



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2020 – 06:48 AM BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

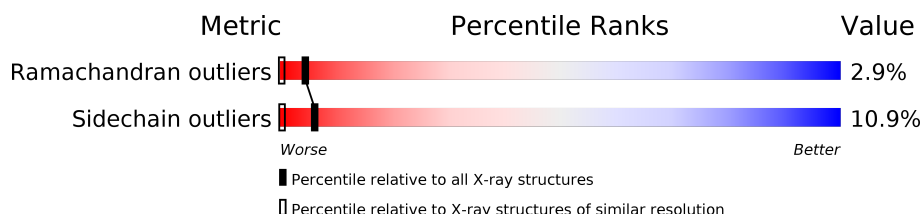
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)


























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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

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















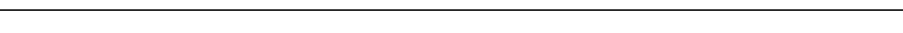




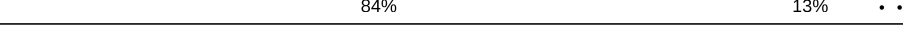





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Mol	Chain	Length	Quality of chain
1	107-A	159	 83% 13% .
1	108-A	159	 84% 14% ..
1	109-A	159	 84% 14% ..
1	11-A	159	 87% 9% ..
1	110-A	159	 85% 12% .
1	111-A	159	 85% 13% ..
1	112-A	159	 85% 13% ..
1	113-A	159	 81% 14% . .
1	114-A	159	 82% 12% 5% .
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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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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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% .















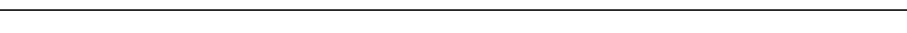




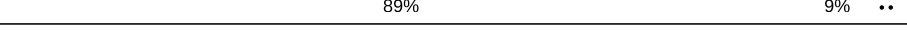





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Mol	Chain	Length	Quality of chain
1	47-A	159	 86% 11% ..
1	48-A	159	 90% 7% ..
1	49-A	159	 87% 10% ..
1	5-A	159	 91% 6% ..
1	50-A	159	 84% 12% ..
1	51-A	159	 86% 11% ..
1	52-A	159	 85% 12% ..
1	53-A	159	 86% 9% ..
1	54-A	159	 87% 12% .
1	55-A	159	 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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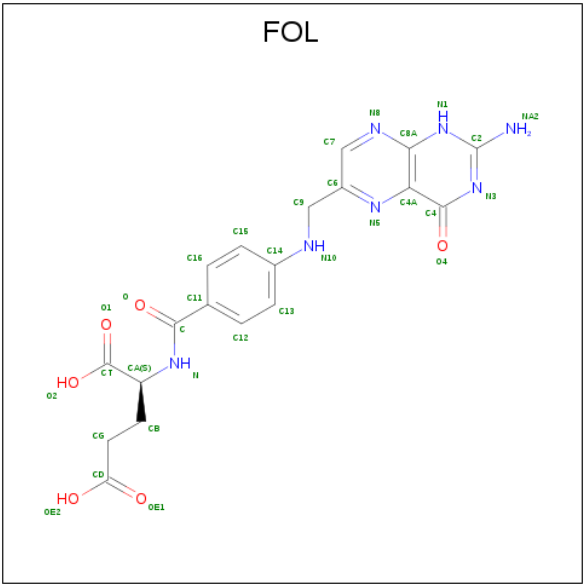
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	143-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	144-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	145-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	7			
1	146-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1223	217	239	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: C₁₉H₁₉N₇O₆).



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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	92-A	1	Total 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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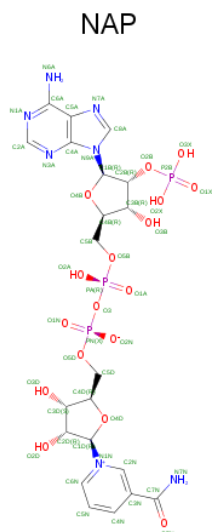
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	107-A	2	Total 2	Ca 2	0	0
3	13-A	2	Total 2	Ca 2	0	0
3	115-A	2	Total 2	Ca 2	0	0
3	74-A	2	Total 2	Ca 2	0	0
3	142-A	2	Total 2	Ca 2	0	0
3	24-A	2	Total 2	Ca 2	0	0
3	156-A	2	Total 2	Ca 2	0	0
3	4-A	2	Total 2	Ca 2	0	0
3	38-A	2	Total 2	Ca 2	0	0
3	132-A	2	Total 2	Ca 2	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: C₂₁H₂₈N₇O₁₇P₃).



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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	162-A	1	Total	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, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

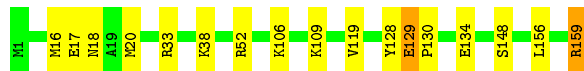
- Molecule 1: Dihydrofolate reductase

Chain 1-A:  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% .




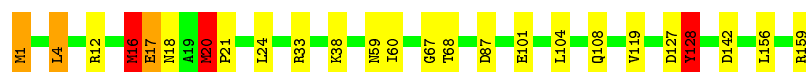
- Molecule 1: Dihydrofolate reductase

Chain 7-A:  82% 15% . .




- Molecule 1: Dihydrofolate reductase

Chain 8-A:  84% 12% . .



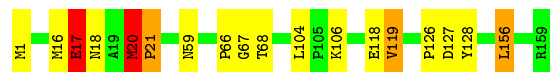
- Molecule 1: Dihydrofolate reductase

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% ..



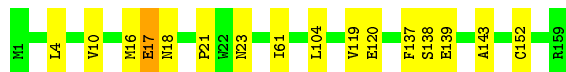
- Molecule 1: Dihydrofolate reductase

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% .



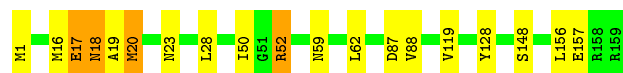
- Molecule 1: Dihydrofolate reductase

Chain 22-A:  89% 9% .



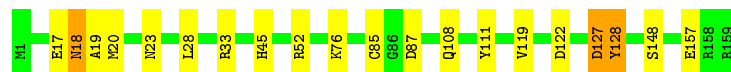
- Molecule 1: Dihydrofolate reductase

Chain 23-A:  88% 9% .




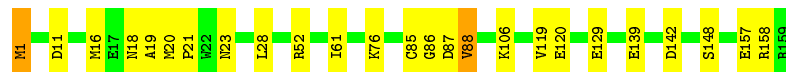
- Molecule 1: Dihydrofolate reductase

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% . .




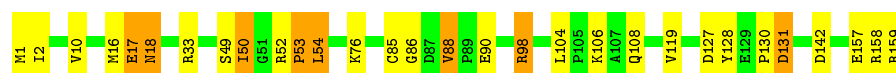
- Molecule 1: Dihydrofolate reductase

Chain 29-A:  81% 16% . .




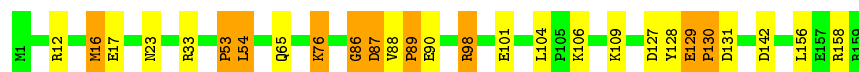
- Molecule 1: Dihydrofolate reductase

Chain 30-A:  81% 14% 5%




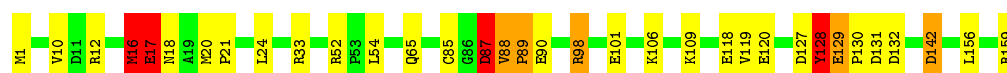
- Molecule 1: Dihydrofolate reductase

Chain 31-A:  83% 11% 6%




- Molecule 1: Dihydrofolate reductase

Chain 32-A:  79% 16% . .




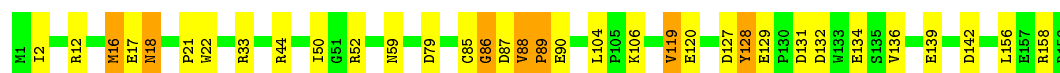
- Molecule 1: Dihydrofolate reductase

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% ..




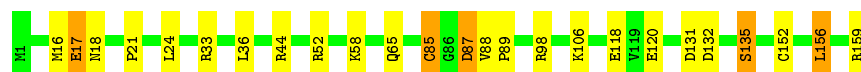
- Molecule 1: Dihydrofolate reductase

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

Category	Count (approx.)
M1	100
M20	100
R33	100
L36	200
R44	100
R52	100
C95	400
G86	400
D87	200
Y88	200
R98	100
Q108	100
E118	100
V119	100
D131	100
S148	100
L156	100
R159	100

- MI M20 R33 L36 R44 R52 Q65 T68 D69 C85 C86 D87 V88 E108 Q110 V118 E120 D127 D131 S135 D144 R158 R159

- | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|
| M1 | N18 | N23 | L28 | R33 | L36 | R44 | R52 | K58 | Q65 | A84 | C85 | G86 | D87 | Y88 | R98 | E119 | E120 | D127 | Y128 | E129 | D143 | G145 | D144 | L156 | R159 |
|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|


- | | | | | | | | | | | | | | | | | | | | | | | | |
|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|
| R1 | D11 | R12 | P21 | R33 | L36 | R44 | R52 | N59 | D70 | K76 | C85 | G86 | D87 | V88 | R98 | K109 | V119 | E120 | D127 | V128 | E129 | L156 | R159 |
|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|

- | | | | | | | | | | | | | | | | | | | | | | | | | | |
|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|
| E1 | D11 | M16 | E17 | N18 | N23 | R33 | L36 | R44 | R52 | Q65 | D70 | A84 | C85 | G86 | D87 | V88 | R98 | L104 | V119 | E120 | E129 | D132 | E139 | L156 | R159 |
|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|

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|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|
| M1 | D11 | L24 | R33 | L36 | R52 | N59 | C85 | G56 | D37 | V88 | R98 | E101 | L104 | E118 | V119 | E120 | D127 | Y128 | S138 | E139 | L156 | E157 | R158 | R159 |
|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|

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|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|
| M1 | E17 | P21 | W22 | L24 | R33 | E48 | K58 | N59 | K76 | D87 | V88 | L104 | P105 | K106 | E118 | D122 | D127 | Y128 | E139 | E154 | I155 | L156 | R159 |
|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|

- 

Chain 55-A:  87% 12% .



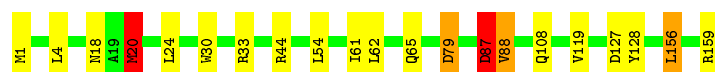
- Molecule 1: Dihydrofolate reductase

Chain 56-A:  87% 9% .



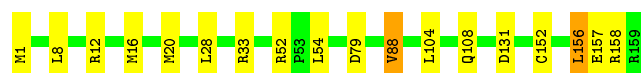
- Molecule 1: Dihydrofolate reductase

Chain 57-A:  87% 10% ..



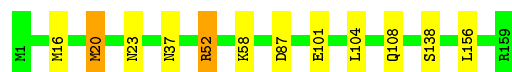
- Molecule 1: Dihydrofolate reductase

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%



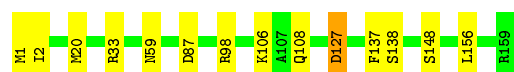
- Molecule 1: Dihydrofolate reductase

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% .



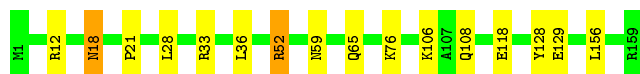
- Molecule 1: Dihydrofolate reductase

Chain 76-A:  85% 14% .



- Molecule 1: Dihydrofolate reductase

Chain 77-A:  90% 9% .




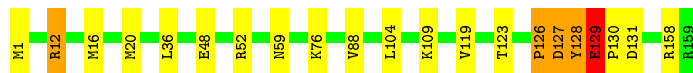
- Molecule 1: Dihydrofolate reductase

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% .



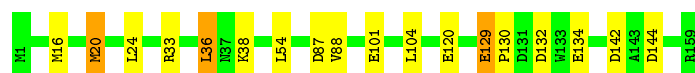
- Molecule 1: Dihydrofolate reductase

Chain 90-A:  87% 10% •



- Molecule 1: Dihydrofolate reductase

Chain 91-A:  89% 9% •



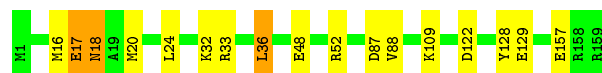
- Molecule 1: Dihydrofolate reductase

Chain 92-A:  88% 10% •




- Molecule 1: Dihydrofolate reductase

Chain 93-A:  89% 9% •




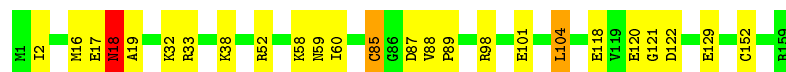
- Molecule 1: Dihydrofolate reductase

Chain 94-A:  84% 15% •



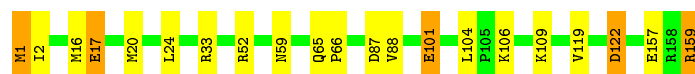
- Molecule 1: Dihydrofolate reductase

Chain 95-A:  84% 14% ••




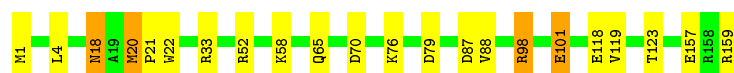
- Molecule 1: Dihydrofolate reductase

Chain 96-A:  87% 10% •




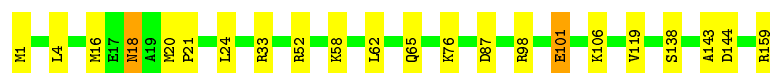
- Molecule 1: Dihydrofolate reductase

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% .



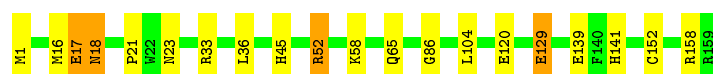
- Molecule 1: Dihydrofolate reductase

Chain 102-A:  90% 9% ..



- Molecule 1: Dihydrofolate reductase

Chain 103-A:  87% 10% .



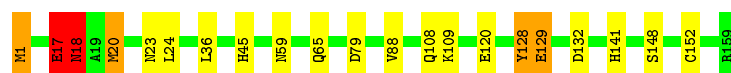
- Molecule 1: Dihydrofolate reductase

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% .



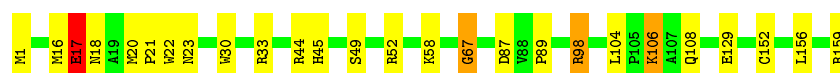
- Molecule 1: Dihydrofolate reductase

Chain 108-A:  84% 14% ..



- Molecule 1: Dihydrofolate reductase

Chain 109-A:  84% 14% ..




- Molecule 1: Dihydrofolate reductase

Chain 110-A:  85% 12% .



- Molecule 1: Dihydrofolate reductase

Chain 111-A:  85% 13% ..




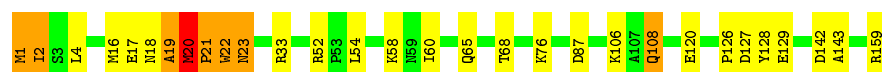
- Molecule 1: Dihydrofolate reductase

Chain 112-A:  85% 13% ..




- Molecule 1: Dihydrofolate reductase

Chain 113-A:  81% 14% . .




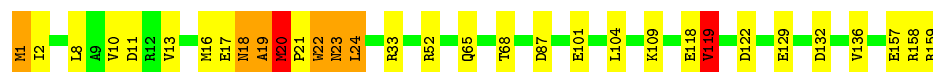
- Molecule 1: Dihydrofolate reductase

Chain 114-A:  82% 12% 5% .



- Molecule 1: Dihydrofolate reductase

Chain 115-A:  80% 15% . .




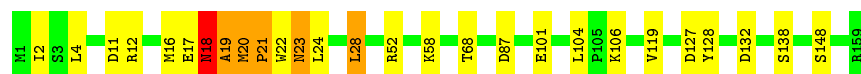
- Molecule 1: Dihydrofolate reductase

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% .



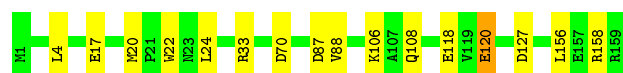
- Molecule 1: Dihydrofolate reductase

Chain 125-A:  87% 12%



- Molecule 1: Dihydrofolate reductase

Chain 126-A:  90% 9%



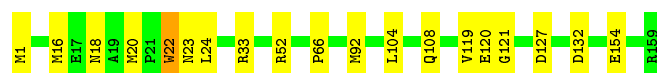
- Molecule 1: Dihydrofolate reductase

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%



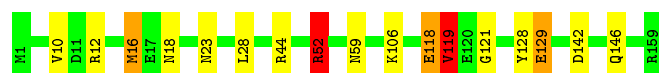
- Molecule 1: Dihydrofolate reductase

Chain 131-A:  86% 13%



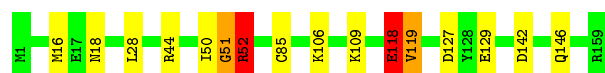
- Molecule 1: Dihydrofolate reductase

Chain 132-A:  89% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 133-A:  90% 8% ..



- Molecule 1: Dihydrofolate reductase

Chain 134-A:  89% 9% .



- Molecule 1: Dihydrofolate reductase

Chain 135-A:  92% 7% ..



- Molecule 1: Dihydrofolate reductase

Chain 136-A:  86% 11% ..



- Molecule 1: Dihydrofolate reductase

Chain 137-A:  87% 8% ..



- 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 146-A:  84% 13% ..



- Molecule 1: Dihydrofolate reductase

Chain 147-A:  87% 11% ..



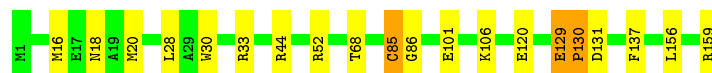
- Molecule 1: Dihydrofolate reductase

Chain 148-A:  86% 11% ..




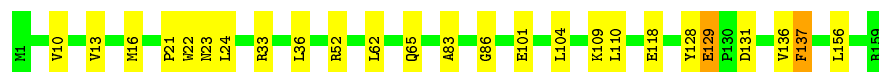
- Molecule 1: Dihydrofolate reductase

Chain 149-A:  87% 11% .




- Molecule 1: Dihydrofolate reductase

Chain 150-A:  84% 14% .



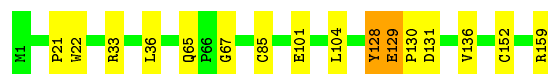
- Molecule 1: Dihydrofolate reductase

Chain 151-A:  85% 13% .



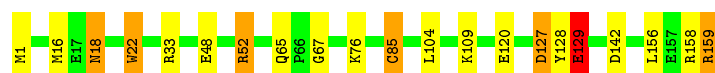
- Molecule 1: Dihydrofolate reductase

Chain 152-A:  90% 9% .



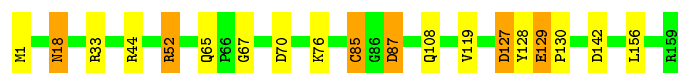
- Molecule 1: Dihydrofolate reductase

Chain 153-A:  87% 9% . .



• Molecule 1: Dihydrofolate reductase

Chain 154-A:  88% 8% .




• Molecule 1: Dihydrofolate reductase

Chain 155-A:  86% 11% .




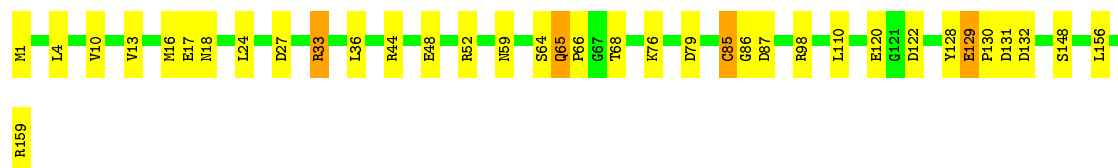
• Molecule 1: Dihydrofolate reductase

Chain 156-A:  81% 17% .



• Molecule 1: Dihydrofolate reductase

Chain 157-A:  77% 20% .



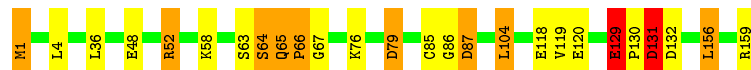
• Molecule 1: Dihydrofolate reductase

Chain 158-A:  86% 10% . .



• Molecule 1: Dihydrofolate reductase

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



• Molecule 1: Dihydrofolate reductase

Chain 160-A:  86% 12% ..

• Molecule 1: Dihydrofolate reductase

Chain 161-A:  86% 10% . .

• Molecule 1: Dihydrofolate reductase

Chain 162-A:  86% 10% . .

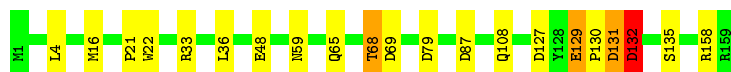
• Molecule 1: Dihydrofolate reductase

Chain 163-A:  86% 12% .

• Molecule 1: Dihydrofolate reductase

Chain 164-A:  86% 9% . .


• Molecule 1: Dihydrofolate reductase

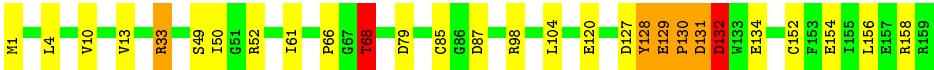
Chain 165-A:  87% 11% . .

• Molecule 1: Dihydrofolate reductase

Chain 166-A:  88% 10% ..

• Molecule 1: Dihydrofolate reductase

Chain 167-A:  82% 13% . .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	34.32Å 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
$\langle I/\sigma(I) \rangle$ ¹	1.87 (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 ²)	11.2	Xtriage
Anisotropy	0.170	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	451154	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FOL, 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%)	5	0
1	2-A	157/159 (99%)	143 (91%)	11 (7%)	3 (2%)	8	0
1	3-A	157/159 (99%)	150 (96%)	4 (2%)	3 (2%)	8	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4-A	157/159 (99%)	146 (93%)	6 (4%)	5 (3%)	4	0
1	5-A	157/159 (99%)	147 (94%)	4 (2%)	6 (4%)	3	0
1	6-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	5	0
1	7-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	8	0
1	8-A	157/159 (99%)	142 (90%)	11 (7%)	4 (2%)	5	0
1	9-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	5	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%)	3	0
1	12-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	5	0
1	13-A	157/159 (99%)	145 (92%)	10 (6%)	2 (1%)	12	1
1	14-A	157/159 (99%)	146 (93%)	8 (5%)	3 (2%)	8	0
1	15-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	5	0
1	16-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	4	0
1	17-A	157/159 (99%)	146 (93%)	5 (3%)	6 (4%)	3	0
1	18-A	157/159 (99%)	142 (90%)	10 (6%)	5 (3%)	4	0
1	19-A	157/159 (99%)	148 (94%)	4 (2%)	5 (3%)	4	0
1	20-A	157/159 (99%)	148 (94%)	8 (5%)	1 (1%)	25	6
1	21-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	5	0
1	22-A	157/159 (99%)	145 (92%)	9 (6%)	3 (2%)	8	0
1	23-A	157/159 (99%)	148 (94%)	5 (3%)	4 (2%)	5	0
1	24-A	157/159 (99%)	147 (94%)	4 (2%)	6 (4%)	3	0
1	25-A	157/159 (99%)	145 (92%)	6 (4%)	6 (4%)	3	0
1	26-A	157/159 (99%)	142 (90%)	9 (6%)	6 (4%)	3	0
1	27-A	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	5	0
1	28-A	157/159 (99%)	143 (91%)	7 (4%)	7 (4%)	2	0
1	29-A	157/159 (99%)	139 (88%)	8 (5%)	10 (6%)	1	0
1	30-A	157/159 (99%)	138 (88%)	10 (6%)	9 (6%)	1	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%)	1	0
1	36-A	157/159 (99%)	140 (89%)	8 (5%)	9 (6%)	1	0
1	37-A	157/159 (99%)	137 (87%)	10 (6%)	10 (6%)	1	0
1	38-A	157/159 (99%)	146 (93%)	5 (3%)	6 (4%)	3	0
1	39-A	157/159 (99%)	142 (90%)	9 (6%)	6 (4%)	3	0
1	40-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	4	0
1	41-A	157/159 (99%)	142 (90%)	8 (5%)	7 (4%)	2	0
1	42-A	157/159 (99%)	146 (93%)	4 (2%)	7 (4%)	2	0
1	43-A	157/159 (99%)	142 (90%)	9 (6%)	6 (4%)	3	0
1	44-A	157/159 (99%)	146 (93%)	6 (4%)	5 (3%)	4	0
1	45-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	4	0
1	46-A	157/159 (99%)	148 (94%)	5 (3%)	4 (2%)	5	0
1	47-A	157/159 (99%)	147 (94%)	4 (2%)	6 (4%)	3	0
1	48-A	157/159 (99%)	148 (94%)	4 (2%)	5 (3%)	4	0
1	49-A	157/159 (99%)	145 (92%)	5 (3%)	7 (4%)	2	0
1	50-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	5	0
1	51-A	157/159 (99%)	146 (93%)	4 (2%)	7 (4%)	2	0
1	52-A	157/159 (99%)	144 (92%)	10 (6%)	3 (2%)	8	0
1	53-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	1
1	54-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	8	0
1	55-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	1
1	56-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	8	0
1	57-A	157/159 (99%)	145 (92%)	10 (6%)	2 (1%)	12	1
1	58-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	6
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%)	8	0
1	61-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	12	1
1	62-A	157/159 (99%)	145 (92%)	9 (6%)	3 (2%)	8	0
1	63-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	12	1
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%)	12	1
1	67-A	157/159 (99%)	147 (94%)	8 (5%)	2 (1%)	12	1
1	68-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	5	0
1	69-A	157/159 (99%)	144 (92%)	10 (6%)	3 (2%)	8	0
1	70-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	3	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%)	2	0
1	73-A	157/159 (99%)	147 (94%)	3 (2%)	7 (4%)	2	0
1	74-A	157/159 (99%)	143 (91%)	8 (5%)	6 (4%)	3	0
1	75-A	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	5	0
1	76-A	157/159 (99%)	143 (91%)	10 (6%)	4 (2%)	5	0
1	77-A	157/159 (99%)	142 (90%)	13 (8%)	2 (1%)	12	1
1	78-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	4	0
1	79-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	5	0
1	80-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	5	0
1	81-A	157/159 (99%)	147 (94%)	8 (5%)	2 (1%)	12	1
1	82-A	157/159 (99%)	143 (91%)	9 (6%)	5 (3%)	4	0
1	83-A	157/159 (99%)	146 (93%)	7 (4%)	4 (2%)	5	0
1	84-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	8	0
1	85-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	3	0
1	86-A	157/159 (99%)	143 (91%)	11 (7%)	3 (2%)	8	0
1	87-A	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	8	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%)	8	0
1	90-A	157/159 (99%)	148 (94%)	7 (4%)	2 (1%)	12	1
1	91-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	1
1	92-A	157/159 (99%)	146 (93%)	7 (4%)	4 (2%)	5	0
1	93-A	157/159 (99%)	147 (94%)	9 (6%)	1 (1%)	25	6
1	94-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	4	0
1	95-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	5	0
1	96-A	157/159 (99%)	146 (93%)	9 (6%)	2 (1%)	12	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	97-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	25	6
1	98-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	8	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%)	8	0
1	101-A	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	8	0
1	102-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	12	1
1	103-A	157/159 (99%)	150 (96%)	3 (2%)	4 (2%)	5	0
1	104-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	12	1
1	105-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	6
1	106-A	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	8	0
1	107-A	157/159 (99%)	144 (92%)	10 (6%)	3 (2%)	8	0
1	108-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	5	0
1	109-A	157/159 (99%)	143 (91%)	9 (6%)	5 (3%)	4	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%)	1	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%)	2	0
1	116-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	3	0
1	117-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	5	0
1	118-A	157/159 (99%)	147 (94%)	4 (2%)	6 (4%)	3	0
1	119-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	6
1	120-A	157/159 (99%)	144 (92%)	11 (7%)	2 (1%)	12	1
1	121-A	157/159 (99%)	148 (94%)	4 (2%)	5 (3%)	4	0
1	122-A	157/159 (99%)	142 (90%)	10 (6%)	5 (3%)	4	0
1	123-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	3	0
1	124-A	157/159 (99%)	144 (92%)	4 (2%)	9 (6%)	1	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%)	12	1
1	127-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	128-A	157/159 (99%)	146 (93%)	7 (4%)	4 (2%)	5	0
1	129-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	25	6
1	130-A	157/159 (99%)	144 (92%)	11 (7%)	2 (1%)	12	1
1	131-A	157/159 (99%)	141 (90%)	11 (7%)	5 (3%)	4	0
1	132-A	157/159 (99%)	140 (89%)	13 (8%)	4 (2%)	5	0
1	133-A	157/159 (99%)	146 (93%)	8 (5%)	3 (2%)	8	0
1	134-A	157/159 (99%)	144 (92%)	10 (6%)	3 (2%)	8	0
1	135-A	157/159 (99%)	143 (91%)	12 (8%)	2 (1%)	12	1
1	136-A	157/159 (99%)	145 (92%)	7 (4%)	5 (3%)	4	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%)	3	0
1	139-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	5	0
1	140-A	157/159 (99%)	149 (95%)	4 (2%)	4 (2%)	5	0
1	141-A	157/159 (99%)	145 (92%)	7 (4%)	5 (3%)	4	0
1	142-A	157/159 (99%)	146 (93%)	5 (3%)	6 (4%)	3	0
1	143-A	157/159 (99%)	146 (93%)	5 (3%)	6 (4%)	3	0
1	144-A	157/159 (99%)	143 (91%)	9 (6%)	5 (3%)	4	0
1	145-A	157/159 (99%)	141 (90%)	11 (7%)	5 (3%)	4	0
1	146-A	157/159 (99%)	143 (91%)	8 (5%)	6 (4%)	3	0
1	147-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	5	0
1	148-A	157/159 (99%)	148 (94%)	4 (2%)	5 (3%)	4	0
1	149-A	157/159 (99%)	146 (93%)	9 (6%)	2 (1%)	12	1
1	150-A	157/159 (99%)	140 (89%)	11 (7%)	6 (4%)	3	0
1	151-A	157/159 (99%)	143 (91%)	11 (7%)	3 (2%)	8	0
1	152-A	157/159 (99%)	149 (95%)	4 (2%)	4 (2%)	5	0
1	153-A	157/159 (99%)	150 (96%)	3 (2%)	4 (2%)	5	0
1	154-A	157/159 (99%)	146 (93%)	8 (5%)	3 (2%)	8	0
1	155-A	157/159 (99%)	142 (90%)	9 (6%)	6 (4%)	3	0
1	156-A	157/159 (99%)	140 (89%)	11 (7%)	6 (4%)	3	0
1	157-A	157/159 (99%)	142 (90%)	10 (6%)	5 (3%)	4	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%)	3	0
1	160-A	157/159 (99%)	141 (90%)	11 (7%)	5 (3%)	4	0
1	161-A	157/159 (99%)	140 (89%)	12 (8%)	5 (3%)	4	0
1	162-A	157/159 (99%)	145 (92%)	7 (4%)	5 (3%)	4	0
1	163-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	5	0
1	164-A	157/159 (99%)	146 (93%)	6 (4%)	5 (3%)	4	0
1	165-A	157/159 (99%)	144 (92%)	6 (4%)	7 (4%)	2	0
1	166-A	157/159 (99%)	142 (90%)	12 (8%)	3 (2%)	8	0
1	167-A	157/159 (99%)	145 (92%)	5 (3%)	7 (4%)	2	0
All	All	26219/26553 (99%)	24212 (92%)	1237 (5%)	770 (3%)	4	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%)	7	0
1	2-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	3-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	4-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	5-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	6-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	7-A	136/136 (100%)	119 (88%)	17 (12%)	4	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	8-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	9-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	10-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	11-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	12-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	13-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	14-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	15-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	16-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	17-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	18-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	19-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	20-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	21-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	22-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	23-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	24-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	25-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	26-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	27-A	136/136 (100%)	117 (86%)	19 (14%)	3	0
1	28-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	29-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	30-A	136/136 (100%)	115 (85%)	21 (15%)	2	0
1	31-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	32-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	33-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	34-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	35-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	36-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	37-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	38-A	136/136 (100%)	119 (88%)	17 (12%)	4	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	39-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	40-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	41-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	42-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	43-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	44-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	45-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	46-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	47-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	48-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	49-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	50-A	136/136 (100%)	115 (85%)	21 (15%)	2	0
1	51-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	52-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	53-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	54-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	55-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	56-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	57-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	58-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	59-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	60-A	136/136 (100%)	114 (84%)	22 (16%)	2	0
1	61-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	62-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	63-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	64-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	65-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	66-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	67-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	68-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	69-A	136/136 (100%)	122 (90%)	14 (10%)	7	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	70-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	71-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	72-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	73-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	74-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	75-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	76-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	77-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	78-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	79-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	80-A	136/136 (100%)	115 (85%)	21 (15%)	2	0
1	81-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	82-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	83-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	84-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	85-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	86-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	87-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	88-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	89-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	90-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	91-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	92-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	93-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	94-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	95-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	96-A	136/136 (100%)	117 (86%)	19 (14%)	3	0
1	97-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	98-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	99-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	100-A	136/136 (100%)	122 (90%)	14 (10%)	7	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	101-A	136/136 (100%)	127 (93%)	9 (7%)	16	1
1	102-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	103-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	104-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	105-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	106-A	136/136 (100%)	114 (84%)	22 (16%)	2	0
1	107-A	136/136 (100%)	114 (84%)	22 (16%)	2	0
1	108-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	109-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	110-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	111-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	112-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	113-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	114-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	115-A	136/136 (100%)	115 (85%)	21 (15%)	2	0
1	116-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	117-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	118-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	119-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	120-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	121-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	122-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	123-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	124-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	125-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	126-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	127-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	128-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	129-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	130-A	136/136 (100%)	128 (94%)	8 (6%)	19	1
1	131-A	136/136 (100%)	124 (91%)	12 (9%)	10	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	132-A	136/136 (100%)	126 (93%)	10 (7%)	13	1
1	133-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	134-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	135-A	136/136 (100%)	125 (92%)	11 (8%)	11	0
1	136-A	136/136 (100%)	122 (90%)	14 (10%)	7	0
1	137-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	138-A	136/136 (100%)	117 (86%)	19 (14%)	3	0
1	139-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	140-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	141-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	142-A	136/136 (100%)	117 (86%)	19 (14%)	3	0
1	143-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	144-A	136/136 (100%)	113 (83%)	23 (17%)	2	0
1	145-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	146-A	136/136 (100%)	117 (86%)	19 (14%)	3	0
1	147-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	148-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	149-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	150-A	136/136 (100%)	120 (88%)	16 (12%)	5	0
1	151-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	152-A	136/136 (100%)	130 (96%)	6 (4%)	28	3
1	153-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	154-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	155-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	156-A	136/136 (100%)	117 (86%)	19 (14%)	3	0
1	157-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	158-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	159-A	136/136 (100%)	121 (89%)	15 (11%)	6	0
1	160-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	161-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	162-A	136/136 (100%)	121 (89%)	15 (11%)	6	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	163-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	164-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	165-A	136/136 (100%)	123 (90%)	13 (10%)	8	0
1	166-A	136/136 (100%)	124 (91%)	12 (9%)	10	0
1	167-A	136/136 (100%)	115 (85%)	21 (15%)	2	0
All	All	22712/22712 (100%)	20232 (89%)	2480 (11%)	6	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 monosaccharides 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
4	NAP	3-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	150-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	26-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	14-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	111-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	71-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	157-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	142-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	27-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	83-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	95-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	156-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	12-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	61-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	121-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	80-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	149-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	71-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	137-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	140-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	6-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	107-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	115-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	70-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	25-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	143-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	128-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	107-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	102-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	19-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	44-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	133-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	136-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	49-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	35-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	88-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	117-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	55-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	155-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	93-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	129-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	164-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	14-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	104-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	74-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	42-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	21-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	135-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	47-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	159-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	38-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	16-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	60-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	76-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	100-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	96-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	69-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	124-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	140-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	2-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	10-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	87-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	112-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	79-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	10-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	146-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	31-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	160-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	82-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	105-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	129-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	39-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	57-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	99-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	125-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	60-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	45-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	122-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	41-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	7-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	54-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	130-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	11-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	149-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	137-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	126-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	45-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	18-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	162-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	49-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	106-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	53-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	148-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	114-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	1-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	85-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	15-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	22-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	108-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	111-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	48-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	75-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	50-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	84-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	25-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	144-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	154-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	5-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	85-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	86-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	59-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	33-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	26-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	29-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	110-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	152-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	77-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	131-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	33-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	29-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	81-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	63-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	70-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	97-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	123-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	28-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	24-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	13-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	94-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	113-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	72-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	141-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	98-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	132-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	166-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	78-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	66-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	68-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	62-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	154-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	134-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	97-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	167-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	81-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	41-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	68-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	87-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	7-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	40-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	13-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	156-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	77-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	116-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	148-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	145-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	106-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	115-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	75-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	125-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	50-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	101-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	32-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	3-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	134-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	24-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	21-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	84-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	89-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	51-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	93-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	58-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	105-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	32-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	153-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	23-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	35-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	132-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	98-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	117-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	133-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	8-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	102-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	122-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	80-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	146-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	28-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	2-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	44-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	34-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	91-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	22-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	69-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	145-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	141-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	43-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	65-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	86-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	99-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	30-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	90-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	19-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	34-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	100-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	165-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	116-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	120-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	11-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	58-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	79-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	109-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	147-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	39-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	124-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	66-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	88-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	144-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	65-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	119-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	162-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	114-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	43-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	4-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	113-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	82-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	166-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	37-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	104-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	167-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	138-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	158-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	143-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	5-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	78-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	20-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	90-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	152-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	120-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	16-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	40-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	95-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	89-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	96-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	118-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	46-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	36-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	157-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	127-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	92-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	18-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	123-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	112-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	6-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	63-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	37-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	9-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	64-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	31-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	158-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	54-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	103-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	38-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	76-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	139-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	136-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	59-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	126-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	128-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	108-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	139-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	94-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	42-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	127-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	151-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	101-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	48-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	15-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAP	91-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	23-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	119-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	56-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	62-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	110-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	52-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	103-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	47-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	130-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	164-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	161-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	56-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	147-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	55-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	64-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	73-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	163-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	30-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	155-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	8-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	12-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	1-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	4-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	27-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	121-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	61-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	142-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	159-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	20-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	17-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	135-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	73-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	131-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	53-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	151-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	51-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	67-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	165-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	57-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	153-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	160-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	163-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	52-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	46-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	17-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	36-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	72-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	92-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	150-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	109-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	161-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
2	FOL	138-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)
4	NAP	118-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	83-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	9-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
4	NAP	74-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	67-A	201	-	28,34,34	1.01	3 (10%)	36,47,47	2.05	9 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	3-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	150-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	26-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	14-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	111-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	71-A	201	-	-	3/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	157-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	142-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	27-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	83-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	95-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	156-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	12-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	61-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	121-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	80-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	149-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	71-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	137-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	140-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	6-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	107-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	115-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	70-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	25-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	143-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	128-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	107-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	102-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	19-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	44-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	133-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	136-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	49-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	35-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	88-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	117-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	55-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	155-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	93-A	204	-	-	2/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	129-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	164-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	14-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	104-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	74-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	42-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	21-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	135-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	47-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	159-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	38-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	16-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	60-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	76-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	100-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	96-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	69-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	124-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	140-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	2-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	10-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	87-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	112-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	79-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	10-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	146-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	31-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	160-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	82-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	105-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	129-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	39-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	57-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	99-A	201	-	-	3/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	125-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	60-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	45-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	122-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	41-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	7-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	54-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	130-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	11-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	149-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	137-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	126-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	45-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	18-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	162-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	49-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	106-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	53-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	148-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	114-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	1-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	85-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	15-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	22-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	108-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	111-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	48-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	75-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	50-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	84-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	25-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	144-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	154-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	5-A	204	-	-	2/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	85-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	86-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	59-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	33-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	26-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	29-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	110-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	152-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	77-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	131-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	33-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	29-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	81-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	63-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	70-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	97-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	123-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	28-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	24-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	13-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	94-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	113-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	72-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	141-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	98-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	132-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	166-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	78-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	66-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	68-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	62-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	154-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	134-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	97-A	204	-	-	2/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	167-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	81-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	41-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	68-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	87-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	7-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	40-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	13-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	156-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	77-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	116-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	148-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	145-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	106-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	115-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	75-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	125-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	50-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	101-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	32-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	3-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	134-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	24-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	21-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	84-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	89-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	51-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	93-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	58-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	105-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	32-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	153-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	23-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	35-A	201	-	-	3/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	132-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	98-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	117-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	133-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	8-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	102-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	122-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	80-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	146-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	28-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	2-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	44-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	34-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	91-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	22-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	69-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	145-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	141-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	43-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	65-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	86-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	99-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	30-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	90-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	19-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	34-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	100-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	165-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	116-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	120-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	11-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	58-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	79-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	109-A	201	-	-	3/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	147-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	39-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	124-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	66-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	88-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	144-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	65-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	119-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	162-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	114-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	43-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	4-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	113-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	82-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	166-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	37-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	104-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	167-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	138-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	158-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	143-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	5-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	78-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	20-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	90-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	152-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	120-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	16-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	40-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	95-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	89-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	96-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	118-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	46-A	201	-	-	3/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	36-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	157-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	127-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	92-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	18-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	123-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	112-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	6-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	63-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	37-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	9-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	64-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	31-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	158-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	54-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	103-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	38-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	76-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	139-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	136-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	59-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	126-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	128-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	108-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	139-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	94-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	42-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	127-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	151-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	101-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	48-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	15-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	91-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	23-A	204	-	-	2/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	119-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	56-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	62-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	110-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	52-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	103-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	47-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	130-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	164-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	161-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	56-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	147-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	55-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	64-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	73-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	163-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	30-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	155-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	8-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	12-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	1-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	4-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	27-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	121-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	61-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	142-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	159-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	20-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	17-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	135-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	73-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	131-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	53-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	151-A	201	-	-	3/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	51-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	67-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	165-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	57-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	153-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	160-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	163-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	52-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	46-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	17-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	36-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	72-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	92-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	150-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	109-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	161-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	138-A	201	-	-	3/16/22/22	0/3/3/3
4	NAP	118-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	83-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	9-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	74-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	67-A	201	-	-	3/16/22/22	0/3/3/3

The worst 5 of 2171 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	157-A	204	NAP	O3B-C3B	-5.81	1.29	1.43
4	26-A	204	NAP	O3B-C3B	-5.81	1.29	1.43
4	111-A	204	NAP	O3B-C3B	-5.81	1.29	1.43
4	156-A	204	NAP	O3B-C3B	-5.81	1.29	1.43
4	61-A	204	NAP	O3B-C3B	-5.81	1.29	1.43

The worst 5 of 3173 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	71-A	201	FOL	N8-C8A-N1	5.51	122.11	115.82
2	80-A	201	FOL	N8-C8A-N1	5.51	122.11	115.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	137-A	201	FOL	N8-C8A-N1	5.51	122.11	115.82
2	25-A	201	FOL	N8-C8A-N1	5.51	122.11	115.82
2	128-A	201	FOL	N8-C8A-N1	5.51	122.11	115.82

There are no chirality outliers.

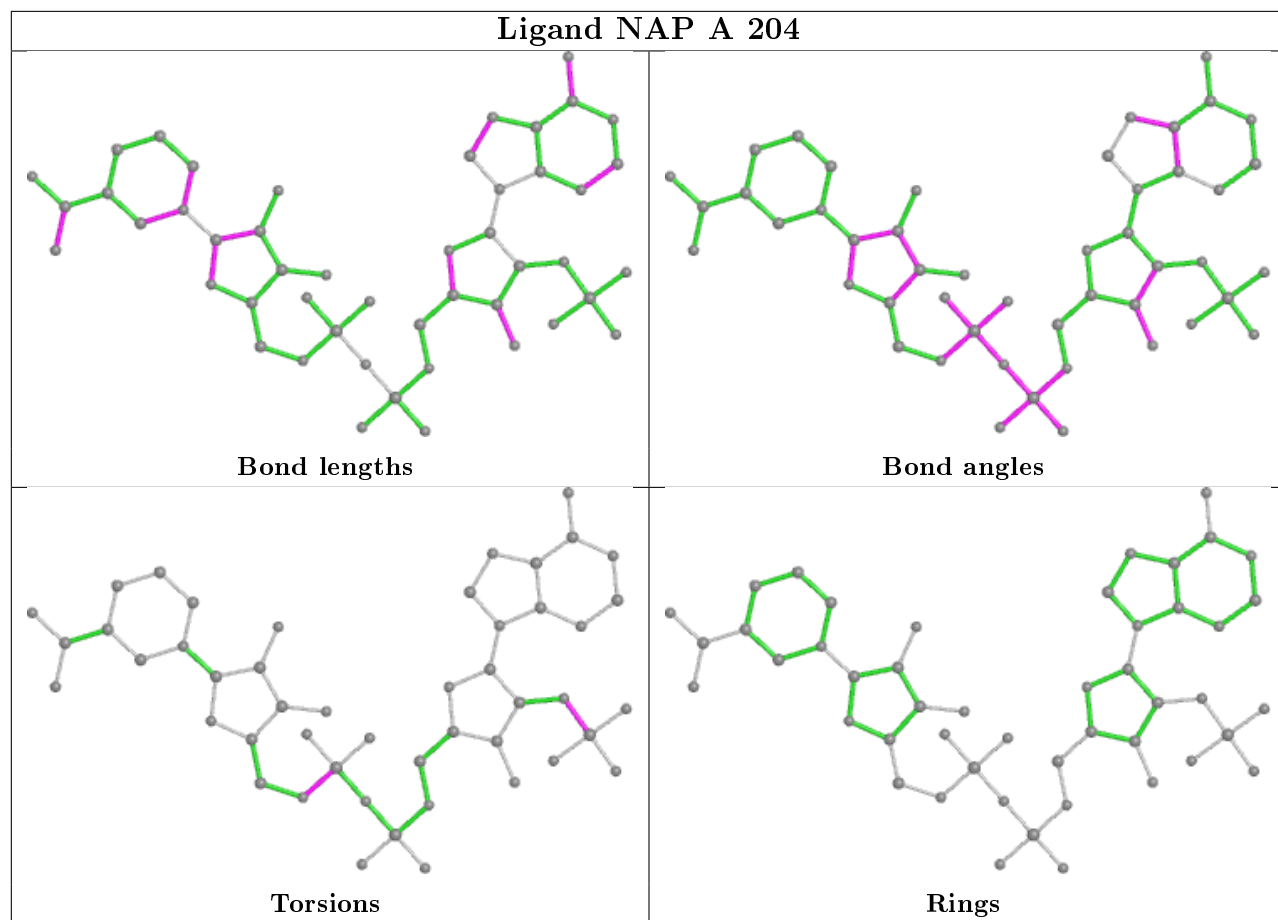
5 of 835 torsion outliers are listed below:

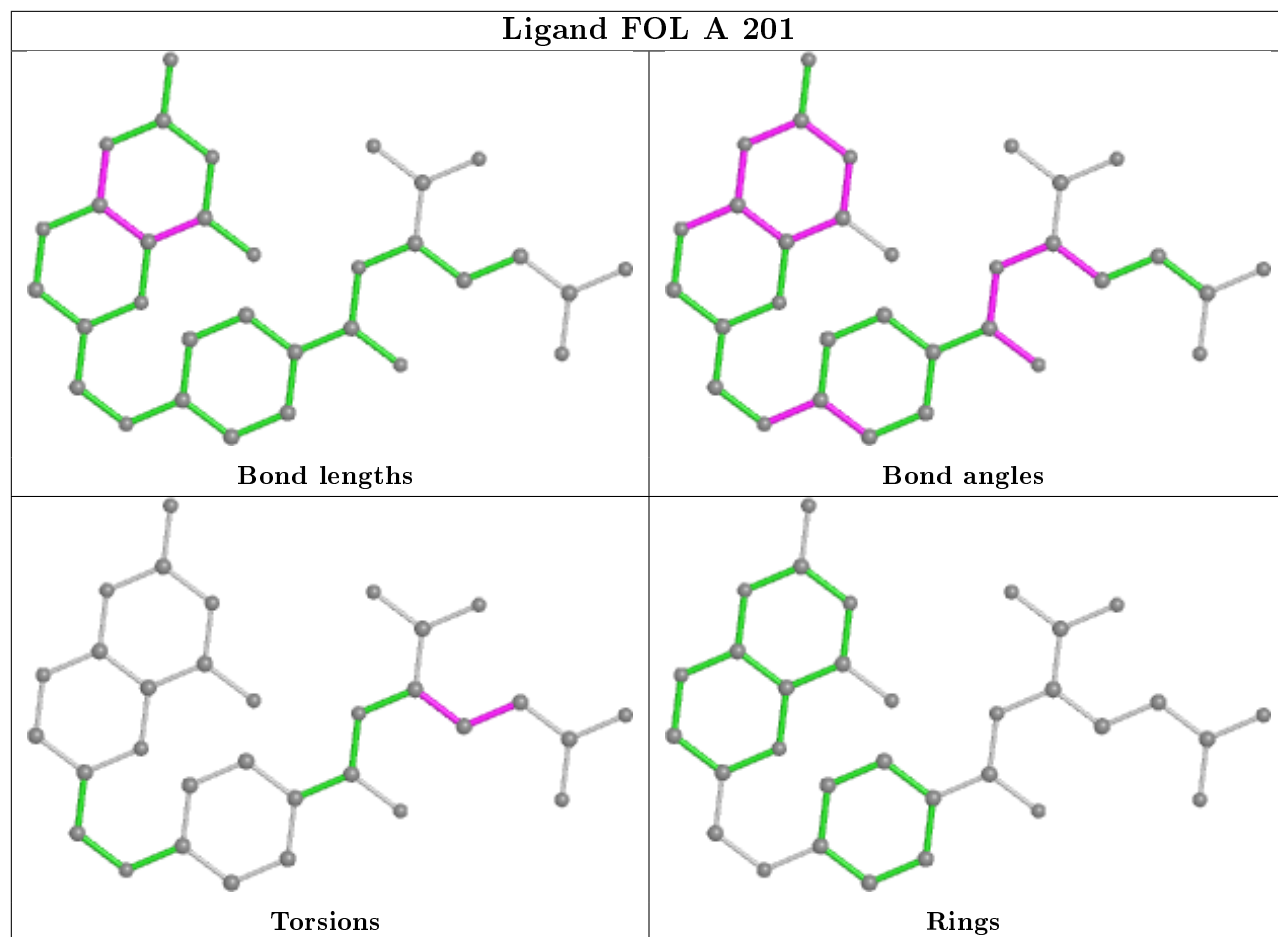
Mol	Chain	Res	Type	Atoms
4	157-A	204	NAP	C5D-O5D-PN-O2N
4	26-A	204	NAP	C5D-O5D-PN-O2N
4	111-A	204	NAP	C5D-O5D-PN-O2N
2	71-A	201	FOL	CT-CA-CB-CG
4	156-A	204	NAP	C5D-O5D-PN-O2N

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

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

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

6.3 Carbohydrates [i](#)

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

6.4 Ligands [i](#)

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

6.5 Other polymers [i](#)

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