	2	0	0	0	0
3	26-A	2	0	0	0	0
3	27-A	2	0	0	0	0
3	28-A	2	0	0	0	0
3	29-A	2	0	0	0	0
3	30-A	2	0	0	0	0
3	31-A	2	0	0	0	0
3	32-A	2	0	0	0	0
3	33-A	2	0	0	0	0
3	34-A	2	0	0	0	0
3	35-A	2	0	0	0	0
3	36-A	2	0	0	0	0
3	37-A	2	0	0	0	0
3	38-A	2	0	0	0	0
3	39-A	2	0	0	0	0
3	40-A	2	0	0	0	0
3	41-A	2	0	0	0	0
3	42-A	2	0	0	0	0
3	43-A	2	0	0	0	0
3	44-A	2	0	0	0	0
3	45-A	2	0	0	0	0
3	46-A	2	0	0	0	0
3	47-A	2	0	0	0	0
3	48-A	2	0	0	0	0
3	49-A	2	0	0	0	0
3	50-A	2	0	0	0	0
3	51-A	2	0	0	0	0
3	52-A	2	0	0	0	0
3	53-A	2	0	0	0	0
3	54-A	2	0	0	0	0
3	55-A	2	0	0	0	0
3	56-A	2	0	0	0	0
3	57-A	2	0	0	0	0
3	58-A	2	0	0	0	0
3	59-A	2	0	0	0	0
3	60-A	2	0	0	0	0
3	61-A	2	0	0	0	0
3	62-A	2	0	0	0	0
3	63-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	64-A	2	0	0	0	0
3	65-A	2	0	0	0	0
3	66-A	2	0	0	0	0
3	67-A	2	0	0	0	0
3	68-A	2	0	0	0	0
3	69-A	2	0	0	0	0
3	70-A	2	0	0	0	0
3	71-A	2	0	0	0	0
3	72-A	2	0	0	0	0
3	73-A	2	0	0	0	0
3	74-A	2	0	0	0	0
3	75-A	2	0	0	0	0
3	76-A	2	0	0	0	0
3	77-A	2	0	0	0	0
3	78-A	2	0	0	0	0
3	79-A	2	0	0	0	0
3	80-A	2	0	0	0	0
3	81-A	2	0	0	0	0
3	82-A	2	0	0	0	0
3	83-A	2	0	0	0	0
3	84-A	2	0	0	0	0
3	85-A	2	0	0	0	0
3	86-A	2	0	0	0	0
3	87-A	2	0	0	0	0
3	88-A	2	0	0	0	0
3	89-A	2	0	0	0	0
3	90-A	2	0	0	0	0
3	91-A	2	0	0	0	0
3	92-A	2	0	0	0	0
3	93-A	2	0	0	0	0
3	94-A	2	0	0	0	0
3	95-A	2	0	0	0	0
3	96-A	2	0	0	0	0
3	97-A	2	0	0	0	0
3	98-A	2	0	0	0	0
3	99-A	2	0	0	0	0
3	100-A	2	0	0	0	0
3	101-A	2	0	0	0	0
3	102-A	2	0	0	0	0
3	103-A	2	0	0	0	0
3	104-A	2	0	0	0	0
3	105-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	106-A	2	0	0	0	0
3	107-A	2	0	0	0	0
3	108-A	2	0	0	0	0
3	109-A	2	0	0	0	0
3	110-A	2	0	0	0	0
3	111-A	2	0	0	0	0
3	112-A	2	0	0	0	0
3	113-A	2	0	0	0	0
3	114-A	2	0	0	0	0
3	115-A	2	0	0	0	0
3	116-A	2	0	0	0	0
3	117-A	2	0	0	0	0
3	118-A	2	0	0	0	0
3	119-A	2	0	0	0	0
3	120-A	2	0	0	0	0
3	121-A	2	0	0	0	0
3	122-A	2	0	0	0	0
3	123-A	2	0	0	0	0
3	124-A	2	0	0	0	0
3	125-A	2	0	0	0	0
3	126-A	2	0	0	0	0
3	127-A	2	0	0	0	0
3	128-A	2	0	0	0	0
3	129-A	2	0	0	0	0
3	130-A	2	0	0	0	0
3	131-A	2	0	0	0	0
3	132-A	2	0	0	0	0
3	133-A	2	0	0	0	0
3	134-A	2	0	0	0	0
3	135-A	2	0	0	0	0
3	136-A	2	0	0	0	0
3	137-A	2	0	0	0	0
3	138-A	2	0	0	0	0
3	139-A	2	0	0	0	0
3	140-A	2	0	0	0	0
3	141-A	2	0	0	0	0
3	142-A	2	0	0	0	0
3	143-A	2	0	0	0	0
3	144-A	2	0	0	0	0
3	145-A	2	0	0	0	0
3	146-A	2	0	0	0	0
3	147-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	148-A	2	0	0	0	0
3	149-A	2	0	0	0	0
3	150-A	2	0	0	0	0
3	151-A	2	0	0	0	0
3	152-A	2	0	0	0	0
3	153-A	2	0	0	0	0
3	154-A	2	0	0	0	0
3	155-A	2	0	0	0	0
3	156-A	2	0	0	0	0
3	157-A	2	0	0	0	0
3	158-A	2	0	0	0	0
3	159-A	2	0	0	0	0
3	160-A	2	0	0	0	0
3	161-A	2	0	0	0	0
3	162-A	2	0	0	0	0
3	163-A	2	0	0	0	0
3	164-A	2	0	0	0	0
3	165-A	2	0	0	0	0
3	166-A	2	0	0	0	0
3	167-A	2	0	0	0	0
4	1-A	48	24	24	0	0
4	2-A	48	24	24	0	0
4	3-A	48	24	24	0	0
4	4-A	48	24	24	0	0
4	5-A	48	24	24	0	0
4	6-A	48	24	24	0	0
4	7-A	48	24	24	0	0
4	8-A	48	24	24	0	0
4	9-A	48	24	24	0	0
4	10-A	48	24	24	0	0
4	11-A	48	24	24	0	0
4	12-A	48	24	24	0	0
4	13-A	48	24	24	0	0
4	14-A	48	24	24	0	0
4	15-A	48	24	24	0	0
4	16-A	48	24	24	0	0
4	17-A	48	24	24	0	0
4	18-A	48	24	24	0	0
4	19-A	48	24	24	0	0
4	20-A	48	24	24	0	0
4	21-A	48	24	24	0	0
4	22-A	48	24	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	23-A	48	24	24	0	0
4	24-A	48	24	24	0	0
4	25-A	48	24	24	0	0
4	26-A	48	24	24	0	0
4	27-A	48	24	24	0	0
4	28-A	48	24	24	0	0
4	29-A	48	24	24	0	0
4	30-A	48	24	24	0	0
4	31-A	48	24	24	0	0
4	32-A	48	24	24	0	0
4	33-A	48	24	24	0	0
4	34-A	48	24	24	0	0
4	35-A	48	24	24	0	0
4	36-A	48	24	24	0	0
4	37-A	48	24	24	0	0
4	38-A	48	24	24	0	0
4	39-A	48	24	24	0	0
4	40-A	48	24	24	0	0
4	41-A	48	24	24	0	0
4	42-A	48	24	24	0	0
4	43-A	48	24	24	0	0
4	44-A	48	24	24	0	0
4	45-A	48	24	24	0	0
4	46-A	48	24	24	0	0
4	47-A	48	24	24	0	0
4	48-A	48	24	24	0	0
4	49-A	48	24	24	0	0
4	50-A	48	24	24	0	0
4	51-A	48	24	24	0	0
4	52-A	48	24	24	0	0
4	53-A	48	24	24	0	0
4	54-A	48	24	24	0	0
4	55-A	48	24	24	0	0
4	56-A	48	24	24	0	0
4	57-A	48	24	24	0	0
4	58-A	48	24	24	0	0
4	59-A	48	24	24	0	0
4	60-A	48	24	24	0	0
4	61-A	48	24	24	0	0
4	62-A	48	24	24	0	0
4	63-A	48	24	24	0	0
4	64-A	48	24	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	65-A	48	24	24	0	0
4	66-A	48	24	24	0	0
4	67-A	48	24	24	0	0
4	68-A	48	24	24	0	0
4	69-A	48	24	24	0	0
4	70-A	48	24	24	0	0
4	71-A	48	24	24	0	0
4	72-A	48	24	24	0	0
4	73-A	48	24	24	0	0
4	74-A	48	24	24	0	0
4	75-A	48	24	24	0	0
4	76-A	48	24	24	0	0
4	77-A	48	24	24	0	0
4	78-A	48	24	24	0	0
4	79-A	48	24	24	0	0
4	80-A	48	24	24	0	0
4	81-A	48	24	24	0	0
4	82-A	48	24	24	0	0
4	83-A	48	24	24	0	0
4	84-A	48	24	24	0	0
4	85-A	48	24	24	0	0
4	86-A	48	24	24	0	0
4	87-A	48	24	24	0	0
4	88-A	48	24	24	0	0
4	89-A	48	24	24	0	0
4	90-A	48	24	24	0	0
4	91-A	48	24	24	0	0
4	92-A	48	24	24	0	0
4	93-A	48	24	24	0	0
4	94-A	48	24	24	0	0
4	95-A	48	24	24	0	0
4	96-A	48	24	24	0	0
4	97-A	48	24	24	0	0
4	98-A	48	24	24	0	0
4	99-A	48	24	24	0	0
4	100-A	48	24	24	0	0
4	101-A	48	24	24	0	0
4	102-A	48	24	24	0	0
4	103-A	48	24	24	0	0
4	104-A	48	24	24	0	0
4	105-A	48	24	24	0	0
4	106-A	48	24	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	107-A	48	24	24	0	0
4	108-A	48	24	24	0	0
4	109-A	48	24	24	0	0
4	110-A	48	24	24	0	0
4	111-A	48	24	24	0	0
4	112-A	48	24	24	0	0
4	113-A	48	24	24	0	0
4	114-A	48	24	24	0	0
4	115-A	48	24	24	0	0
4	116-A	48	24	24	0	0
4	117-A	48	24	24	0	0
4	118-A	48	24	24	0	0
4	119-A	48	24	24	0	0
4	120-A	48	24	24	0	0
4	121-A	48	24	24	0	0
4	122-A	48	24	24	0	0
4	123-A	48	24	24	0	0
4	124-A	48	24	24	0	0
4	125-A	48	24	24	0	0
4	126-A	48	24	24	0	0
4	127-A	48	24	24	0	0
4	128-A	48	24	24	0	0
4	129-A	48	24	24	0	0
4	130-A	48	24	24	0	0
4	131-A	48	24	24	0	0
4	132-A	48	24	24	0	0
4	133-A	48	24	24	0	0
4	134-A	48	24	24	0	0
4	135-A	48	24	24	0	0
4	136-A	48	24	24	0	0
4	137-A	48	24	24	0	0
4	138-A	48	24	24	0	0
4	139-A	48	24	24	0	0
4	140-A	48	24	24	0	0
4	141-A	48	24	24	0	0
4	142-A	48	24	24	0	0
4	143-A	48	24	24	0	0
4	144-A	48	24	24	0	0
4	145-A	48	24	24	0	0
4	146-A	48	24	24	0	0
4	147-A	48	24	24	0	0
4	148-A	48	24	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	149-A	48	24	24	0	0
4	150-A	48	24	24	0	0
4	151-A	48	24	24	0	0
4	152-A	48	24	24	0	0
4	153-A	48	24	24	0	0
4	154-A	48	24	24	0	0
4	155-A	48	24	24	0	0
4	156-A	48	24	24	0	0
4	157-A	48	24	24	0	0
4	158-A	48	24	24	0	0
4	159-A	48	24	24	0	0
4	160-A	48	24	24	0	0
4	161-A	48	24	24	0	0
4	162-A	48	24	24	0	0
4	163-A	48	24	24	0	0
4	164-A	48	24	24	0	0
4	165-A	48	24	24	0	0
4	166-A	48	24	24	0	0
4	167-A	48	24	24	0	0
5	1-A	83	0	0	0	0
5	2-A	83	0	0	0	0
5	3-A	79	0	0	0	0
5	4-A	68	0	0	0	0
5	5-A	75	0	0	0	0
5	6-A	80	0	0	0	0
5	7-A	99	0	0	0	0
5	8-A	89	0	0	0	0
5	9-A	79	0	0	0	0
5	10-A	79	0	0	0	0
5	11-A	82	0	0	0	0
5	12-A	88	0	0	0	0
5	13-A	89	0	0	0	0
5	14-A	96	0	0	0	0
5	15-A	96	0	0	0	0
5	16-A	94	0	0	0	0
5	17-A	84	0	0	0	0
5	18-A	89	0	0	0	0
5	19-A	80	0	0	0	0
5	20-A	73	0	0	0	0
5	21-A	92	0	0	0	0
5	22-A	91	0	0	0	0
5	23-A	94	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	24-A	95	0	0	0	0
5	25-A	76	0	0	0	0
5	26-A	83	0	0	0	0
5	27-A	81	0	0	0	0
5	28-A	81	0	0	0	0
5	29-A	83	0	0	0	0
5	30-A	84	0	0	0	0
5	31-A	86	0	0	0	0
5	32-A	85	0	0	0	0
5	33-A	86	0	0	0	0
5	34-A	93	0	0	0	0
5	35-A	93	0	0	0	0
5	36-A	77	0	0	0	0
5	37-A	82	0	0	0	0
5	38-A	87	0	0	0	0
5	39-A	93	0	0	0	0
5	40-A	84	0	0	0	0
5	41-A	82	0	0	0	0
5	42-A	83	0	0	0	0
5	43-A	95	0	0	0	0
5	44-A	100	0	0	0	0
5	45-A	93	0	0	0	0
5	46-A	92	0	0	0	0
5	47-A	98	0	0	0	0
5	48-A	92	0	0	0	0
5	49-A	89	0	0	0	0
5	50-A	78	0	0	0	0
5	51-A	68	0	0	0	0
5	52-A	77	0	0	0	0
5	53-A	87	0	0	0	0
5	54-A	92	0	0	0	0
5	55-A	92	0	0	0	0
5	56-A	82	0	0	0	0
5	57-A	86	0	0	0	0
5	58-A	89	0	0	0	0
5	59-A	96	0	0	0	0
5	60-A	96	0	0	0	0
5	61-A	98	0	0	0	0
5	62-A	100	0	0	0	0
5	63-A	97	0	0	0	0
5	64-A	87	0	0	0	0
5	65-A	83	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	66-A	77	0	0	0	0
5	67-A	78	0	0	0	0
5	68-A	79	0	0	0	0
5	69-A	79	0	0	0	0
5	70-A	85	0	0	0	0
5	71-A	91	0	0	0	0
5	72-A	101	0	0	0	0
5	73-A	94	0	0	0	0
5	74-A	85	0	0	0	0
5	75-A	92	0	0	0	0
5	76-A	82	0	0	0	0
5	77-A	85	0	0	0	0
5	78-A	84	0	0	0	0
5	79-A	86	0	0	0	0
5	80-A	85	0	0	0	0
5	81-A	92	0	0	0	0
5	82-A	91	0	0	0	0
5	83-A	98	0	0	0	0
5	84-A	94	0	0	0	0
5	85-A	94	0	0	0	0
5	86-A	88	0	0	0	0
5	87-A	84	0	0	0	0
5	88-A	82	0	0	0	0
5	89-A	92	0	0	0	0
5	90-A	98	0	0	0	0
5	91-A	75	0	0	0	0
5	92-A	77	0	0	0	0
5	93-A	78	0	0	0	0
5	94-A	92	0	0	0	0
5	95-A	101	0	0	0	0
5	96-A	106	0	0	0	0
5	97-A	94	0	0	0	0
5	98-A	86	0	0	0	0
5	99-A	87	0	0	0	0
5	100-A	80	0	0	0	0
5	101-A	76	0	0	0	0
5	102-A	80	0	0	0	0
5	103-A	89	0	0	0	0
5	104-A	88	0	0	0	0
5	105-A	97	0	0	0	0
5	106-A	85	0	0	0	0
5	107-A	87	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	108-A	93	0	0	0	0
5	109-A	82	0	0	0	0
5	110-A	82	0	0	0	0
5	111-A	75	0	0	0	0
5	112-A	85	0	0	0	0
5	113-A	97	0	0	0	0
5	114-A	98	0	0	0	0
5	115-A	86	0	0	0	0
5	116-A	89	0	0	0	0
5	117-A	85	0	0	0	0
5	118-A	89	0	0	0	0
5	119-A	88	0	0	0	0
5	120-A	95	0	0	0	0
5	121-A	93	0	0	0	0
5	122-A	90	0	0	0	0
5	123-A	82	0	0	0	0
5	124-A	81	0	0	0	0
5	125-A	84	0	0	0	0
5	126-A	101	0	0	0	0
5	127-A	96	0	0	0	0
5	128-A	90	0	0	0	0
5	129-A	89	0	0	0	0
5	130-A	81	0	0	0	0
5	131-A	75	0	0	0	0
5	132-A	87	0	0	0	0
5	133-A	96	0	0	0	0
5	134-A	89	0	0	0	0
5	135-A	89	0	0	0	0
5	136-A	87	0	0	0	0
5	137-A	88	0	0	0	0
5	138-A	88	0	0	0	0
5	139-A	96	0	0	0	0
5	140-A	88	0	0	0	0
5	141-A	80	0	0	0	0
5	142-A	80	0	0	0	0
5	143-A	83	0	0	0	0
5	144-A	84	0	0	0	0
5	145-A	99	0	0	0	0
5	146-A	101	0	0	0	0
5	147-A	105	0	0	0	0
5	148-A	103	0	0	0	0
5	149-A	86	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	150-A	94	0	0	0	0
5	151-A	92	0	0	0	0
5	152-A	89	0	0	0	0
5	153-A	99	0	0	0	0
5	154-A	98	0	0	0	0
5	155-A	78	0	0	0	0
5	156-A	79	0	0	0	0
5	157-A	80	0	0	0	0
5	158-A	78	0	0	0	0
5	159-A	82	0	0	0	0
5	160-A	82	0	0	0	0
5	161-A	86	0	0	0	0
5	162-A	84	0	0	0	0
5	163-A	91	0	0	0	0
5	164-A	92	0	0	0	0
5	165-A	90	0	0	0	0
5	166-A	81	0	0	0	0
5	167-A	89	0	0	0	0
All	All	240066	211088	211070	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 [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	7	0
1	2-A	157/159 (99%)	143 (91%)	11 (7%)	3 (2%)	10	0
1	3-A	157/159 (99%)	150 (96%)	4 (2%)	3 (2%)	10	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4-A	157/159 (99%)	146 (93%)	6 (4%)	5 (3%)	5	0
1	5-A	157/159 (99%)	147 (94%)	4 (2%)	6 (4%)	4	0
1	6-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	7	0
1	7-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	10	0
1	8-A	157/159 (99%)	142 (90%)	11 (7%)	4 (2%)	7	0
1	9-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	7	0
1	10-A	157/159 (99%)	146 (93%)	3 (2%)	8 (5%)	2	0
1	11-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	4	0
1	12-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	7	0
1	13-A	157/159 (99%)	145 (92%)	10 (6%)	2 (1%)	15	2
1	14-A	157/159 (99%)	146 (93%)	8 (5%)	3 (2%)	10	0
1	15-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	7	0
1	16-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	5	0
1	17-A	157/159 (99%)	146 (93%)	5 (3%)	6 (4%)	4	0
1	18-A	157/159 (99%)	142 (90%)	10 (6%)	5 (3%)	5	0
1	19-A	157/159 (99%)	148 (94%)	4 (2%)	5 (3%)	5	0
1	20-A	157/159 (99%)	148 (94%)	8 (5%)	1 (1%)	30	8
1	21-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	7	0
1	22-A	157/159 (99%)	145 (92%)	9 (6%)	3 (2%)	10	0
1	23-A	157/159 (99%)	148 (94%)	5 (3%)	4 (2%)	7	0
1	24-A	157/159 (99%)	147 (94%)	4 (2%)	6 (4%)	4	0
1	25-A	157/159 (99%)	145 (92%)	6 (4%)	6 (4%)	4	0
1	26-A	157/159 (99%)	142 (90%)	9 (6%)	6 (4%)	4	0
1	27-A	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	7	0
1	28-A	157/159 (99%)	143 (91%)	7 (4%)	7 (4%)	3	0
1	29-A	157/159 (99%)	139 (88%)	8 (5%)	10 (6%)	2	0
1	30-A	157/159 (99%)	138 (88%)	10 (6%)	9 (6%)	2	0
1	31-A	157/159 (99%)	136 (87%)	10 (6%)	11 (7%)	1	0
1	32-A	157/159 (99%)	137 (87%)	7 (4%)	13 (8%)	1	0
1	33-A	157/159 (99%)	137 (87%)	7 (4%)	13 (8%)	1	0
1	34-A	157/159 (99%)	139 (88%)	7 (4%)	11 (7%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	35-A	157/159 (99%)	141 (90%)	7 (4%)	9 (6%)	2	0
1	36-A	157/159 (99%)	140 (89%)	8 (5%)	9 (6%)	2	0
1	37-A	157/159 (99%)	137 (87%)	10 (6%)	10 (6%)	2	0
1	38-A	157/159 (99%)	146 (93%)	5 (3%)	6 (4%)	4	0
1	39-A	157/159 (99%)	142 (90%)	9 (6%)	6 (4%)	4	0
1	40-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	5	0
1	41-A	157/159 (99%)	142 (90%)	8 (5%)	7 (4%)	3	0
1	42-A	157/159 (99%)	146 (93%)	4 (2%)	7 (4%)	3	0
1	43-A	157/159 (99%)	142 (90%)	9 (6%)	6 (4%)	4	0
1	44-A	157/159 (99%)	146 (93%)	6 (4%)	5 (3%)	5	0
1	45-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	5	0
1	46-A	157/159 (99%)	148 (94%)	5 (3%)	4 (2%)	7	0
1	47-A	157/159 (99%)	147 (94%)	4 (2%)	6 (4%)	4	0
1	48-A	157/159 (99%)	148 (94%)	4 (2%)	5 (3%)	5	0
1	49-A	157/159 (99%)	145 (92%)	5 (3%)	7 (4%)	3	0
1	50-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	7	0
1	51-A	157/159 (99%)	146 (93%)	4 (2%)	7 (4%)	3	0
1	52-A	157/159 (99%)	144 (92%)	10 (6%)	3 (2%)	10	0
1	53-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	15	2
1	54-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	10	0
1	55-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	15	2
1	56-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	10	0
1	57-A	157/159 (99%)	145 (92%)	10 (6%)	2 (1%)	15	2
1	58-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	30	8
1	59-A	157/159 (99%)	148 (94%)	9 (6%)	0	100	100
1	60-A	157/159 (99%)	152 (97%)	2 (1%)	3 (2%)	10	0
1	61-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	15	2
1	62-A	157/159 (99%)	145 (92%)	9 (6%)	3 (2%)	10	0
1	63-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	15	2
1	64-A	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
1	65-A	157/159 (99%)	149 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	66-A	157/159 (99%)	147 (94%)	8 (5%)	2 (1%)	15	2
1	67-A	157/159 (99%)	147 (94%)	8 (5%)	2 (1%)	15	2
1	68-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	7	0
1	69-A	157/159 (99%)	144 (92%)	10 (6%)	3 (2%)	10	0
1	70-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	4	0
1	71-A	157/159 (99%)	144 (92%)	5 (3%)	8 (5%)	2	0
1	72-A	157/159 (99%)	144 (92%)	6 (4%)	7 (4%)	3	0
1	73-A	157/159 (99%)	147 (94%)	3 (2%)	7 (4%)	3	0
1	74-A	157/159 (99%)	143 (91%)	8 (5%)	6 (4%)	4	0
1	75-A	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	7	0
1	76-A	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	7	0
1	77-A	157/159 (99%)	142 (90%)	13 (8%)	2 (1%)	15	2
1	78-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	5	0
1	79-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	7	0
1	80-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	7	0
1	81-A	157/159 (99%)	147 (94%)	8 (5%)	2 (1%)	15	2
1	82-A	157/159 (99%)	143 (91%)	9 (6%)	5 (3%)	5	0
1	83-A	157/159 (99%)	146 (93%)	7 (4%)	4 (2%)	7	0
1	84-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	10	0
1	85-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	4	0
1	86-A	157/159 (99%)	143 (91%)	11 (7%)	3 (2%)	10	0
1	87-A	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	10	0
1	88-A	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
1	89-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	10	0
1	90-A	157/159 (99%)	148 (94%)	7 (4%)	2 (1%)	15	2
1	91-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	15	2
1	92-A	157/159 (99%)	146 (93%)	7 (4%)	4 (2%)	7	0
1	93-A	157/159 (99%)	147 (94%)	9 (6%)	1 (1%)	30	8
1	94-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	5	0
1	95-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	7	0
1	96-A	157/159 (99%)	146 (93%)	9 (6%)	2 (1%)	15	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	97-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	30	8
1	98-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	10	0
1	99-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	100-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	10	0
1	101-A	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	10	0
1	102-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	15	2
1	103-A	157/159 (99%)	150 (96%)	3 (2%)	4 (2%)	7	0
1	104-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	15	2
1	105-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	30	8
1	106-A	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	10	0
1	107-A	157/159 (99%)	144 (92%)	10 (6%)	3 (2%)	10	0
1	108-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	7	0
1	109-A	157/159 (99%)	143 (91%)	9 (6%)	5 (3%)	5	0
1	110-A	157/159 (99%)	139 (88%)	10 (6%)	8 (5%)	2	0
1	111-A	157/159 (99%)	142 (90%)	6 (4%)	9 (6%)	2	0
1	112-A	157/159 (99%)	141 (90%)	8 (5%)	8 (5%)	2	0
1	113-A	157/159 (99%)	141 (90%)	5 (3%)	11 (7%)	1	0
1	114-A	157/159 (99%)	138 (88%)	11 (7%)	8 (5%)	2	0
1	115-A	157/159 (99%)	145 (92%)	5 (3%)	7 (4%)	3	0
1	116-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	4	0
1	117-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	7	0
1	118-A	157/159 (99%)	147 (94%)	4 (2%)	6 (4%)	4	0
1	119-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	30	8
1	120-A	157/159 (99%)	144 (92%)	11 (7%)	2 (1%)	15	2
1	121-A	157/159 (99%)	148 (94%)	4 (2%)	5 (3%)	5	0
1	122-A	157/159 (99%)	142 (90%)	10 (6%)	5 (3%)	5	0
1	123-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	4	0
1	124-A	157/159 (99%)	144 (92%)	4 (2%)	9 (6%)	2	0
1	125-A	157/159 (99%)	142 (90%)	7 (4%)	8 (5%)	2	0
1	126-A	157/159 (99%)	148 (94%)	7 (4%)	2 (1%)	15	2
1	127-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	30	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	128-A	157/159 (99%)	146 (93%)	7 (4%)	4 (2%)	7	0
1	129-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	30	8
1	130-A	157/159 (99%)	144 (92%)	11 (7%)	2 (1%)	15	2
1	131-A	157/159 (99%)	141 (90%)	11 (7%)	5 (3%)	5	0
1	132-A	157/159 (99%)	140 (89%)	13 (8%)	4 (2%)	7	0
1	133-A	157/159 (99%)	146 (93%)	8 (5%)	3 (2%)	10	0
1	134-A	157/159 (99%)	144 (92%)	10 (6%)	3 (2%)	10	0
1	135-A	157/159 (99%)	143 (91%)	12 (8%)	2 (1%)	15	2
1	136-A	157/159 (99%)	145 (92%)	7 (4%)	5 (3%)	5	0
1	137-A	157/159 (99%)	144 (92%)	5 (3%)	8 (5%)	2	0
1	138-A	157/159 (99%)	146 (93%)	5 (3%)	6 (4%)	4	0
1	139-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	7	0
1	140-A	157/159 (99%)	149 (95%)	4 (2%)	4 (2%)	7	0
1	141-A	157/159 (99%)	145 (92%)	7 (4%)	5 (3%)	5	0
1	142-A	157/159 (99%)	146 (93%)	5 (3%)	6 (4%)	4	0
1	143-A	157/159 (99%)	146 (93%)	5 (3%)	6 (4%)	4	0
1	144-A	157/159 (99%)	143 (91%)	9 (6%)	5 (3%)	5	0
1	145-A	157/159 (99%)	141 (90%)	11 (7%)	5 (3%)	5	0
1	146-A	157/159 (99%)	143 (91%)	8 (5%)	6 (4%)	4	0
1	147-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	7	0
1	148-A	157/159 (99%)	148 (94%)	4 (2%)	5 (3%)	5	0
1	149-A	157/159 (99%)	146 (93%)	9 (6%)	2 (1%)	15	2
1	150-A	157/159 (99%)	140 (89%)	11 (7%)	6 (4%)	4	0
1	151-A	157/159 (99%)	143 (91%)	11 (7%)	3 (2%)	10	0
1	152-A	157/159 (99%)	149 (95%)	4 (2%)	4 (2%)	7	0
1	153-A	157/159 (99%)	150 (96%)	3 (2%)	4 (2%)	7	0
1	154-A	157/159 (99%)	146 (93%)	8 (5%)	3 (2%)	10	0
1	155-A	157/159 (99%)	142 (90%)	9 (6%)	6 (4%)	4	0
1	156-A	157/159 (99%)	140 (89%)	11 (7%)	6 (4%)	4	0
1	157-A	157/159 (99%)	142 (90%)	10 (6%)	5 (3%)	5	0
1	158-A	157/159 (99%)	140 (89%)	9 (6%)	8 (5%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	159-A	157/159 (99%)	140 (89%)	11 (7%)	6 (4%)	4	0
1	160-A	157/159 (99%)	141 (90%)	11 (7%)	5 (3%)	5	0
1	161-A	157/159 (99%)	140 (89%)	12 (8%)	5 (3%)	5	0
1	162-A	157/159 (99%)	145 (92%)	7 (4%)	5 (3%)	5	0
1	163-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	7	0
1	164-A	157/159 (99%)	146 (93%)	6 (4%)	5 (3%)	5	0
1	165-A	157/159 (99%)	144 (92%)	6 (4%)	7 (4%)	3	0
1	166-A	157/159 (99%)	142 (90%)	12 (8%)	3 (2%)	10	0
1	167-A	157/159 (99%)	145 (92%)	5 (3%)	7 (4%)	3	0
All	All	26219/26553 (99%)	24212 (92%)	1237 (5%)	770 (3%)	6	0

5 of 770 Ramachandran outliers are listed below:

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

### 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%)	122 (90%)	14 (10%)	9	0
1	2-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	3-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	4-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	5-A	136/136 (100%)	127 (93%)	9 (7%)	21	1
1	6-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	7-A	136/136 (100%)	119 (88%)	17 (12%)	6	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	9-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	10-A	136/136 (100%)	126 (93%)	10 (7%)	17	1
1	11-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	12-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	13-A	136/136 (100%)	127 (93%)	9 (7%)	21	1
1	14-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	15-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	16-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	17-A	136/136 (100%)	125 (92%)	11 (8%)	15	1
1	18-A	136/136 (100%)	128 (94%)	8 (6%)	24	2
1	19-A	136/136 (100%)	125 (92%)	11 (8%)	15	1
1	20-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	21-A	136/136 (100%)	126 (93%)	10 (7%)	17	1
1	22-A	136/136 (100%)	124 (91%)	12 (9%)	12	0
1	23-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	24-A	136/136 (100%)	124 (91%)	12 (9%)	12	0
1	25-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	26-A	136/136 (100%)	124 (91%)	12 (9%)	12	0
1	27-A	136/136 (100%)	117 (86%)	19 (14%)	4	0
1	28-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	29-A	136/136 (100%)	116 (85%)	20 (15%)	4	0
1	30-A	136/136 (100%)	115 (85%)	21 (15%)	3	0
1	31-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	32-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	33-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	34-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	35-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	36-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	37-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	38-A	136/136 (100%)	119 (88%)	17 (12%)	6	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	39-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	40-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	41-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	42-A	136/136 (100%)	125 (92%)	11 (8%)	15	1
1	43-A	136/136 (100%)	125 (92%)	11 (8%)	15	1
1	44-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	45-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	46-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	47-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	48-A	136/136 (100%)	124 (91%)	12 (9%)	12	0
1	49-A	136/136 (100%)	125 (92%)	11 (8%)	15	1
1	50-A	136/136 (100%)	115 (85%)	21 (15%)	3	0
1	51-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	52-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	53-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	54-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	55-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	56-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	57-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	58-A	136/136 (100%)	125 (92%)	11 (8%)	15	1
1	59-A	136/136 (100%)	127 (93%)	9 (7%)	21	1
1	60-A	136/136 (100%)	114 (84%)	22 (16%)	3	0
1	61-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	62-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	63-A	136/136 (100%)	126 (93%)	10 (7%)	17	1
1	64-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	65-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	66-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	67-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	68-A	136/136 (100%)	124 (91%)	12 (9%)	12	0
1	69-A	136/136 (100%)	122 (90%)	14 (10%)	9	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	70-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	71-A	136/136 (100%)	127 (93%)	9 (7%)	21	1
1	72-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	73-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	74-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	75-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	76-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	77-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	78-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	79-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	80-A	136/136 (100%)	115 (85%)	21 (15%)	3	0
1	81-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	82-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	83-A	136/136 (100%)	127 (93%)	9 (7%)	21	1
1	84-A	136/136 (100%)	127 (93%)	9 (7%)	21	1
1	85-A	136/136 (100%)	124 (91%)	12 (9%)	12	0
1	86-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	87-A	136/136 (100%)	125 (92%)	11 (8%)	15	1
1	88-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	89-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	90-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	91-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	92-A	136/136 (100%)	124 (91%)	12 (9%)	12	0
1	93-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	94-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	95-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	96-A	136/136 (100%)	117 (86%)	19 (14%)	4	0
1	97-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	98-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	99-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	100-A	136/136 (100%)	122 (90%)	14 (10%)	9	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	101-A	136/136 (100%)	127 (93%)	9 (7%)	21	1
1	102-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	103-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	104-A	136/136 (100%)	125 (92%)	11 (8%)	15	1
1	105-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	106-A	136/136 (100%)	114 (84%)	22 (16%)	3	0
1	107-A	136/136 (100%)	114 (84%)	22 (16%)	3	0
1	108-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	109-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	110-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	111-A	136/136 (100%)	124 (91%)	12 (9%)	12	0
1	112-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	113-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	114-A	136/136 (100%)	116 (85%)	20 (15%)	4	0
1	115-A	136/136 (100%)	115 (85%)	21 (15%)	3	0
1	116-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	117-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	118-A	136/136 (100%)	116 (85%)	20 (15%)	4	0
1	119-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	120-A	136/136 (100%)	126 (93%)	10 (7%)	17	1
1	121-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	122-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	123-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	124-A	136/136 (100%)	124 (91%)	12 (9%)	12	0
1	125-A	136/136 (100%)	124 (91%)	12 (9%)	12	0
1	126-A	136/136 (100%)	125 (92%)	11 (8%)	15	1
1	127-A	136/136 (100%)	125 (92%)	11 (8%)	15	1
1	128-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	129-A	136/136 (100%)	126 (93%)	10 (7%)	17	1
1	130-A	136/136 (100%)	128 (94%)	8 (6%)	24	2
1	131-A	136/136 (100%)	124 (91%)	12 (9%)	12	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	132-A	136/136 (100%)	126 (93%)	10 (7%)	17	1
1	133-A	136/136 (100%)	125 (92%)	11 (8%)	15	1
1	134-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	135-A	136/136 (100%)	125 (92%)	11 (8%)	15	1
1	136-A	136/136 (100%)	122 (90%)	14 (10%)	9	0
1	137-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	138-A	136/136 (100%)	117 (86%)	19 (14%)	4	0
1	139-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	140-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	141-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	142-A	136/136 (100%)	117 (86%)	19 (14%)	4	0
1	143-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	144-A	136/136 (100%)	113 (83%)	23 (17%)	2	0
1	145-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	146-A	136/136 (100%)	117 (86%)	19 (14%)	4	0
1	147-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	148-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	149-A	136/136 (100%)	124 (91%)	12 (9%)	12	0
1	150-A	136/136 (100%)	120 (88%)	16 (12%)	6	0
1	151-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	152-A	136/136 (100%)	130 (96%)	6 (4%)	35	5
1	153-A	136/136 (100%)	116 (85%)	20 (15%)	4	0
1	154-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	155-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	156-A	136/136 (100%)	117 (86%)	19 (14%)	4	0
1	157-A	136/136 (100%)	116 (85%)	20 (15%)	4	0
1	158-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	159-A	136/136 (100%)	121 (89%)	15 (11%)	8	0
1	160-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	161-A	136/136 (100%)	116 (85%)	20 (15%)	4	0
1	162-A	136/136 (100%)	121 (89%)	15 (11%)	8	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	163-A	136/136 (100%)	118 (87%)	18 (13%)	5	0
1	164-A	136/136 (100%)	119 (88%)	17 (12%)	6	0
1	165-A	136/136 (100%)	123 (90%)	13 (10%)	10	0
1	166-A	136/136 (100%)	124 (91%)	12 (9%)	12	0
1	167-A	136/136 (100%)	115 (85%)	21 (15%)	3	0
All	All	22712/22712 (100%)	20232 (89%)	2480 (11%)	8	0

5 of 2480 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	78-A	18	ASN
1	96-A	119	VAL
1	156-A	76	LYS
1	80-A	33	ARG
1	88-A	104	LEU

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FOL	1-A	201	-	27,34,34	1.36	3 (11%)	28,47,47	1.95	7 (25%)
4	NAP	1-A	204	-	45,52,52	1.70	9 (20%)	55,80,80	1.41	12 (21%)
2	FOL	10-A	201	-	27,34,34	1.36	3 (11%)	28,47,47	2.11	8 (28%)
4	NAP	10-A	204	-	45,52,52	1.74	9 (20%)	55,80,80	1.25	8 (14%)
2	FOL	100-A	201	-	27,34,34	1.70	4 (14%)	28,47,47	2.13	7 (25%)
4	NAP	100-A	204	-	45,52,52	1.77	10 (22%)	55,80,80	1.36	11 (20%)
2	FOL	101-A	201	-	27,34,34	1.38	3 (11%)	28,47,47	1.62	4 (14%)
4	NAP	101-A	204	-	45,52,52	1.72	10 (22%)	55,80,80	1.32	10 (18%)
2	FOL	102-A	201	-	27,34,34	1.21	3 (11%)	28,47,47	1.84	6 (21%)
4	NAP	102-A	204	-	45,52,52	1.77	10 (22%)	55,80,80	1.34	11 (20%)
2	FOL	103-A	201	-	27,34,34	1.36	3 (11%)	28,47,47	1.90	6 (21%)
4	NAP	103-A	204	-	45,52,52	1.82	11 (24%)	55,80,80	1.36	10 (18%)
2	FOL	104-A	201	-	27,34,34	1.40	5 (18%)	28,47,47	2.06	7 (25%)
4	NAP	104-A	204	-	45,52,52	1.80	11 (24%)	55,80,80	1.54	13 (23%)
2	FOL	105-A	201	-	27,34,34	1.54	4 (14%)	28,47,47	2.06	6 (21%)
4	NAP	105-A	204	-	45,52,52	1.78	9 (20%)	55,80,80	1.28	9 (16%)
2	FOL	106-A	201	-	27,34,34	1.39	4 (14%)	28,47,47	1.89	6 (21%)
4	NAP	106-A	204	-	45,52,52	1.81	11 (24%)	55,80,80	1.26	10 (18%)
2	FOL	107-A	201	-	27,34,34	1.45	4 (14%)	28,47,47	2.03	7 (25%)
4	NAP	107-A	204	-	45,52,52	1.76	11 (24%)	55,80,80	1.34	12 (21%)
2	FOL	108-A	201	-	27,34,34	1.29	3 (11%)	28,47,47	2.23	9 (32%)
4	NAP	108-A	204	-	45,52,52	1.71	12 (26%)	55,80,80	1.38	7 (12%)
2	FOL	109-A	201	-	27,34,34	1.33	3 (11%)	28,47,47	1.91	6 (21%)
4	NAP	109-A	204	-	45,52,52	1.66	11 (24%)	55,80,80	1.27	9 (16%)
2	FOL	11-A	201	-	27,34,34	1.29	3 (11%)	28,47,47	1.95	4 (14%)
4	NAP	11-A	204	-	45,52,52	1.74	11 (24%)	55,80,80	1.36	12 (21%)
2	FOL	110-A	201	-	27,34,34	1.41	3 (11%)	28,47,47	2.62	7 (25%)
4	NAP	110-A	204	-	45,52,52	1.76	12 (26%)	55,80,80	1.31	12 (21%)
2	FOL	111-A	201	-	27,34,34	1.48	3 (11%)	28,47,47	2.05	4 (14%)
4	NAP	111-A	204	-	45,52,52	1.73	11 (24%)	55,80,80	1.37	12 (21%)
2	FOL	112-A	201	-	27,34,34	1.28	3 (11%)	28,47,47	2.38	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAP	112-A	204	-	45,52,52	1.75	9 (20%)	55,80,80	1.32	10 (18%)
2	FOL	113-A	201	-	27,34,34	1.45	3 (11%)	28,47,47	1.94	5 (17%)
4	NAP	113-A	204	-	45,52,52	1.76	9 (20%)	55,80,80	1.31	9 (16%)
2	FOL	114-A	201	-	27,34,34	1.39	3 (11%)	28,47,47	2.23	5 (17%)
4	NAP	114-A	204	-	45,52,52	1.74	11 (24%)	55,80,80	1.33	10 (18%)
2	FOL	115-A	201	-	27,34,34	1.41	3 (11%)	28,47,47	2.54	8 (28%)
4	NAP	115-A	204	-	45,52,52	1.83	12 (26%)	55,80,80	1.49	11 (20%)
2	FOL	116-A	201	-	27,34,34	1.38	4 (14%)	28,47,47	1.81	7 (25%)
4	NAP	116-A	204	-	45,52,52	1.77	10 (22%)	55,80,80	1.30	10 (18%)
2	FOL	117-A	201	-	27,34,34	1.52	4 (14%)	28,47,47	1.60	4 (14%)
4	NAP	117-A	204	-	45,52,52	1.74	10 (22%)	55,80,80	1.63	13 (23%)
2	FOL	118-A	201	-	27,34,34	1.53	3 (11%)	28,47,47	2.35	12 (42%)
4	NAP	118-A	204	-	45,52,52	1.71	9 (20%)	55,80,80	2.62	12 (21%)
2	FOL	119-A	201	-	27,34,34	1.45	3 (11%)	28,47,47	1.94	6 (21%)
4	NAP	119-A	204	-	45,52,52	1.84	11 (24%)	55,80,80	1.98	11 (20%)
2	FOL	12-A	201	-	27,34,34	1.55	3 (11%)	28,47,47	1.83	5 (17%)
4	NAP	12-A	204	-	45,52,52	1.69	9 (20%)	55,80,80	1.37	13 (23%)
2	FOL	120-A	201	-	27,34,34	1.50	5 (18%)	28,47,47	1.91	6 (21%)
4	NAP	120-A	204	-	45,52,52	1.71	10 (22%)	55,80,80	1.20	6 (10%)
2	FOL	121-A	201	-	27,34,34	1.55	3 (11%)	28,47,47	1.88	5 (17%)
4	NAP	121-A	204	-	45,52,52	1.66	10 (22%)	55,80,80	1.27	10 (18%)
2	FOL	122-A	201	-	27,34,34	1.48	4 (14%)	28,47,47	1.82	5 (17%)
4	NAP	122-A	204	-	45,52,52	1.73	9 (20%)	55,80,80	1.36	11 (20%)
2	FOL	123-A	201	-	27,34,34	1.52	5 (18%)	28,47,47	1.75	4 (14%)
4	NAP	123-A	204	-	45,52,52	1.68	10 (22%)	55,80,80	1.39	11 (20%)
2	FOL	124-A	201	-	27,34,34	1.41	3 (11%)	28,47,47	2.05	8 (28%)
4	NAP	124-A	204	-	45,52,52	1.65	8 (17%)	55,80,80	1.33	11 (20%)
2	FOL	125-A	201	-	27,34,34	1.41	4 (14%)	28,47,47	1.97	5 (17%)
4	NAP	125-A	204	-	45,52,52	1.64	7 (15%)	55,80,80	1.30	9 (16%)
2	FOL	126-A	201	-	27,34,34	1.69	5 (18%)	28,47,47	2.59	10 (35%)
4	NAP	126-A	204	-	45,52,52	1.65	9 (20%)	55,80,80	1.23	10 (18%)
2	FOL	127-A	201	-	27,34,34	1.37	3 (11%)	28,47,47	2.11	8 (28%)
4	NAP	127-A	204	-	45,52,52	1.69	9 (20%)	55,80,80	1.36	11 (20%)
2	FOL	128-A	201	-	27,34,34	1.37	4 (14%)	28,47,47	2.14	7 (25%)
4	NAP	128-A	204	-	45,52,52	1.70	9 (20%)	55,80,80	1.43	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FOL	129-A	201	-	27,34,34	1.55	3 (11%)	28,47,47	2.20	10 (35%)
4	NAP	129-A	204	-	45,52,52	1.72	9 (20%)	55,80,80	1.45	11 (20%)
2	FOL	13-A	201	-	27,34,34	1.52	4 (14%)	28,47,47	2.76	9 (32%)
4	NAP	13-A	204	-	45,52,52	1.72	10 (22%)	55,80,80	1.23	8 (14%)
2	FOL	130-A	201	-	27,34,34	1.43	3 (11%)	28,47,47	1.94	7 (25%)
4	NAP	130-A	204	-	45,52,52	1.71	9 (20%)	55,80,80	1.42	13 (23%)
2	FOL	131-A	201	-	27,34,34	1.39	4 (14%)	28,47,47	1.96	6 (21%)
4	NAP	131-A	204	-	45,52,52	1.63	9 (20%)	55,80,80	1.24	6 (10%)
2	FOL	132-A	201	-	27,34,34	1.55	5 (18%)	28,47,47	1.76	5 (17%)
4	NAP	132-A	204	-	45,52,52	1.53	7 (15%)	55,80,80	1.19	5 (9%)
2	FOL	133-A	201	-	27,34,34	1.41	3 (11%)	28,47,47	2.14	3 (10%)
4	NAP	133-A	204	-	45,52,52	1.61	10 (22%)	55,80,80	1.09	2 (3%)
2	FOL	134-A	201	-	27,34,34	1.52	4 (14%)	28,47,47	2.27	8 (28%)
4	NAP	134-A	204	-	45,52,52	1.58	8 (17%)	55,80,80	1.14	5 (9%)
2	FOL	135-A	201	-	27,34,34	1.46	4 (14%)	28,47,47	1.83	5 (17%)
4	NAP	135-A	204	-	45,52,52	1.72	9 (20%)	55,80,80	1.33	9 (16%)
2	FOL	136-A	201	-	27,34,34	1.34	3 (11%)	28,47,47	2.13	9 (32%)
4	NAP	136-A	204	-	45,52,52	1.71	9 (20%)	55,80,80	1.30	9 (16%)
2	FOL	137-A	201	-	27,34,34	1.46	3 (11%)	28,47,47	1.74	5 (17%)
4	NAP	137-A	204	-	45,52,52	1.71	8 (17%)	55,80,80	1.29	8 (14%)
2	FOL	138-A	201	-	27,34,34	1.29	3 (11%)	28,47,47	2.31	9 (32%)
4	NAP	138-A	204	-	45,52,52	1.67	9 (20%)	55,80,80	1.32	11 (20%)
2	FOL	139-A	201	-	27,34,34	1.45	4 (14%)	28,47,47	2.23	8 (28%)
4	NAP	139-A	204	-	45,52,52	1.69	9 (20%)	55,80,80	1.39	10 (18%)
2	FOL	14-A	201	-	27,34,34	1.42	4 (14%)	28,47,47	2.45	6 (21%)
4	NAP	14-A	204	-	45,52,52	1.74	11 (24%)	55,80,80	1.26	10 (18%)
2	FOL	140-A	201	-	27,34,34	1.26	3 (11%)	28,47,47	1.82	6 (21%)
4	NAP	140-A	204	-	45,52,52	1.73	9 (20%)	55,80,80	1.33	10 (18%)
2	FOL	141-A	201	-	27,34,34	1.36	3 (11%)	28,47,47	1.84	6 (21%)
4	NAP	141-A	204	-	45,52,52	1.70	9 (20%)	55,80,80	1.25	9 (16%)
2	FOL	142-A	201	-	27,34,34	1.29	3 (11%)	28,47,47	2.00	6 (21%)
4	NAP	142-A	204	-	45,52,52	1.66	8 (17%)	55,80,80	1.32	12 (21%)
2	FOL	143-A	201	-	27,34,34	1.52	4 (14%)	28,47,47	2.00	7 (25%)
4	NAP	143-A	204	-	45,52,52	1.72	9 (20%)	55,80,80	1.24	10 (18%)
2	FOL	144-A	201	-	27,34,34	1.41	4 (14%)	28,47,47	2.13	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAP	144-A	204	-	45,52,52	1.71	9 (20%)	55,80,80	1.25	10 (18%)
2	FOL	145-A	201	-	27,34,34	1.37	3 (11%)	28,47,47	1.89	5 (17%)
4	NAP	145-A	204	-	45,52,52	1.75	10 (22%)	55,80,80	1.22	10 (18%)
2	FOL	146-A	201	-	27,34,34	1.42	3 (11%)	28,47,47	1.80	5 (17%)
4	NAP	146-A	204	-	45,52,52	1.73	10 (22%)	55,80,80	1.25	9 (16%)
2	FOL	147-A	201	-	27,34,34	1.47	3 (11%)	28,47,47	1.90	8 (28%)
4	NAP	147-A	204	-	45,52,52	1.77	12 (26%)	55,80,80	1.31	10 (18%)
2	FOL	148-A	201	-	27,34,34	1.53	4 (14%)	28,47,47	1.84	5 (17%)
4	NAP	148-A	204	-	45,52,52	1.72	10 (22%)	55,80,80	1.33	11 (20%)
2	FOL	149-A	201	-	27,34,34	1.42	3 (11%)	28,47,47	1.86	6 (21%)
4	NAP	149-A	204	-	45,52,52	1.73	9 (20%)	55,80,80	1.34	9 (16%)
2	FOL	15-A	201	-	27,34,34	1.64	4 (14%)	28,47,47	1.90	5 (17%)
4	NAP	15-A	204	-	45,52,52	1.71	10 (22%)	55,80,80	1.37	12 (21%)
2	FOL	150-A	201	-	27,34,34	1.40	4 (14%)	28,47,47	1.73	4 (14%)
4	NAP	150-A	204	-	45,52,52	1.66	9 (20%)	55,80,80	1.34	11 (20%)
2	FOL	151-A	201	-	27,34,34	1.52	3 (11%)	28,47,47	2.05	5 (17%)
4	NAP	151-A	204	-	45,52,52	1.66	10 (22%)	55,80,80	1.40	12 (21%)
2	FOL	152-A	201	-	27,34,34	1.66	4 (14%)	28,47,47	1.77	4 (14%)
4	NAP	152-A	204	-	45,52,52	1.63	7 (15%)	55,80,80	1.20	8 (14%)
2	FOL	153-A	201	-	27,34,34	1.39	4 (14%)	28,47,47	1.96	9 (32%)
4	NAP	153-A	204	-	45,52,52	1.68	10 (22%)	55,80,80	1.21	7 (12%)
2	FOL	154-A	201	-	27,34,34	1.49	3 (11%)	28,47,47	1.95	5 (17%)
4	NAP	154-A	204	-	45,52,52	1.66	10 (22%)	55,80,80	1.36	10 (18%)
2	FOL	155-A	201	-	27,34,34	1.44	3 (11%)	28,47,47	2.07	8 (28%)
4	NAP	155-A	204	-	45,52,52	1.67	9 (20%)	55,80,80	1.31	8 (14%)
2	FOL	156-A	201	-	27,34,34	1.57	6 (22%)	28,47,47	2.22	4 (14%)
4	NAP	156-A	204	-	45,52,52	1.70	9 (20%)	55,80,80	1.45	12 (21%)
2	FOL	157-A	201	-	27,34,34	1.44	3 (11%)	28,47,47	1.80	7 (25%)
4	NAP	157-A	204	-	45,52,52	1.59	8 (17%)	55,80,80	1.11	4 (7%)
2	FOL	158-A	201	-	27,34,34	1.47	3 (11%)	28,47,47	1.95	8 (28%)
4	NAP	158-A	204	-	45,52,52	1.56	9 (20%)	55,80,80	1.20	5 (9%)
2	FOL	159-A	201	-	27,34,34	1.40	5 (18%)	28,47,47	1.71	4 (14%)
4	NAP	159-A	204	-	45,52,52	1.53	6 (13%)	55,80,80	1.27	10 (18%)
2	FOL	16-A	201	-	27,34,34	1.48	5 (18%)	28,47,47	1.95	5 (17%)
4	NAP	16-A	204	-	45,52,52	1.74	10 (22%)	55,80,80	1.31	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FOL	160-A	201	-	27,34,34	1.50	4 (14%)	28,47,47	2.11	5 (17%)
4	NAP	160-A	204	-	45,52,52	1.70	10 (22%)	55,80,80	1.25	9 (16%)
2	FOL	161-A	201	-	27,34,34	1.29	5 (18%)	28,47,47	1.92	5 (17%)
4	NAP	161-A	204	-	45,52,52	1.69	9 (20%)	55,80,80	1.31	10 (18%)
2	FOL	162-A	201	-	27,34,34	1.49	4 (14%)	28,47,47	1.73	6 (21%)
4	NAP	162-A	204	-	45,52,52	1.69	10 (22%)	55,80,80	1.27	10 (18%)
2	FOL	163-A	201	-	27,34,34	1.32	5 (18%)	28,47,47	1.93	5 (17%)
4	NAP	163-A	204	-	45,52,52	1.70	10 (22%)	55,80,80	1.27	9 (16%)
2	FOL	164-A	201	-	27,34,34	1.44	4 (14%)	28,47,47	1.96	3 (10%)
4	NAP	164-A	204	-	45,52,52	1.66	9 (20%)	55,80,80	1.37	11 (20%)
2	FOL	165-A	201	-	27,34,34	1.47	5 (18%)	28,47,47	2.19	6 (21%)
4	NAP	165-A	204	-	45,52,52	1.77	10 (22%)	55,80,80	1.31	9 (16%)
2	FOL	166-A	201	-	27,34,34	1.51	4 (14%)	28,47,47	1.61	5 (17%)
4	NAP	166-A	204	-	45,52,52	1.63	9 (20%)	55,80,80	1.37	10 (18%)
2	FOL	167-A	201	-	27,34,34	1.50	3 (11%)	28,47,47	2.28	6 (21%)
4	NAP	167-A	204	-	45,52,52	1.73	10 (22%)	55,80,80	1.34	10 (18%)
2	FOL	17-A	201	-	27,34,34	1.47	3 (11%)	28,47,47	1.55	4 (14%)
4	NAP	17-A	204	-	45,52,52	1.75	10 (22%)	55,80,80	1.35	12 (21%)
2	FOL	18-A	201	-	27,34,34	1.45	4 (14%)	28,47,47	1.85	5 (17%)
4	NAP	18-A	204	-	45,52,52	1.78	11 (24%)	55,80,80	1.44	12 (21%)
2	FOL	19-A	201	-	27,34,34	1.53	3 (11%)	28,47,47	1.85	5 (17%)
4	NAP	19-A	204	-	45,52,52	1.75	9 (20%)	55,80,80	1.30	9 (16%)
2	FOL	2-A	201	-	27,34,34	1.47	3 (11%)	28,47,47	1.64	5 (17%)
4	NAP	2-A	204	-	45,52,52	1.68	8 (17%)	55,80,80	1.30	11 (20%)
2	FOL	20-A	201	-	27,34,34	1.43	3 (11%)	28,47,47	1.78	6 (21%)
4	NAP	20-A	204	-	45,52,52	1.75	10 (22%)	55,80,80	1.25	7 (12%)
2	FOL	21-A	201	-	27,34,34	1.67	3 (11%)	28,47,47	2.11	9 (32%)
4	NAP	21-A	204	-	45,52,52	1.71	9 (20%)	55,80,80	1.33	11 (20%)
2	FOL	22-A	201	-	27,34,34	1.44	3 (11%)	28,47,47	1.82	4 (14%)
4	NAP	22-A	204	-	45,52,52	1.80	12 (26%)	55,80,80	1.21	7 (12%)
2	FOL	23-A	201	-	27,34,34	1.34	3 (11%)	28,47,47	1.92	7 (25%)
4	NAP	23-A	204	-	45,52,52	1.77	10 (22%)	55,80,80	1.39	13 (23%)
2	FOL	24-A	201	-	27,34,34	1.36	4 (14%)	28,47,47	2.04	9 (32%)
4	NAP	24-A	204	-	45,52,52	1.75	10 (22%)	55,80,80	1.27	9 (16%)
2	FOL	25-A	201	-	27,34,34	1.54	4 (14%)	28,47,47	2.33	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAP	25-A	204	-	45,52,52	1.79	11 (24%)	55,80,80	1.40	11 (20%)
2	FOL	26-A	201	-	27,34,34	1.56	4 (14%)	28,47,47	2.25	9 (32%)
4	NAP	26-A	204	-	45,52,52	1.74	10 (22%)	55,80,80	1.32	10 (18%)
2	FOL	27-A	201	-	27,34,34	1.53	3 (11%)	28,47,47	1.97	4 (14%)
4	NAP	27-A	204	-	45,52,52	1.77	10 (22%)	55,80,80	1.32	10 (18%)
2	FOL	28-A	201	-	27,34,34	1.54	3 (11%)	28,47,47	1.83	3 (10%)
4	NAP	28-A	204	-	45,52,52	1.76	12 (26%)	55,80,80	1.34	9 (16%)
2	FOL	29-A	201	-	27,34,34	1.37	4 (14%)	28,47,47	2.01	7 (25%)
4	NAP	29-A	204	-	45,52,52	1.74	11 (24%)	55,80,80	1.32	9 (16%)
2	FOL	3-A	201	-	27,34,34	1.33	3 (11%)	28,47,47	1.63	4 (14%)
4	NAP	3-A	204	-	45,52,52	1.73	9 (20%)	55,80,80	1.34	11 (20%)
2	FOL	30-A	201	-	27,34,34	1.59	3 (11%)	28,47,47	1.79	6 (21%)
4	NAP	30-A	204	-	45,52,52	1.82	10 (22%)	55,80,80	1.35	9 (16%)
2	FOL	31-A	201	-	27,34,34	1.36	3 (11%)	28,47,47	1.93	7 (25%)
4	NAP	31-A	204	-	45,52,52	1.67	11 (24%)	55,80,80	1.34	5 (9%)
2	FOL	32-A	201	-	27,34,34	1.42	3 (11%)	28,47,47	1.80	6 (21%)
4	NAP	32-A	204	-	45,52,52	1.64	11 (24%)	55,80,80	1.23	6 (10%)
2	FOL	33-A	201	-	27,34,34	1.45	3 (11%)	28,47,47	1.84	6 (21%)
4	NAP	33-A	204	-	45,52,52	1.78	10 (22%)	55,80,80	1.41	10 (18%)
2	FOL	34-A	201	-	27,34,34	1.44	3 (11%)	28,47,47	2.29	13 (46%)
4	NAP	34-A	204	-	45,52,52	1.56	8 (17%)	55,80,80	1.21	6 (10%)
2	FOL	35-A	201	-	27,34,34	1.39	4 (14%)	28,47,47	1.70	5 (17%)
4	NAP	35-A	204	-	45,52,52	1.75	12 (26%)	55,80,80	1.42	10 (18%)
2	FOL	36-A	201	-	27,34,34	1.42	4 (14%)	28,47,47	1.88	6 (21%)
4	NAP	36-A	204	-	45,52,52	1.70	11 (24%)	55,80,80	1.28	10 (18%)
2	FOL	37-A	201	-	27,34,34	1.41	3 (11%)	28,47,47	2.02	8 (28%)
4	NAP	37-A	204	-	45,52,52	1.71	11 (24%)	55,80,80	1.25	9 (16%)
2	FOL	38-A	201	-	27,34,34	1.21	3 (11%)	28,47,47	1.98	5 (17%)
4	NAP	38-A	204	-	45,52,52	1.77	10 (22%)	55,80,80	1.33	12 (21%)
2	FOL	39-A	201	-	27,34,34	1.45	4 (14%)	28,47,47	2.46	6 (21%)
4	NAP	39-A	204	-	45,52,52	1.82	11 (24%)	55,80,80	1.31	11 (20%)
2	FOL	4-A	201	-	27,34,34	1.54	3 (11%)	28,47,47	2.08	7 (25%)
4	NAP	4-A	204	-	45,52,52	1.74	8 (17%)	55,80,80	1.42	12 (21%)
2	FOL	40-A	201	-	27,34,34	1.46	3 (11%)	28,47,47	2.00	7 (25%)
4	NAP	40-A	204	-	45,52,52	1.76	9 (20%)	55,80,80	1.37	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FOL	41-A	201	-	27,34,34	1.52	3 (11%)	28,47,47	2.02	7 (25%)
4	NAP	41-A	204	-	45,52,52	1.76	11 (24%)	55,80,80	1.37	11 (20%)
2	FOL	42-A	201	-	27,34,34	1.63	3 (11%)	28,47,47	2.01	8 (28%)
4	NAP	42-A	204	-	45,52,52	1.78	11 (24%)	55,80,80	1.52	11 (20%)
2	FOL	43-A	201	-	27,34,34	1.38	3 (11%)	28,47,47	2.19	5 (17%)
4	NAP	43-A	204	-	45,52,52	1.71	8 (17%)	55,80,80	1.35	10 (18%)
2	FOL	44-A	201	-	27,34,34	1.49	3 (11%)	28,47,47	2.06	5 (17%)
4	NAP	44-A	204	-	45,52,52	1.74	10 (22%)	55,80,80	1.23	8 (14%)
2	FOL	45-A	201	-	27,34,34	1.43	3 (11%)	28,47,47	1.69	4 (14%)
4	NAP	45-A	204	-	45,52,52	1.72	10 (22%)	55,80,80	1.21	9 (16%)
2	FOL	46-A	201	-	27,34,34	1.51	5 (18%)	28,47,47	2.03	6 (21%)
4	NAP	46-A	204	-	45,52,52	1.68	9 (20%)	55,80,80	1.20	8 (14%)
2	FOL	47-A	201	-	27,34,34	1.54	3 (11%)	28,47,47	1.95	5 (17%)
4	NAP	47-A	204	-	45,52,52	1.76	9 (20%)	55,80,80	1.26	8 (14%)
2	FOL	48-A	201	-	27,34,34	1.45	3 (11%)	28,47,47	2.16	9 (32%)
4	NAP	48-A	204	-	45,52,52	1.75	9 (20%)	55,80,80	1.38	10 (18%)
2	FOL	49-A	201	-	27,34,34	1.32	3 (11%)	28,47,47	1.92	5 (17%)
4	NAP	49-A	204	-	45,52,52	1.76	10 (22%)	55,80,80	1.55	14 (25%)
2	FOL	5-A	201	-	27,34,34	1.48	4 (14%)	28,47,47	2.02	8 (28%)
4	NAP	5-A	204	-	45,52,52	1.70	8 (17%)	55,80,80	1.47	12 (21%)
2	FOL	50-A	201	-	27,34,34	1.50	3 (11%)	28,47,47	1.84	4 (14%)
4	NAP	50-A	204	-	45,52,52	1.76	9 (20%)	55,80,80	1.32	11 (20%)
2	FOL	51-A	201	-	27,34,34	1.49	3 (11%)	28,47,47	1.95	5 (17%)
4	NAP	51-A	204	-	45,52,52	1.76	10 (22%)	55,80,80	1.31	10 (18%)
2	FOL	52-A	201	-	27,34,34	1.69	5 (18%)	28,47,47	2.19	9 (32%)
4	NAP	52-A	204	-	45,52,52	1.78	9 (20%)	55,80,80	1.39	9 (16%)
2	FOL	53-A	201	-	27,34,34	1.52	3 (11%)	28,47,47	2.10	4 (14%)
4	NAP	53-A	204	-	45,52,52	1.75	9 (20%)	55,80,80	1.25	8 (14%)
2	FOL	54-A	201	-	27,34,34	1.37	4 (14%)	28,47,47	2.01	6 (21%)
4	NAP	54-A	204	-	45,52,52	1.72	10 (22%)	55,80,80	1.40	10 (18%)
2	FOL	55-A	201	-	27,34,34	1.37	4 (14%)	28,47,47	1.92	7 (25%)
4	NAP	55-A	204	-	45,52,52	1.75	10 (22%)	55,80,80	1.25	10 (18%)
2	FOL	56-A	201	-	27,34,34	1.51	4 (14%)	28,47,47	2.20	5 (17%)
4	NAP	56-A	204	-	45,52,52	1.64	7 (15%)	55,80,80	2.30	12 (21%)
2	FOL	57-A	201	-	27,34,34	1.61	4 (14%)	28,47,47	2.28	11 (39%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAP	57-A	204	-	45,52,52	1.59	8 (17%)	55,80,80	2.51	6 (10%)
2	FOL	58-A	201	-	27,34,34	1.46	3 (11%)	28,47,47	2.13	9 (32%)
4	NAP	58-A	204	-	45,52,52	1.67	8 (17%)	55,80,80	1.07	2 (3%)
2	FOL	59-A	201	-	27,34,34	1.60	3 (11%)	28,47,47	1.80	6 (21%)
4	NAP	59-A	204	-	45,52,52	1.64	8 (17%)	55,80,80	1.34	8 (14%)
2	FOL	6-A	201	-	27,34,34	1.75	4 (14%)	28,47,47	1.93	5 (17%)
4	NAP	6-A	204	-	45,52,52	1.63	8 (17%)	55,80,80	1.22	6 (10%)
2	FOL	60-A	201	-	27,34,34	1.45	3 (11%)	28,47,47	2.07	6 (21%)
4	NAP	60-A	204	-	45,52,52	1.80	10 (22%)	55,80,80	1.31	7 (12%)
2	FOL	61-A	201	-	27,34,34	1.38	3 (11%)	28,47,47	1.95	5 (17%)
4	NAP	61-A	204	-	45,52,52	1.73	9 (20%)	55,80,80	1.26	8 (14%)
2	FOL	62-A	201	-	27,34,34	1.43	3 (11%)	28,47,47	2.20	7 (25%)
4	NAP	62-A	204	-	45,52,52	1.74	7 (15%)	55,80,80	1.34	10 (18%)
2	FOL	63-A	201	-	27,34,34	1.35	3 (11%)	28,47,47	2.29	8 (28%)
4	NAP	63-A	204	-	45,52,52	1.69	8 (17%)	55,80,80	1.39	9 (16%)
2	FOL	64-A	201	-	27,34,34	1.37	3 (11%)	28,47,47	2.05	9 (32%)
4	NAP	64-A	204	-	45,52,52	1.75	8 (17%)	55,80,80	1.22	7 (12%)
2	FOL	65-A	201	-	27,34,34	1.71	4 (14%)	28,47,47	1.90	7 (25%)
4	NAP	65-A	204	-	45,52,52	1.78	10 (22%)	55,80,80	1.24	7 (12%)
2	FOL	66-A	201	-	27,34,34	1.39	3 (11%)	28,47,47	2.12	8 (28%)
4	NAP	66-A	204	-	45,52,52	1.74	11 (24%)	55,80,80	1.29	10 (18%)
2	FOL	67-A	201	-	27,34,34	1.38	3 (11%)	28,47,47	1.92	5 (17%)
4	NAP	67-A	204	-	45,52,52	1.74	11 (24%)	55,80,80	1.25	8 (14%)
2	FOL	68-A	201	-	27,34,34	1.50	3 (11%)	28,47,47	1.85	4 (14%)
4	NAP	68-A	204	-	45,52,52	1.74	11 (24%)	55,80,80	1.15	6 (10%)
2	FOL	69-A	201	-	27,34,34	1.48	4 (14%)	28,47,47	2.15	6 (21%)
4	NAP	69-A	204	-	45,52,52	1.80	10 (22%)	55,80,80	1.32	9 (16%)
2	FOL	7-A	201	-	27,34,34	1.57	3 (11%)	28,47,47	1.97	5 (17%)
4	NAP	7-A	204	-	45,52,52	1.59	10 (22%)	55,80,80	1.01	2 (3%)
2	FOL	70-A	201	-	27,34,34	1.55	4 (14%)	28,47,47	2.17	8 (28%)
4	NAP	70-A	204	-	45,52,52	1.79	10 (22%)	55,80,80	1.39	11 (20%)
2	FOL	71-A	201	-	27,34,34	1.41	3 (11%)	28,47,47	1.86	5 (17%)
4	NAP	71-A	204	-	45,52,52	1.74	11 (24%)	55,80,80	1.35	10 (18%)
2	FOL	72-A	201	-	27,34,34	1.38	3 (11%)	28,47,47	2.11	5 (17%)
4	NAP	72-A	204	-	45,52,52	1.74	12 (26%)	55,80,80	1.28	10 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FOL	73-A	201	-	27,34,34	1.58	3 (11%)	28,47,47	1.76	6 (21%)
4	NAP	73-A	204	-	45,52,52	1.71	11 (24%)	55,80,80	1.29	9 (16%)
2	FOL	74-A	201	-	27,34,34	1.62	3 (11%)	28,47,47	1.94	6 (21%)
4	NAP	74-A	204	-	45,52,52	1.75	12 (26%)	55,80,80	1.35	10 (18%)
2	FOL	75-A	201	-	27,34,34	1.40	4 (14%)	28,47,47	1.96	5 (17%)
4	NAP	75-A	204	-	45,52,52	1.75	10 (22%)	55,80,80	1.36	10 (18%)
2	FOL	76-A	201	-	27,34,34	1.62	3 (11%)	28,47,47	2.31	6 (21%)
4	NAP	76-A	204	-	45,52,52	1.75	10 (22%)	55,80,80	1.30	10 (18%)
2	FOL	77-A	201	-	27,34,34	1.54	5 (18%)	28,47,47	2.22	5 (17%)
4	NAP	77-A	204	-	45,52,52	1.71	10 (22%)	55,80,80	1.35	9 (16%)
2	FOL	78-A	201	-	27,34,34	1.35	3 (11%)	28,47,47	2.06	7 (25%)
4	NAP	78-A	204	-	45,52,52	1.71	9 (20%)	55,80,80	1.33	8 (14%)
2	FOL	79-A	201	-	27,34,34	1.32	3 (11%)	28,47,47	1.86	7 (25%)
4	NAP	79-A	204	-	45,52,52	1.75	10 (22%)	55,80,80	1.52	12 (21%)
2	FOL	8-A	201	-	27,34,34	1.50	3 (11%)	28,47,47	2.04	4 (14%)
4	NAP	8-A	204	-	45,52,52	1.60	9 (20%)	55,80,80	1.11	4 (7%)
2	FOL	80-A	201	-	27,34,34	1.56	4 (14%)	28,47,47	2.30	9 (32%)
4	NAP	80-A	204	-	45,52,52	1.76	10 (22%)	55,80,80	1.40	11 (20%)
2	FOL	81-A	201	-	27,34,34	1.47	4 (14%)	28,47,47	2.03	6 (21%)
4	NAP	81-A	204	-	45,52,52	1.67	9 (20%)	55,80,80	1.24	7 (12%)
2	FOL	82-A	201	-	27,34,34	1.53	5 (18%)	28,47,47	2.16	7 (25%)
4	NAP	82-A	204	-	45,52,52	1.65	9 (20%)	55,80,80	1.17	5 (9%)
2	FOL	83-A	201	-	27,34,34	1.67	4 (14%)	28,47,47	2.32	8 (28%)
4	NAP	83-A	204	-	45,52,52	1.62	9 (20%)	55,80,80	1.29	6 (10%)
2	FOL	84-A	201	-	27,34,34	1.40	3 (11%)	28,47,47	2.13	7 (25%)
4	NAP	84-A	204	-	45,52,52	1.62	8 (17%)	55,80,80	1.19	5 (9%)
2	FOL	85-A	201	-	27,34,34	1.44	4 (14%)	28,47,47	1.97	5 (17%)
4	NAP	85-A	204	-	45,52,52	1.71	10 (22%)	55,80,80	1.35	10 (18%)
2	FOL	86-A	201	-	27,34,34	1.34	3 (11%)	28,47,47	1.77	6 (21%)
4	NAP	86-A	204	-	45,52,52	1.68	10 (22%)	55,80,80	1.25	10 (18%)
2	FOL	87-A	201	-	27,34,34	1.41	4 (14%)	28,47,47	1.92	7 (25%)
4	NAP	87-A	204	-	45,52,52	1.70	9 (20%)	55,80,80	1.24	6 (10%)
2	FOL	88-A	201	-	27,34,34	1.31	3 (11%)	28,47,47	1.79	5 (17%)
4	NAP	88-A	204	-	45,52,52	1.69	10 (22%)	55,80,80	1.31	9 (16%)
2	FOL	89-A	201	-	27,34,34	1.51	3 (11%)	28,47,47	1.83	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAP	89-A	204	-	45,52,52	1.70	10 (22%)	55,80,80	1.36	9 (16%)
2	FOL	9-A	201	-	27,34,34	1.54	3 (11%)	28,47,47	1.86	8 (28%)
4	NAP	9-A	204	-	45,52,52	1.63	8 (17%)	55,80,80	1.14	6 (10%)
2	FOL	90-A	201	-	27,34,34	1.36	3 (11%)	28,47,47	1.78	6 (21%)
4	NAP	90-A	204	-	45,52,52	1.66	8 (17%)	55,80,80	1.44	12 (21%)
2	FOL	91-A	201	-	27,34,34	1.31	2 (7%)	28,47,47	1.90	6 (21%)
4	NAP	91-A	204	-	45,52,52	1.69	11 (24%)	55,80,80	1.19	9 (16%)
2	FOL	92-A	201	-	27,34,34	1.47	3 (11%)	28,47,47	2.02	7 (25%)
4	NAP	92-A	204	-	45,52,52	1.70	10 (22%)	55,80,80	1.27	9 (16%)
2	FOL	93-A	201	-	27,34,34	1.43	4 (14%)	28,47,47	2.11	6 (21%)
4	NAP	93-A	204	-	45,52,52	1.69	11 (24%)	55,80,80	1.34	10 (18%)
2	FOL	94-A	201	-	27,34,34	1.45	3 (11%)	28,47,47	1.93	9 (32%)
4	NAP	94-A	204	-	45,52,52	1.70	9 (20%)	55,80,80	1.26	7 (12%)
2	FOL	95-A	201	-	27,34,34	1.33	3 (11%)	28,47,47	1.73	6 (21%)
4	NAP	95-A	204	-	45,52,52	1.65	9 (20%)	55,80,80	1.31	8 (14%)
2	FOL	96-A	201	-	27,34,34	1.42	3 (11%)	28,47,47	1.66	6 (21%)
4	NAP	96-A	204	-	45,52,52	1.74	10 (22%)	55,80,80	1.23	7 (12%)
2	FOL	97-A	201	-	27,34,34	1.38	4 (14%)	28,47,47	1.88	5 (17%)
4	NAP	97-A	204	-	45,52,52	1.76	11 (24%)	55,80,80	1.20	7 (12%)
2	FOL	98-A	201	-	27,34,34	1.45	3 (11%)	28,47,47	2.07	4 (14%)
4	NAP	98-A	204	-	45,52,52	1.75	10 (22%)	55,80,80	1.32	10 (18%)
2	FOL	99-A	201	-	27,34,34	1.45	3 (11%)	28,47,47	2.02	7 (25%)
4	NAP	99-A	204	-	45,52,52	1.79	11 (24%)	55,80,80	1.42	9 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	1-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	1-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	10-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	10-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	100-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	100-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	101-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	101-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	102-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	102-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	103-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	103-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	104-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	104-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	105-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	105-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	106-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	106-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	107-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	107-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	108-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	108-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	109-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	109-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	11-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	11-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	110-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	110-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	111-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	111-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	112-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	112-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	113-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	113-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	114-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	114-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	115-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	115-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	116-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	116-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	117-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	117-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	118-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	118-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	119-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	119-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	12-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	12-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	120-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	120-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	121-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	121-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	122-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	122-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	123-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	123-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	124-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	124-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	125-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	125-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	126-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	126-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	127-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	127-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	128-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	128-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	129-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	129-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	13-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	13-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	130-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	130-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	131-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	131-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	132-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	132-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	133-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	133-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	134-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	134-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	135-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	135-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	136-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	136-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	137-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	137-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	138-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	138-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	139-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	139-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	14-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	14-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	140-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	140-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	141-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	141-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	142-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	142-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	143-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	143-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	144-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	144-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	145-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	145-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	146-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	146-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	147-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	147-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	148-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	148-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	149-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	149-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	15-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	15-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	150-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	150-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	151-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	151-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	152-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	152-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	153-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	153-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	154-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	154-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	155-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	155-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	156-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	156-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	157-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	157-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	158-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	158-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	159-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	159-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	16-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	16-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	160-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	160-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	161-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	161-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	162-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	162-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	163-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	163-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	164-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	164-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	165-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	165-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	166-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	166-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	167-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	167-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	17-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	17-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	18-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	18-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	19-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	19-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	2-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	2-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	20-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	20-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	21-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	21-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	22-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	22-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	23-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	23-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	24-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	24-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	25-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	25-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	26-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	26-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	27-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	27-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	28-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	28-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	29-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	29-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	3-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	3-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	30-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	30-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	31-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	31-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	32-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	32-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	33-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	33-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	34-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	34-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	35-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	35-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	36-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	36-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	37-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	37-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	38-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	38-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	39-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	39-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	4-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	4-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	40-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	40-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	41-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	41-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	42-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	42-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	43-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	43-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	44-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	44-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	45-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	45-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	46-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	46-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	47-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	47-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	48-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	48-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	49-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	49-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	5-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	5-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	50-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	50-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	51-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	51-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	52-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	52-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	53-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	53-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	54-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	54-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	55-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	55-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	56-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	56-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	57-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	57-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	58-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	58-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	59-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	59-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	6-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	6-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	60-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	60-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	61-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	61-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	62-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	62-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	63-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	63-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	64-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	64-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	65-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	65-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	66-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	66-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	67-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	67-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	68-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	68-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	69-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	69-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	7-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	7-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	70-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	70-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	71-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	71-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	72-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	72-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	73-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	73-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	74-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	74-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	75-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	75-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	76-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	76-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	77-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	77-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	78-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	78-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	79-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	79-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	8-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	8-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	80-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	80-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	81-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	81-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	82-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	82-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	83-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	83-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	84-A	201	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	84-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	85-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	85-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	86-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	86-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	87-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	87-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	88-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	88-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	89-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	89-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	9-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	9-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	90-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	90-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	91-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	91-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	92-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	92-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	93-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	93-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	94-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	94-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	95-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	95-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	96-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	96-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	97-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	97-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	98-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	98-A	204	-	-	0/27/67/67	0/5/5/5
2	FOL	99-A	201	-	-	0/16/22/22	0/3/3/3
4	NAP	99-A	204	-	-	0/27/67/67	0/5/5/5

The worst 5 of 2193 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	6-A	201	FOL	C8A-N1	-6.65	1.30	1.37
2	152-A	201	FOL	C8A-N1	-6.44	1.30	1.37
2	12-A	201	FOL	C8A-N1	-6.43	1.30	1.37
4	69-A	204	NAP	O3B-C3B	-6.42	1.27	1.43
4	25-A	204	NAP	O3B-C3B	-6.41	1.27	1.43

The worst 5 of 2601 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	118-A	204	NAP	O2N-PN-O3	-11.07	57.84	105.27
4	57-A	204	NAP	O2N-PN-O3	-10.58	59.95	105.27
4	56-A	204	NAP	O2N-PN-O3	-9.07	66.38	105.27
2	156-A	201	FOL	CB-CA-N	-7.64	97.99	109.92
2	133-A	201	FOL	C4A-C4-N3	-7.58	113.61	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS failed to run properly - this section will therefore be empty.