wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 17, 2023 – 08:40 AM EST

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)

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

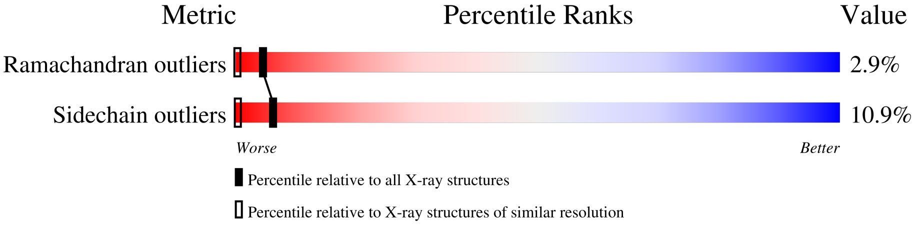
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	
1	25-A	159	
1	26-A	159	
1	27-A	159	
1	28-A	159	
1	29-A	159	
1	3-A	159	
1	30-A	159	
1	31-A	159	
1	32-A	159	
1	33-A	159	
1	34-A	159	
1	35-A	159	
1	36-A	159	
1	37-A	159	
1	38-A	159	
1	39-A	159	
1	4-A	159	
1	40-A	159	
1	41-A	159	
1	42-A	159	
1	43-A	159	
1	44-A	159	
1	45-A	159	
1	46-A	159	

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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	
1	93-A	159	
1	94-A	159	
1	95-A	159	
1	96-A	159	
1	97-A	159	
1	98-A	159	
1	99-A	159	

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

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

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

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

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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 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	102-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	103-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	104-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	105-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	106-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	107-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	108-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	109-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	110-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	111-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	112-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	113-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	114-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	115-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	116-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	117-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	118-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	119-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	120-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	121-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	122-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	123-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	124-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	125-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	126-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	127-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	128-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	129-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	130-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	131-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	132-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	133-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	134-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	135-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	136-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	137-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	138-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	139-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	140-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	141-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	142-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	143-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	144-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	145-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	146-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	147-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	148-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	149-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	150-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	151-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	152-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	153-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	154-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	155-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	156-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	157-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	158-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	159-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	160-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	161-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	162-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0
1	163-A	159	Total C H N O S 2491 805 1223 217 239 7	0	0	0

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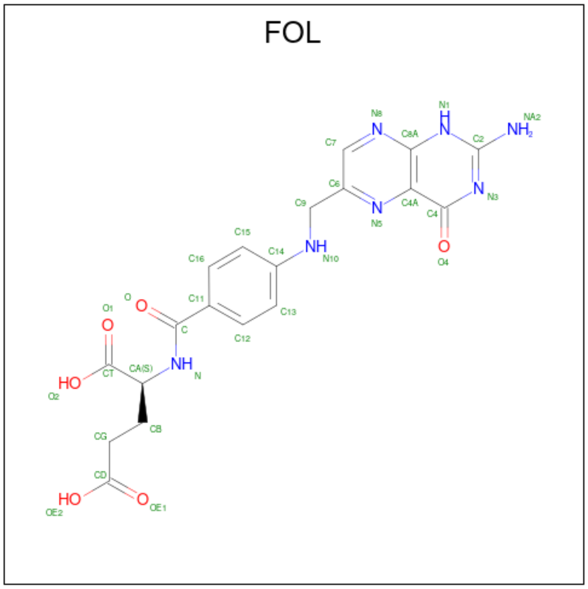
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	164-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	165-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	166-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0
1	167-A	159	Total 2491	C 805	H 1223	N 217	O 239	S 7	0	0	0

- Molecule 2 is FOLIC ACID (three-letter code: FOL) (formula: $C_{19}H_{19}N_7O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	1-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	2-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	3-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	4-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	5-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	6-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	7-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	8-A	1	Total C H N O 49 19 17 7 6	0	0
2	9-A	1	Total C H N O 49 19 17 7 6	0	0
2	10-A	1	Total C H N O 49 19 17 7 6	0	0
2	11-A	1	Total C H N O 49 19 17 7 6	0	0
2	12-A	1	Total C H N O 49 19 17 7 6	0	0
2	13-A	1	Total C H N O 49 19 17 7 6	0	0
2	14-A	1	Total C H N O 49 19 17 7 6	0	0
2	15-A	1	Total C H N O 49 19 17 7 6	0	0
2	16-A	1	Total C H N O 49 19 17 7 6	0	0
2	17-A	1	Total C H N O 49 19 17 7 6	0	0
2	18-A	1	Total C H N O 49 19 17 7 6	0	0
2	19-A	1	Total C H N O 49 19 17 7 6	0	0
2	20-A	1	Total C H N O 49 19 17 7 6	0	0
2	21-A	1	Total C H N O 49 19 17 7 6	0	0
2	22-A	1	Total C H N O 49 19 17 7 6	0	0
2	23-A	1	Total C H N O 49 19 17 7 6	0	0
2	24-A	1	Total C H N O 49 19 17 7 6	0	0
2	25-A	1	Total C H N O 49 19 17 7 6	0	0
2	26-A	1	Total C H N O 49 19 17 7 6	0	0
2	27-A	1	Total C H N O 49 19 17 7 6	0	0
2	28-A	1	Total C H N O 49 19 17 7 6	0	0

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	1-A	2	Total Ca 2 2	0	0
3	2-A	2	Total Ca 2 2	0	0
3	3-A	2	Total Ca 2 2	0	0
3	4-A	2	Total Ca 2 2	0	0
3	5-A	2	Total Ca 2 2	0	0
3	6-A	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	7-A	2	Total Ca 2 2	0	0
3	8-A	2	Total Ca 2 2	0	0
3	9-A	2	Total Ca 2 2	0	0
3	10-A	2	Total Ca 2 2	0	0
3	11-A	2	Total Ca 2 2	0	0
3	12-A	2	Total Ca 2 2	0	0
3	13-A	2	Total Ca 2 2	0	0
3	14-A	2	Total Ca 2 2	0	0
3	15-A	2	Total Ca 2 2	0	0
3	16-A	2	Total Ca 2 2	0	0
3	17-A	2	Total Ca 2 2	0	0
3	18-A	2	Total Ca 2 2	0	0
3	19-A	2	Total Ca 2 2	0	0
3	20-A	2	Total Ca 2 2	0	0
3	21-A	2	Total Ca 2 2	0	0
3	22-A	2	Total Ca 2 2	0	0
3	23-A	2	Total Ca 2 2	0	0
3	24-A	2	Total Ca 2 2	0	0
3	25-A	2	Total Ca 2 2	0	0
3	26-A	2	Total Ca 2 2	0	0
3	27-A	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	28-A	2	Total Ca 2 2	0	0
3	29-A	2	Total Ca 2 2	0	0
3	30-A	2	Total Ca 2 2	0	0
3	31-A	2	Total Ca 2 2	0	0
3	32-A	2	Total Ca 2 2	0	0
3	33-A	2	Total Ca 2 2	0	0
3	34-A	2	Total Ca 2 2	0	0
3	35-A	2	Total Ca 2 2	0	0
3	36-A	2	Total Ca 2 2	0	0
3	37-A	2	Total Ca 2 2	0	0
3	38-A	2	Total Ca 2 2	0	0
3	39-A	2	Total Ca 2 2	0	0
3	40-A	2	Total Ca 2 2	0	0
3	41-A	2	Total Ca 2 2	0	0
3	42-A	2	Total Ca 2 2	0	0
3	43-A	2	Total Ca 2 2	0	0
3	44-A	2	Total Ca 2 2	0	0
3	45-A	2	Total Ca 2 2	0	0
3	46-A	2	Total Ca 2 2	0	0
3	47-A	2	Total Ca 2 2	0	0
3	48-A	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	49-A	2	Total Ca 2 2	0	0
3	50-A	2	Total Ca 2 2	0	0
3	51-A	2	Total Ca 2 2	0	0
3	52-A	2	Total Ca 2 2	0	0
3	53-A	2	Total Ca 2 2	0	0
3	54-A	2	Total Ca 2 2	0	0
3	55-A	2	Total Ca 2 2	0	0
3	56-A	2	Total Ca 2 2	0	0
3	57-A	2	Total Ca 2 2	0	0
3	58-A	2	Total Ca 2 2	0	0
3	59-A	2	Total Ca 2 2	0	0
3	60-A	2	Total Ca 2 2	0	0
3	61-A	2	Total Ca 2 2	0	0
3	62-A	2	Total Ca 2 2	0	0
3	63-A	2	Total Ca 2 2	0	0
3	64-A	2	Total Ca 2 2	0	0
3	65-A	2	Total Ca 2 2	0	0
3	66-A	2	Total Ca 2 2	0	0
3	67-A	2	Total Ca 2 2	0	0
3	68-A	2	Total Ca 2 2	0	0
3	69-A	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	70-A	2	Total Ca 2 2	0	0
3	71-A	2	Total Ca 2 2	0	0
3	72-A	2	Total Ca 2 2	0	0
3	73-A	2	Total Ca 2 2	0	0
3	74-A	2	Total Ca 2 2	0	0
3	75-A	2	Total Ca 2 2	0	0
3	76-A	2	Total Ca 2 2	0	0
3	77-A	2	Total Ca 2 2	0	0
3	78-A	2	Total Ca 2 2	0	0
3	79-A	2	Total Ca 2 2	0	0
3	80-A	2	Total Ca 2 2	0	0
3	81-A	2	Total Ca 2 2	0	0
3	82-A	2	Total Ca 2 2	0	0
3	83-A	2	Total Ca 2 2	0	0
3	84-A	2	Total Ca 2 2	0	0
3	85-A	2	Total Ca 2 2	0	0
3	86-A	2	Total Ca 2 2	0	0
3	87-A	2	Total Ca 2 2	0	0
3	88-A	2	Total Ca 2 2	0	0
3	89-A	2	Total Ca 2 2	0	0
3	90-A	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	91-A	2	Total Ca 2 2	0	0
3	92-A	2	Total Ca 2 2	0	0
3	93-A	2	Total Ca 2 2	0	0
3	94-A	2	Total Ca 2 2	0	0
3	95-A	2	Total Ca 2 2	0	0
3	96-A	2	Total Ca 2 2	0	0
3	97-A	2	Total Ca 2 2	0	0
3	98-A	2	Total Ca 2 2	0	0
3	99-A	2	Total Ca 2 2	0	0
3	100-A	2	Total Ca 2 2	0	0
3	101-A	2	Total Ca 2 2	0	0
3	102-A	2	Total Ca 2 2	0	0
3	103-A	2	Total Ca 2 2	0	0
3	104-A	2	Total Ca 2 2	0	0
3	105-A	2	Total Ca 2 2	0	0
3	106-A	2	Total Ca 2 2	0	0
3	107-A	2	Total Ca 2 2	0	0
3	108-A	2	Total Ca 2 2	0	0
3	109-A	2	Total Ca 2 2	0	0
3	110-A	2	Total Ca 2 2	0	0
3	111-A	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	112-A	2	Total Ca 2 2	0	0
3	113-A	2	Total Ca 2 2	0	0
3	114-A	2	Total Ca 2 2	0	0
3	115-A	2	Total Ca 2 2	0	0
3	116-A	2	Total Ca 2 2	0	0
3	117-A	2	Total Ca 2 2	0	0
3	118-A	2	Total Ca 2 2	0	0
3	119-A	2	Total Ca 2 2	0	0
3	120-A	2	Total Ca 2 2	0	0
3	121-A	2	Total Ca 2 2	0	0
3	122-A	2	Total Ca 2 2	0	0
3	123-A	2	Total Ca 2 2	0	0
3	124-A	2	Total Ca 2 2	0	0
3	125-A	2	Total Ca 2 2	0	0
3	126-A	2	Total Ca 2 2	0	0
3	127-A	2	Total Ca 2 2	0	0
3	128-A	2	Total Ca 2 2	0	0
3	129-A	2	Total Ca 2 2	0	0
3	130-A	2	Total Ca 2 2	0	0
3	131-A	2	Total Ca 2 2	0	0
3	132-A	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	133-A	2	Total Ca 2 2	0	0
3	134-A	2	Total Ca 2 2	0	0
3	135-A	2	Total Ca 2 2	0	0
3	136-A	2	Total Ca 2 2	0	0
3	137-A	2	Total Ca 2 2	0	0
3	138-A	2	Total Ca 2 2	0	0
3	139-A	2	Total Ca 2 2	0	0
3	140-A	2	Total Ca 2 2	0	0
3	141-A	2	Total Ca 2 2	0	0
3	142-A	2	Total Ca 2 2	0	0
3	143-A	2	Total Ca 2 2	0	0
3	144-A	2	Total Ca 2 2	0	0
3	145-A	2	Total Ca 2 2	0	0
3	146-A	2	Total Ca 2 2	0	0
3	147-A	2	Total Ca 2 2	0	0
3	148-A	2	Total Ca 2 2	0	0
3	149-A	2	Total Ca 2 2	0	0
3	150-A	2	Total Ca 2 2	0	0
3	151-A	2	Total Ca 2 2	0	0
3	152-A	2	Total Ca 2 2	0	0
3	153-A	2	Total Ca 2 2	0	0

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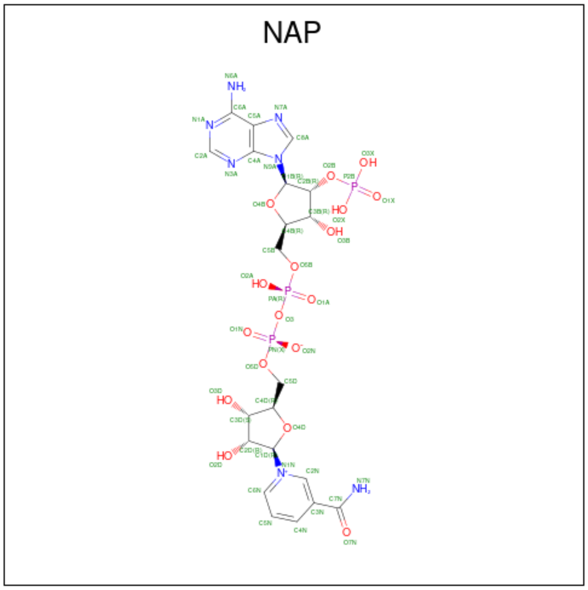
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	154-A	2	Total Ca 2 2	0	0
3	155-A	2	Total Ca 2 2	0	0
3	156-A	2	Total Ca 2 2	0	0
3	157-A	2	Total Ca 2 2	0	0
3	158-A	2	Total Ca 2 2	0	0
3	159-A	2	Total Ca 2 2	0	0
3	160-A	2	Total Ca 2 2	0	0
3	161-A	2	Total Ca 2 2	0	0
3	162-A	2	Total Ca 2 2	0	0
3	163-A	2	Total Ca 2 2	0	0
3	164-A	2	Total Ca 2 2	0	0
3	165-A	2	Total Ca 2 2	0	0
3	166-A	2	Total Ca 2 2	0	0
3	167-A	2	Total Ca 2 2	0	0

- Molecule 4 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	78-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	79-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	80-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	81-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	82-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	83-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	84-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	85-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	86-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	87-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	88-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	89-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	90-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	91-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	92-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	93-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	94-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	95-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	96-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	97-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	98-A	1	Total C H N O P 72 21 24 7 17 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 C H N O P 72 21 24 7 17 3	0	0
4	121-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	122-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	123-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	124-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	125-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	126-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	127-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	128-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	129-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	130-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	131-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	132-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	133-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	134-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	135-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	136-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	137-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	138-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	139-A	1	Total C H N O P 72 21 24 7 17 3	0	0
4	140-A	1	Total C H N O P 72 21 24 7 17 3	0	0

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

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

- Molecule 5 is water.

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

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

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

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

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

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

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

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

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

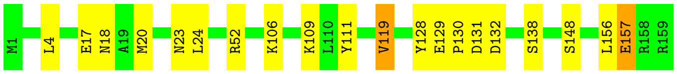
3 Residue-property plots ⓘ

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.

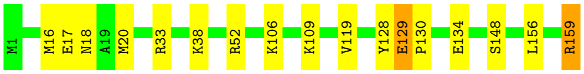
- Molecule 1: Dihydrofolate reductase

Chain 1-A:



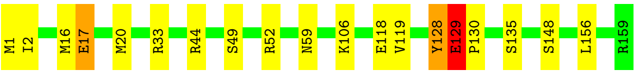
- Molecule 1: Dihydrofolate reductase

Chain 2-A:



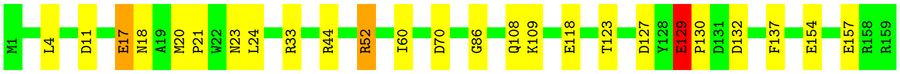
- Molecule 1: Dihydrofolate reductase

Chain 3-A:



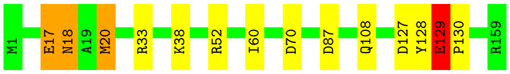
- Molecule 1: Dihydrofolate reductase

Chain 4-A:



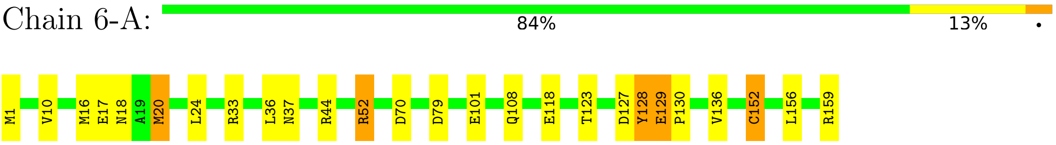
- Molecule 1: Dihydrofolate reductase

Chain 5-A:



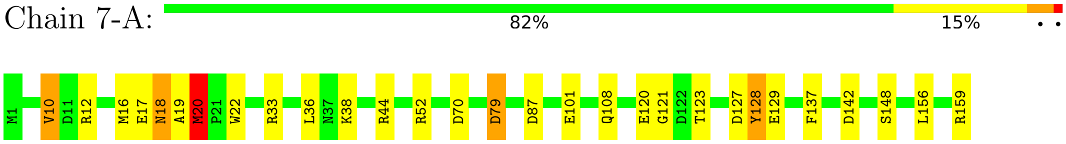
- Molecule 1: Dihydrofolate reductase

Chain 6-A:



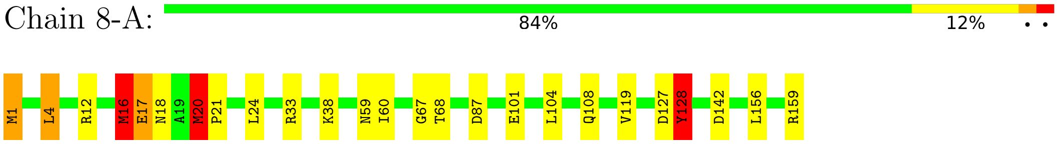
- Molecule 1: Dihydrofolate reductase

Chain 7-A:



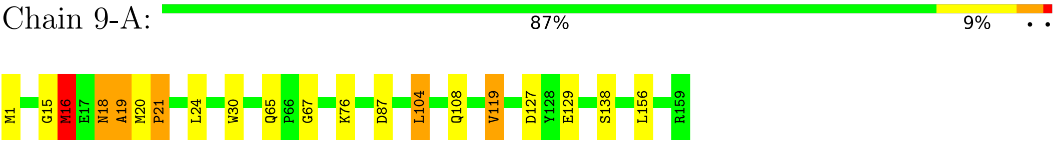
- Molecule 1: Dihydrofolate reductase

Chain 8-A:



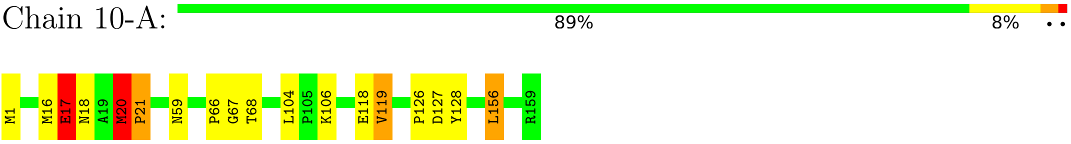
- Molecule 1: Dihydrofolate reductase

Chain 9-A:



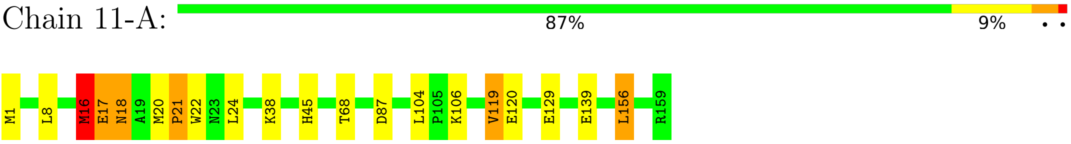
- Molecule 1: Dihydrofolate reductase

Chain 10-A:



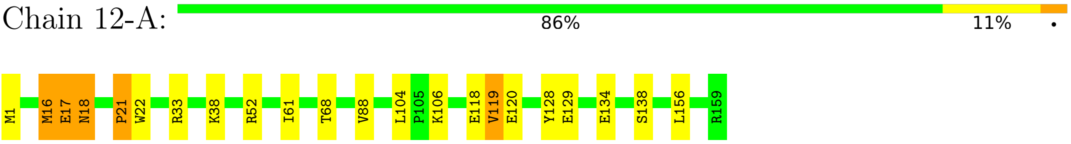
- Molecule 1: Dihydrofolate reductase

Chain 11-A:



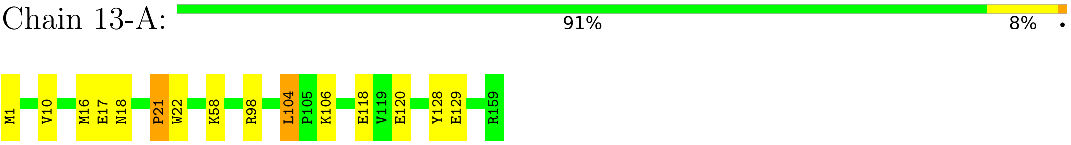
- Molecule 1: Dihydrofolate reductase

Chain 12-A:



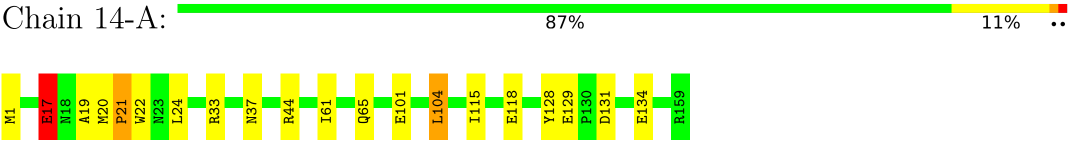
- Molecule 1: Dihydrofolate reductase

Chain 13-A:



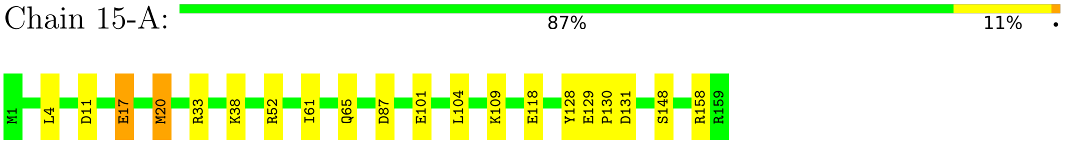
- Molecule 1: Dihydrofolate reductase

Chain 14-A:



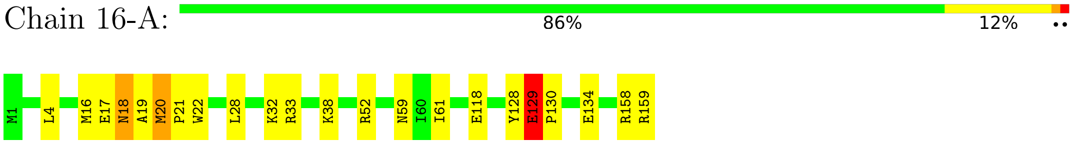
- Molecule 1: Dihydrofolate reductase

Chain 15-A:



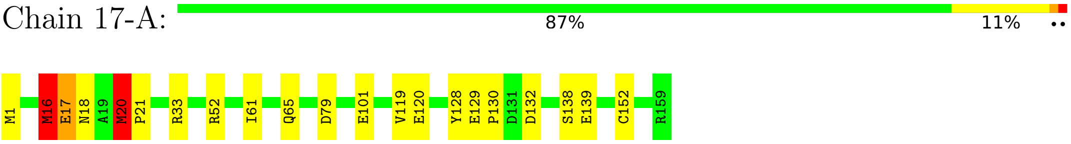
- Molecule 1: Dihydrofolate reductase

Chain 16-A:



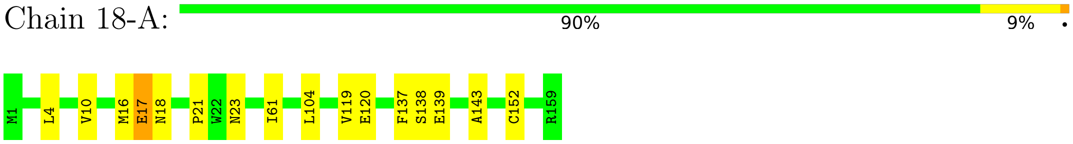
- Molecule 1: Dihydrofolate reductase

Chain 17-A:



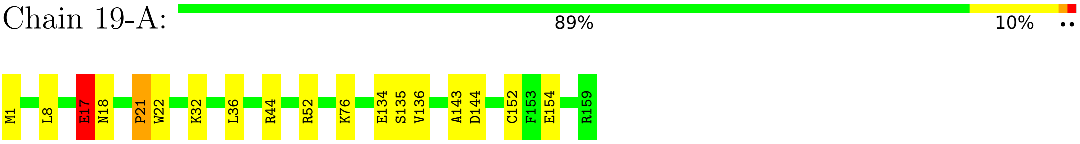
- Molecule 1: Dihydrofolate reductase

Chain 18-A:



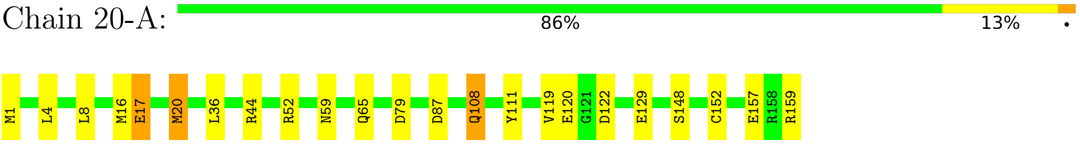
- Molecule 1: Dihydrofolate reductase

Chain 19-A:



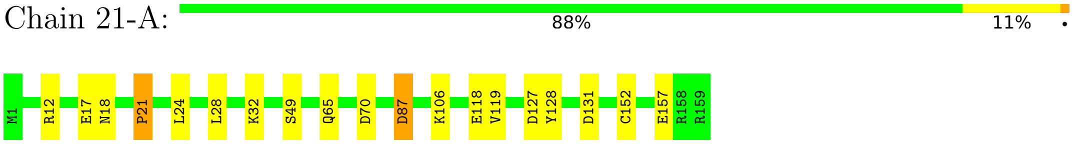
- Molecule 1: Dihydrofolate reductase

Chain 20-A:



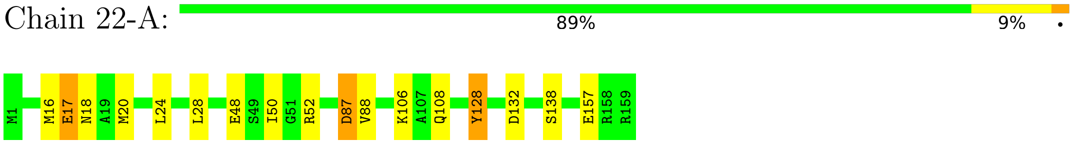
- Molecule 1: Dihydrofolate reductase

Chain 21-A:



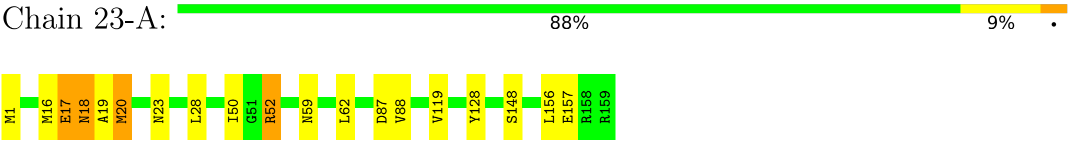
- Molecule 1: Dihydrofolate reductase

Chain 22-A:



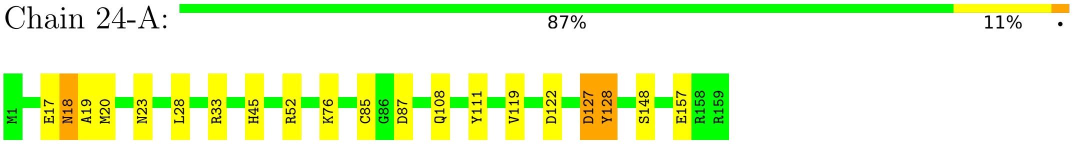
- Molecule 1: Dihydrofolate reductase

Chain 23-A:



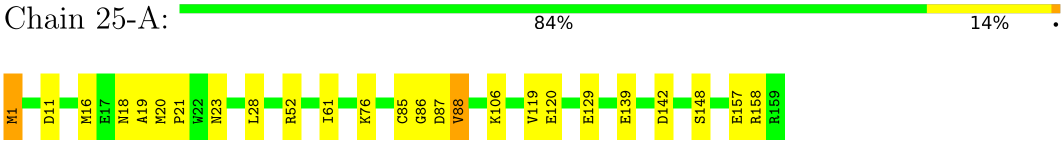
- Molecule 1: Dihydrofolate reductase

Chain 24-A:



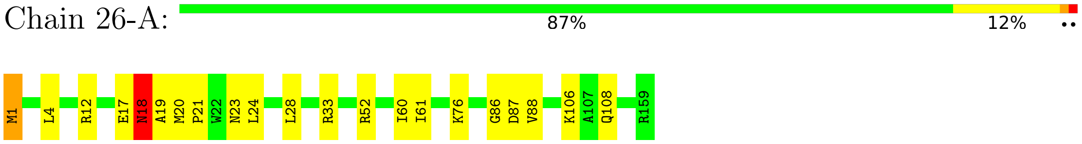
- Molecule 1: Dihydrofolate reductase

Chain 25-A:



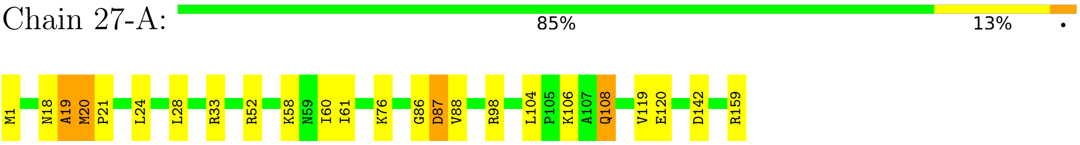
- Molecule 1: Dihydrofolate reductase

Chain 26-A:



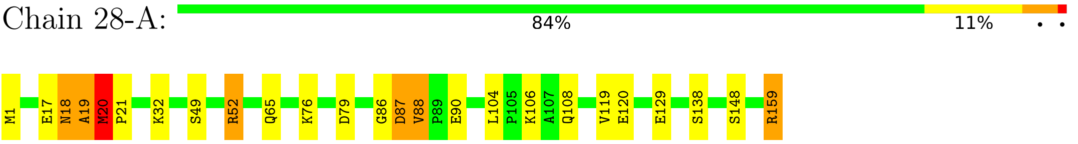
- Molecule 1: Dihydrofolate reductase

Chain 27-A:



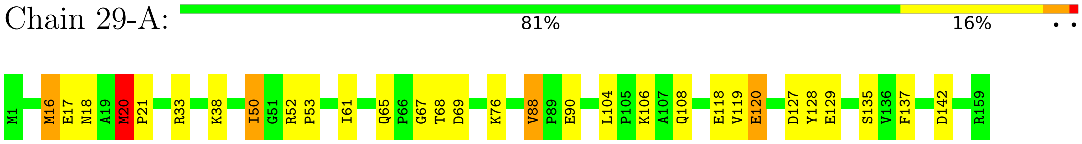
- Molecule 1: Dihydrofolate reductase

Chain 28-A:



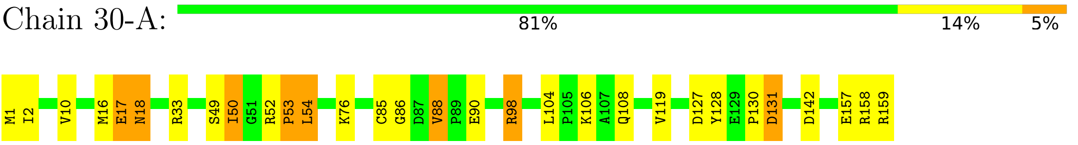
- Molecule 1: Dihydrofolate reductase

Chain 29-A:



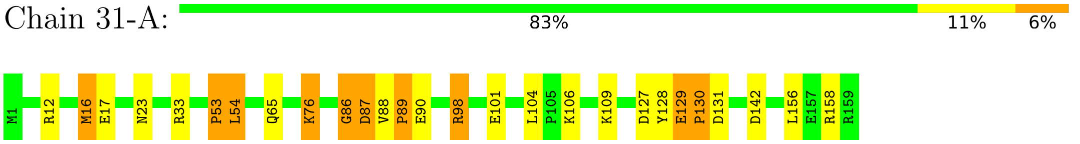
- Molecule 1: Dihydrofolate reductase

Chain 30-A:



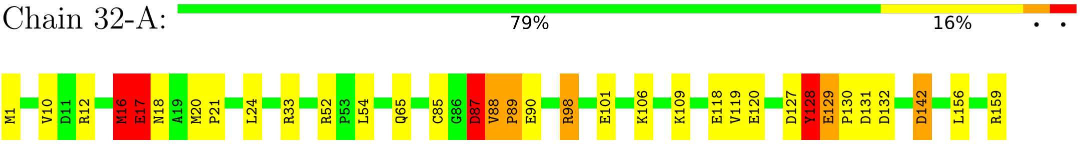
- Molecule 1: Dihydrofolate reductase

Chain 31-A:



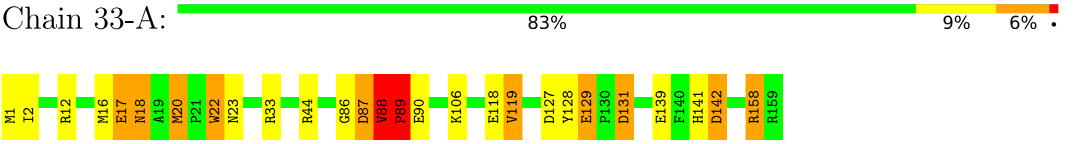
- Molecule 1: Dihydrofolate reductase

Chain 32-A:

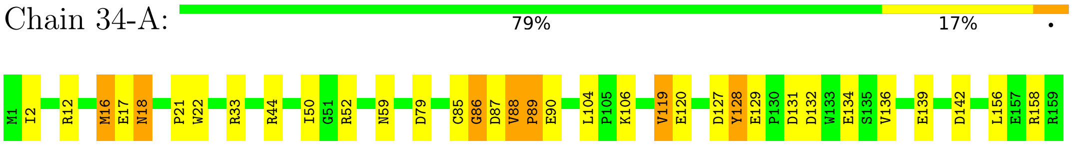


- Molecule 1: Dihydrofolate reductase

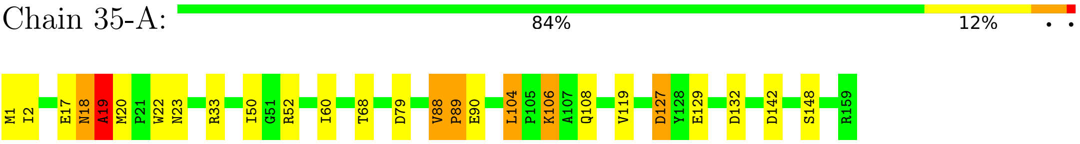
Chain 33-A:



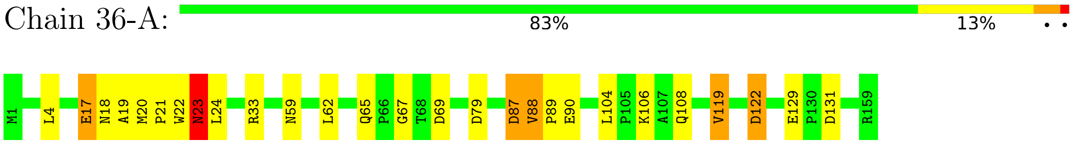
- Molecule 1: Dihydrofolate reductase



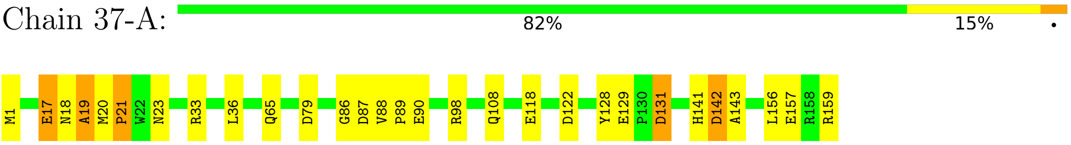
- Molecule 1: Dihydrofolate reductase



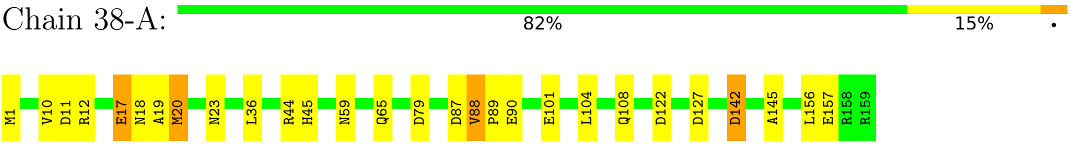
- Molecule 1: Dihydrofolate reductase



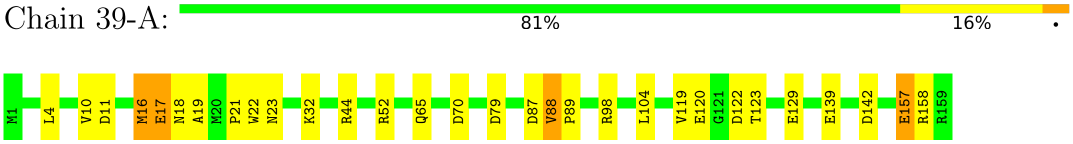
- Molecule 1: Dihydrofolate reductase



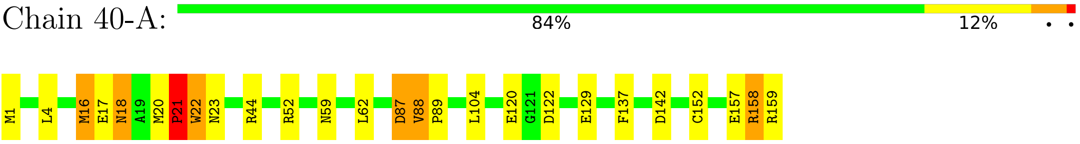
- Molecule 1: Dihydrofolate reductase



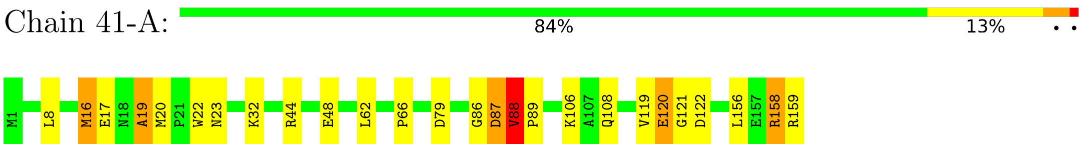
- Molecule 1: Dihydrofolate reductase



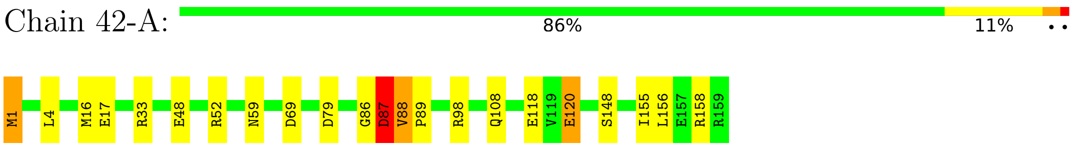
- Molecule 1: Dihydrofolate reductase



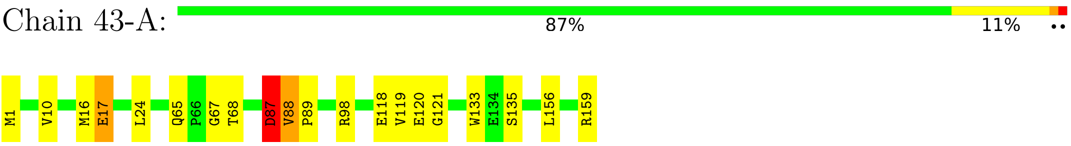
- Molecule 1: Dihydrofolate reductase



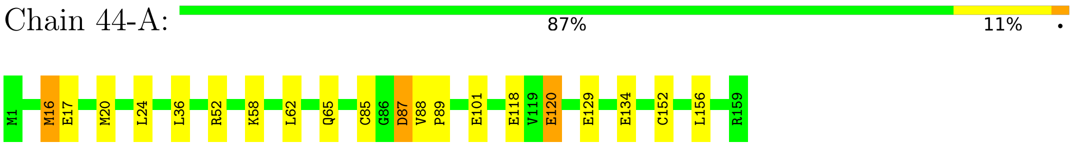
• Molecule 1: Dihydrofolate reductase



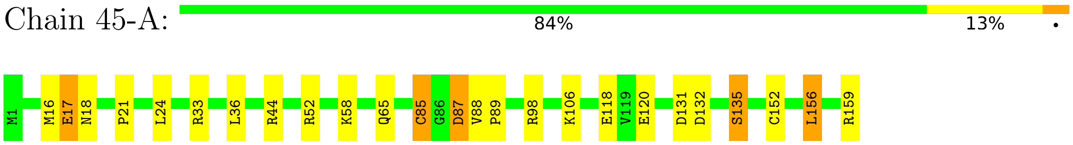
• Molecule 1: Dihydrofolate reductase



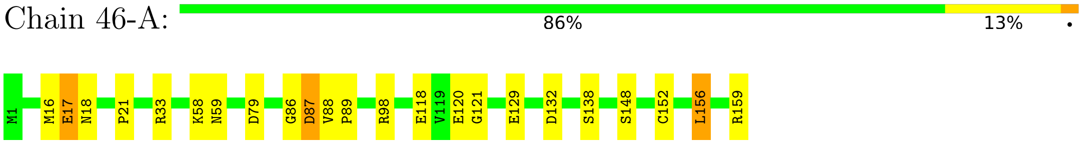
• Molecule 1: Dihydrofolate reductase



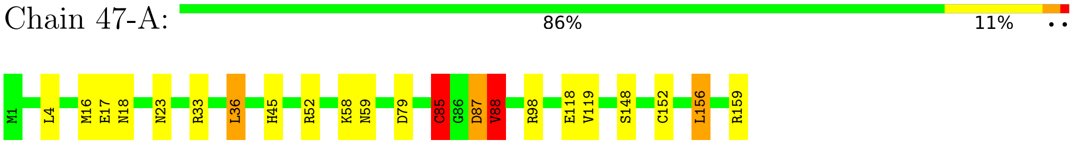
• Molecule 1: Dihydrofolate reductase



• Molecule 1: Dihydrofolate reductase

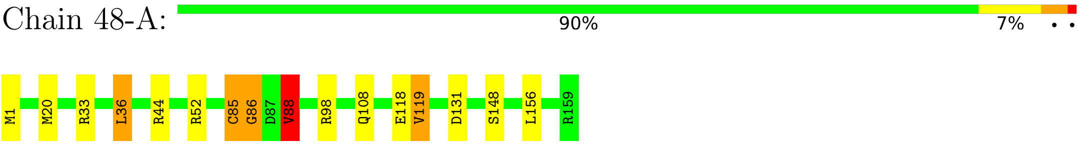


• Molecule 1: Dihydrofolate reductase



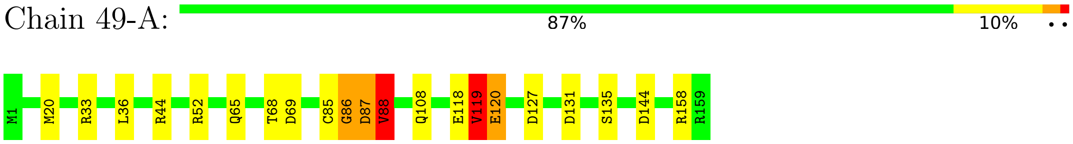
• Molecule 1: Dihydrofolate reductase

Chain 48-A:



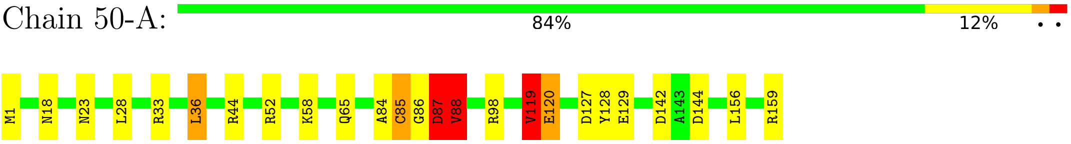
- Molecule 1: Dihydrofolate reductase

Chain 49-A:



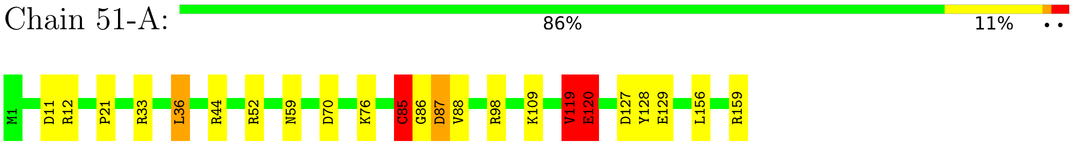
- Molecule 1: Dihydrofolate reductase

Chain 50-A:



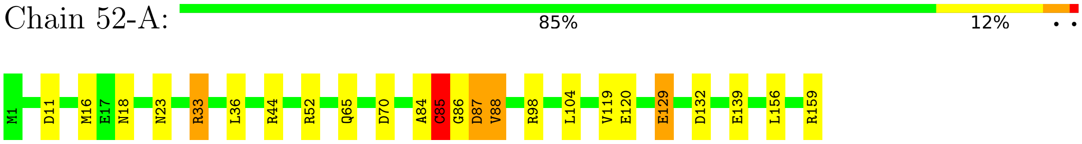
- Molecule 1: Dihydrofolate reductase

Chain 51-A:



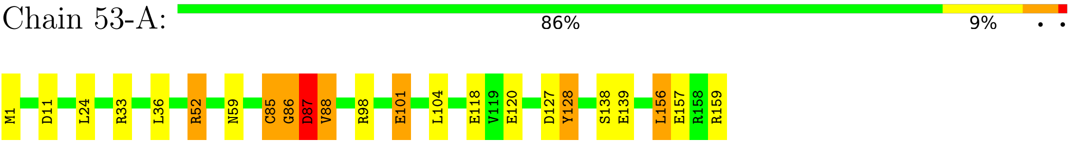
- Molecule 1: Dihydrofolate reductase

Chain 52-A:



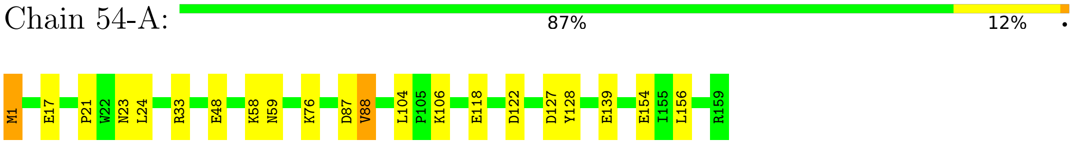
- Molecule 1: Dihydrofolate reductase

Chain 53-A:



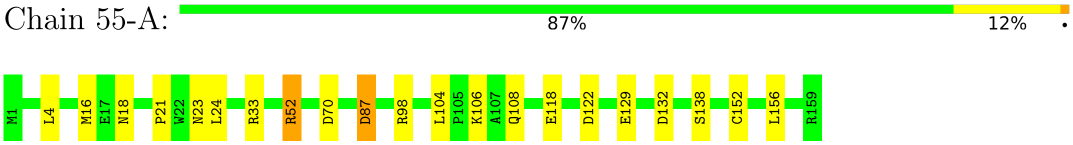
- Molecule 1: Dihydrofolate reductase

Chain 54-A:



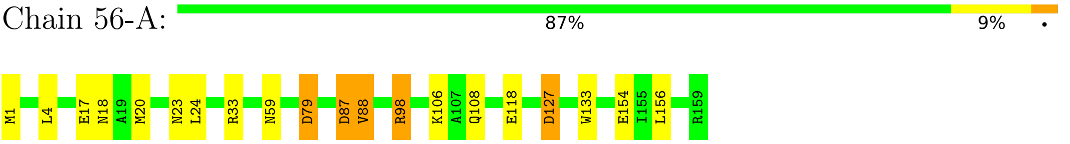
- Molecule 1: Dihydrofolate reductase

Chain 55-A:



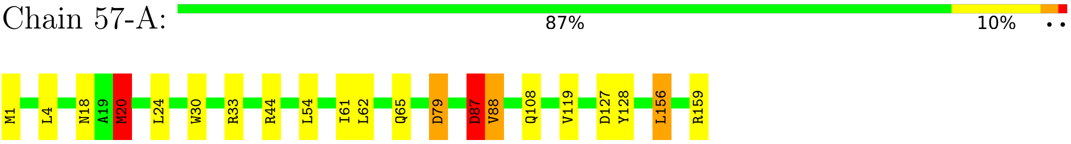
- Molecule 1: Dihydrofolate reductase

Chain 56-A:



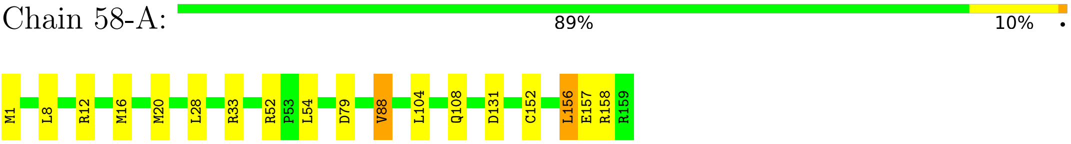
- Molecule 1: Dihydrofolate reductase

Chain 57-A:



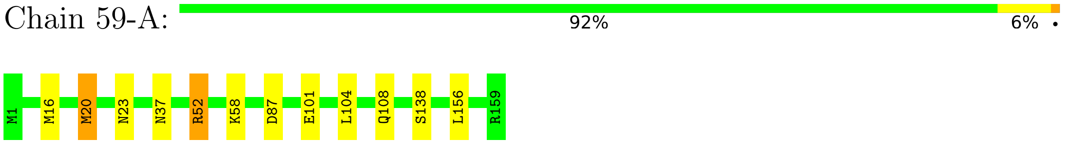
- Molecule 1: Dihydrofolate reductase

Chain 58-A:



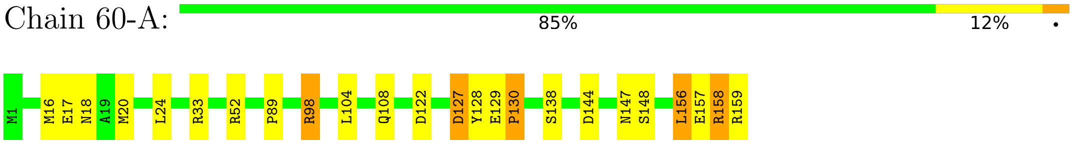
- Molecule 1: Dihydrofolate reductase

Chain 59-A:



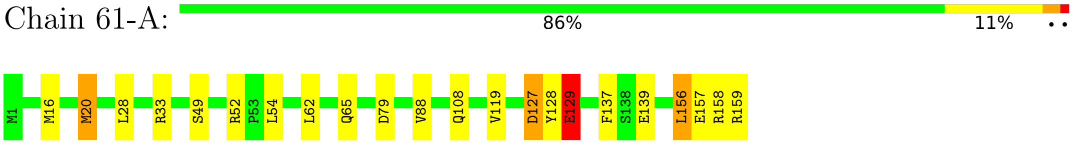
- Molecule 1: Dihydrofolate reductase

Chain 60-A:



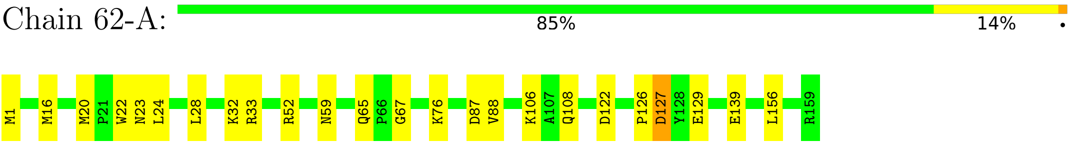
- Molecule 1: Dihydrofolate reductase

Chain 61-A:



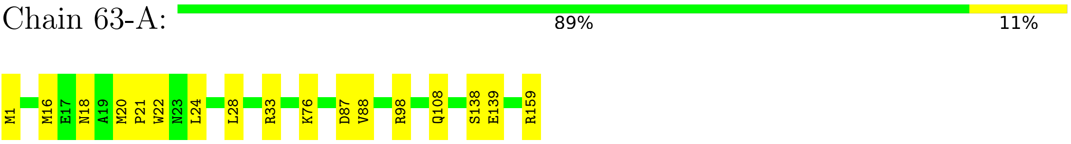
- Molecule 1: Dihydrofolate reductase

Chain 62-A:



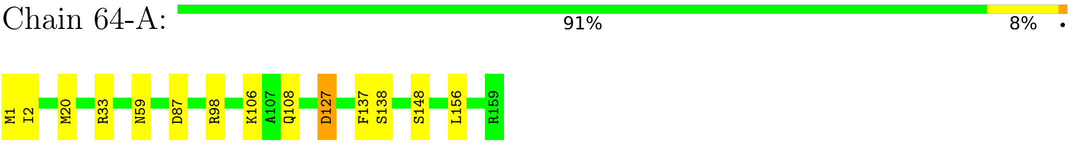
- Molecule 1: Dihydrofolate reductase

Chain 63-A:



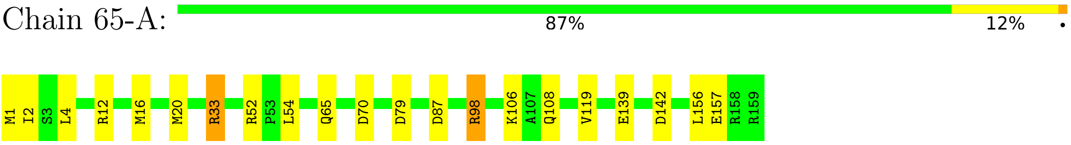
- Molecule 1: Dihydrofolate reductase

Chain 64-A:



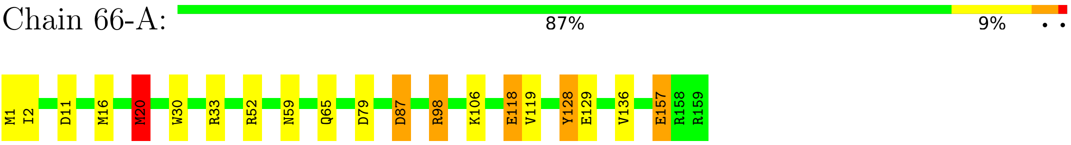
- Molecule 1: Dihydrofolate reductase

Chain 65-A:



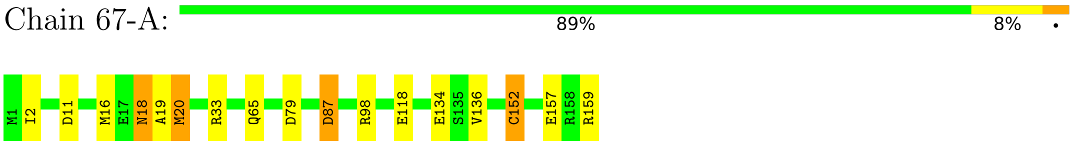
- Molecule 1: Dihydrofolate reductase

Chain 66-A:



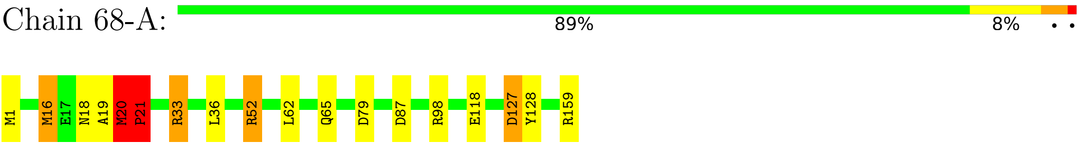
- Molecule 1: Dihydrofolate reductase

Chain 67-A:



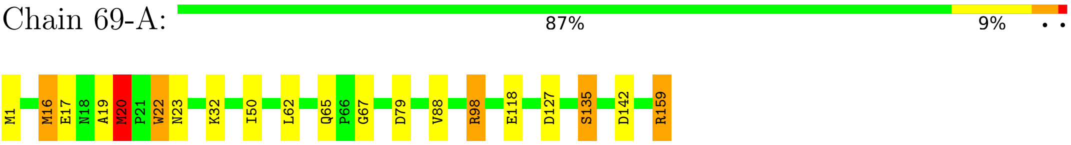
- Molecule 1: Dihydrofolate reductase

Chain 68-A:



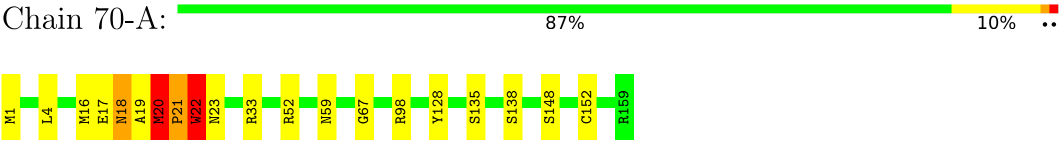
- Molecule 1: Dihydrofolate reductase

Chain 69-A:



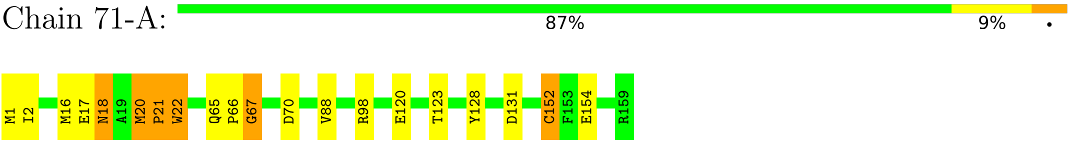
- Molecule 1: Dihydrofolate reductase

Chain 70-A:



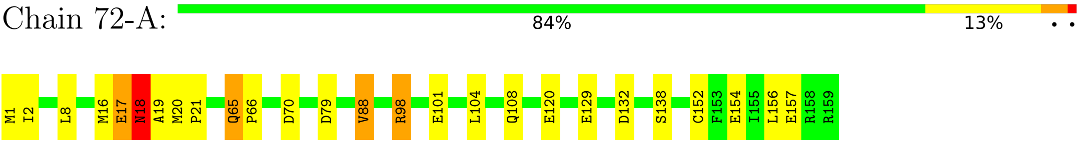
- Molecule 1: Dihydrofolate reductase

Chain 71-A:



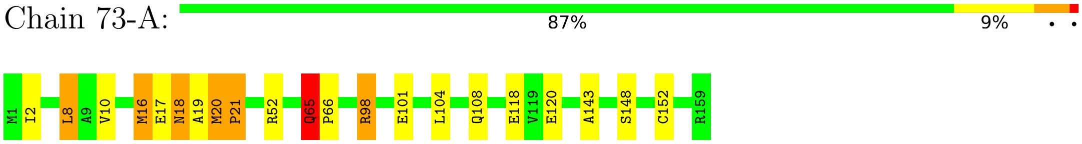
- Molecule 1: Dihydrofolate reductase

Chain 72-A:



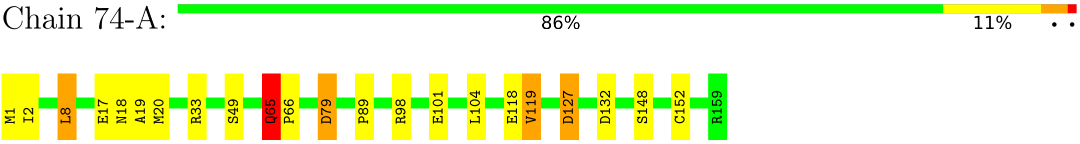
- Molecule 1: Dihydrofolate reductase

Chain 73-A:



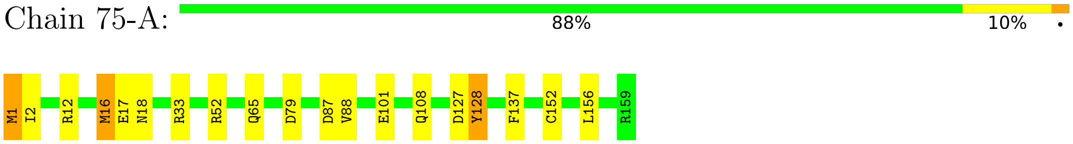
- Molecule 1: Dihydrofolate reductase

Chain 74-A:



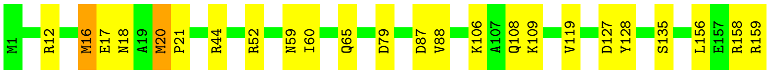
- Molecule 1: Dihydrofolate reductase

Chain 75-A:



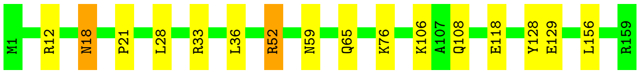
- Molecule 1: Dihydrofolate reductase

Chain 76-A:



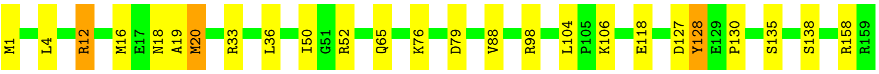
- Molecule 1: Dihydrofolate reductase

Chain 77-A:



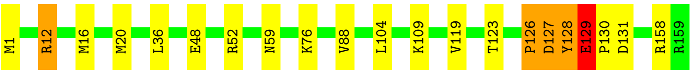
- Molecule 1: Dihydrofolate reductase

Chain 78-A:



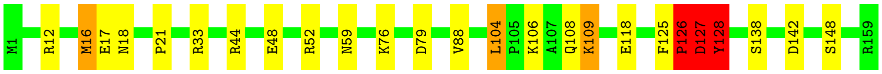
- Molecule 1: Dihydrofolate reductase

Chain 79-A:



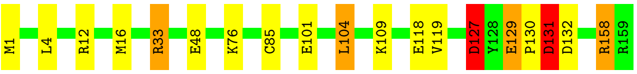
- Molecule 1: Dihydrofolate reductase

Chain 80-A:



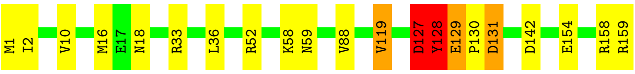
- Molecule 1: Dihydrofolate reductase

Chain 81-A:



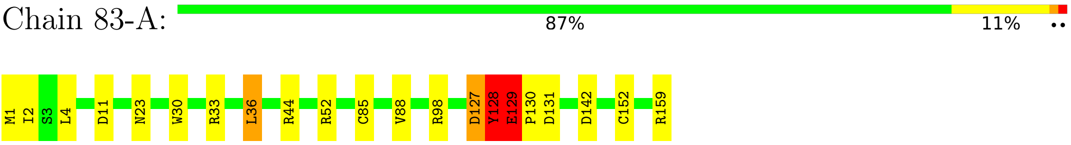
- Molecule 1: Dihydrofolate reductase

Chain 82-A:



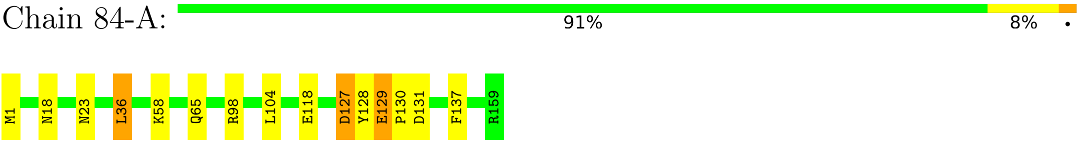
- Molecule 1: Dihydrofolate reductase

Chain 83-A:



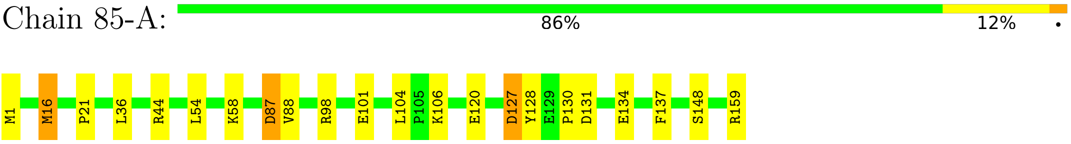
- Molecule 1: Dihydrofolate reductase

Chain 84-A:



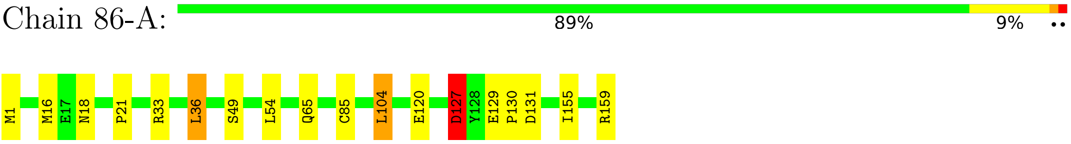
- Molecule 1: Dihydrofolate reductase

Chain 85-A:



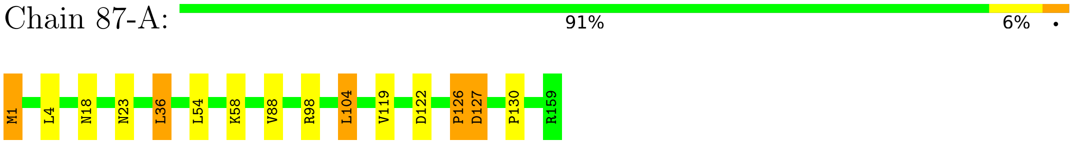
- Molecule 1: Dihydrofolate reductase

Chain 86-A:



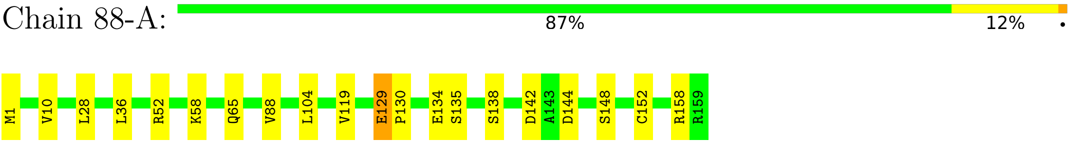
- Molecule 1: Dihydrofolate reductase

Chain 87-A:



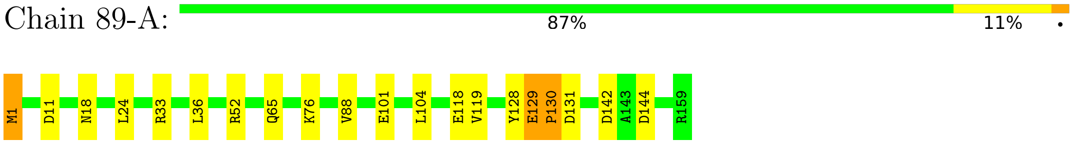
- Molecule 1: Dihydrofolate reductase

Chain 88-A:



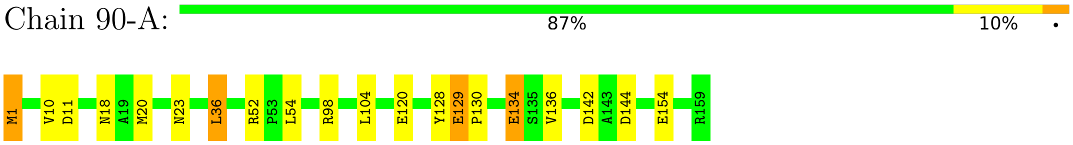
- Molecule 1: Dihydrofolate reductase

Chain 89-A:



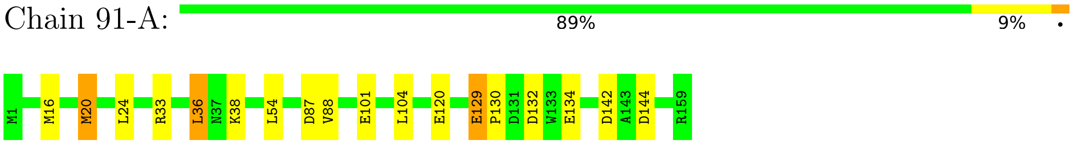
- Molecule 1: Dihydrofolate reductase

Chain 90-A:



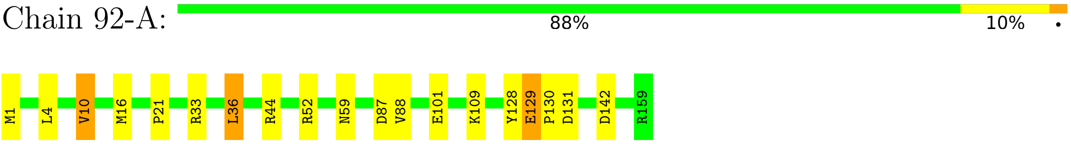
- Molecule 1: Dihydrofolate reductase

Chain 91-A:



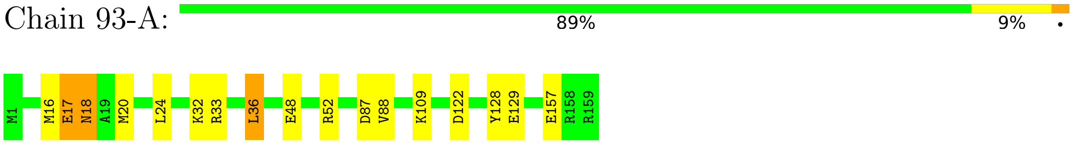
- Molecule 1: Dihydrofolate reductase

Chain 92-A:



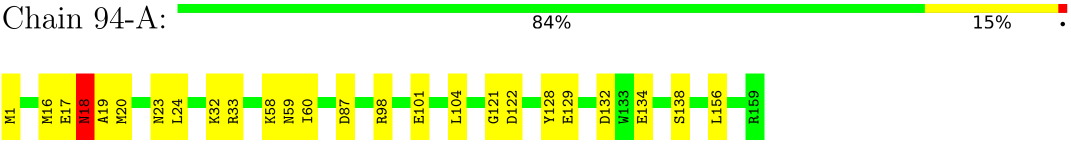
- Molecule 1: Dihydrofolate reductase

Chain 93-A:



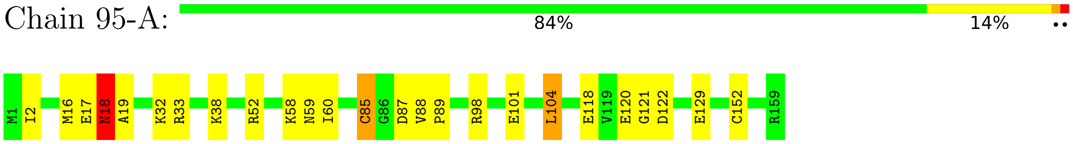
- Molecule 1: Dihydrofolate reductase

Chain 94-A:



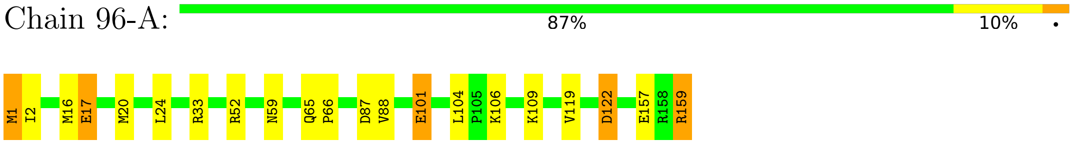
- Molecule 1: Dihydrofolate reductase

Chain 95-A:

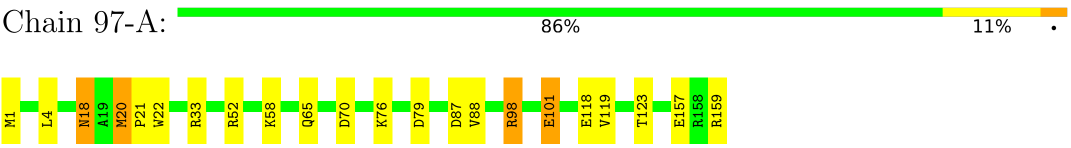


- Molecule 1: Dihydrofolate reductase

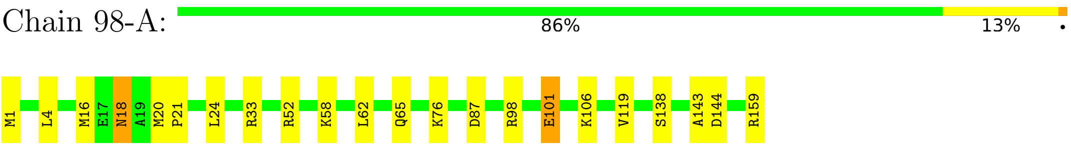
Chain 96-A:



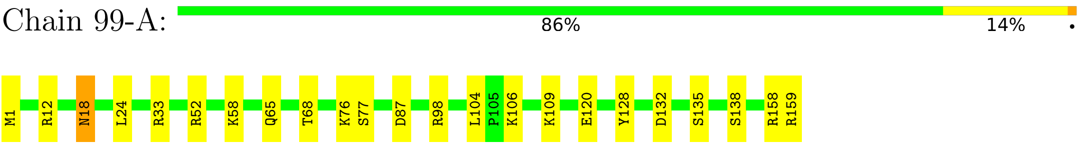
- Molecule 1: Dihydrofolate reductase



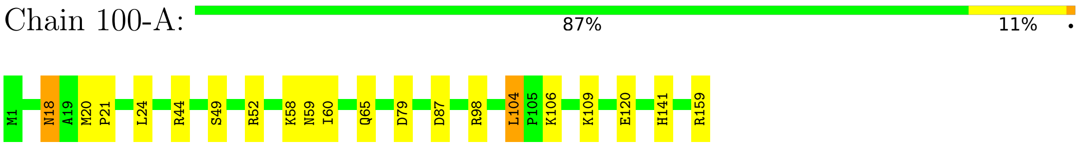
- Molecule 1: Dihydrofolate reductase



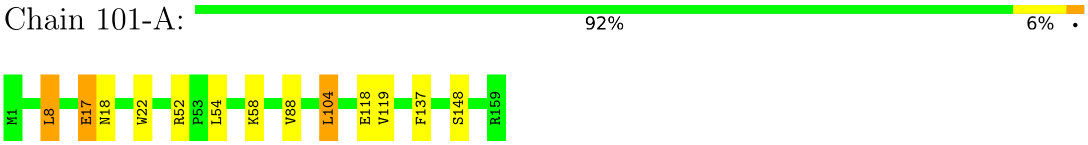
- Molecule 1: Dihydrofolate reductase



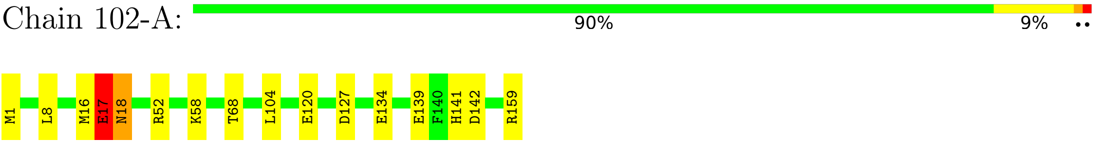
- Molecule 1: Dihydrofolate reductase



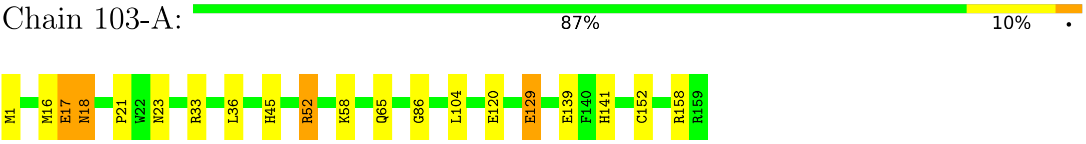
- Molecule 1: Dihydrofolate reductase



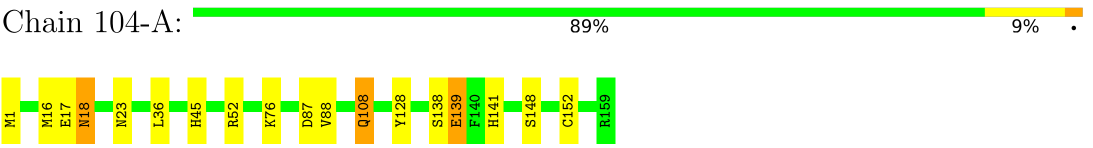
- Molecule 1: Dihydrofolate reductase



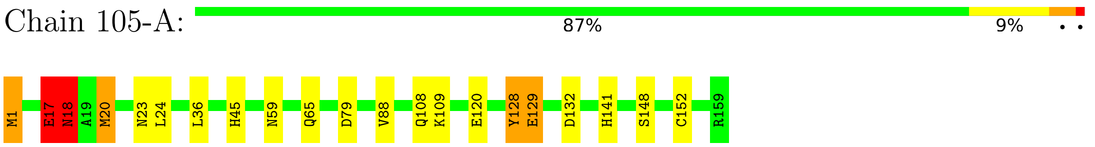
- Molecule 1: Dihydrofolate reductase



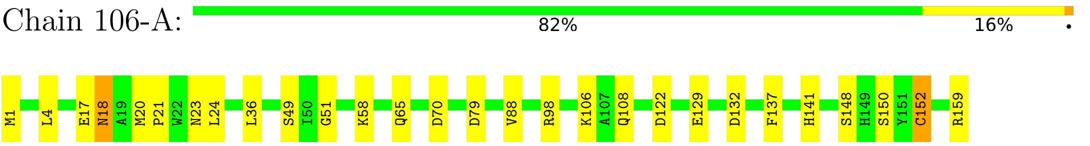
- Molecule 1: Dihydrofolate reductase



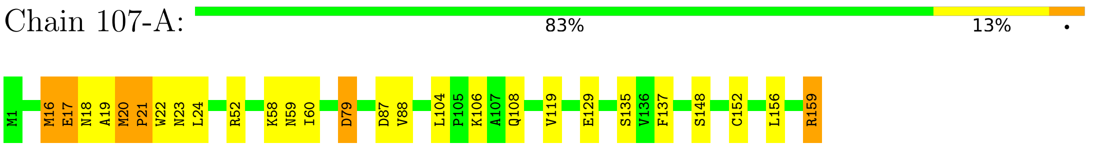
• Molecule 1: Dihydrofolate reductase



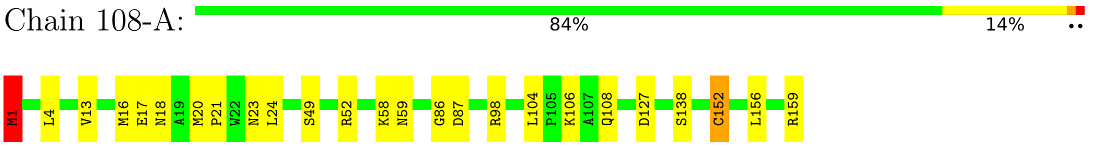
• Molecule 1: Dihydrofolate reductase



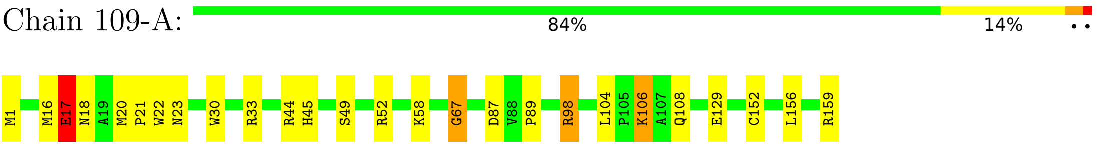
• Molecule 1: Dihydrofolate reductase



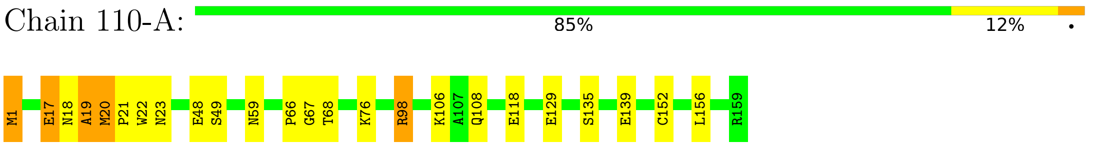
• Molecule 1: Dihydrofolate reductase



• Molecule 1: Dihydrofolate reductase

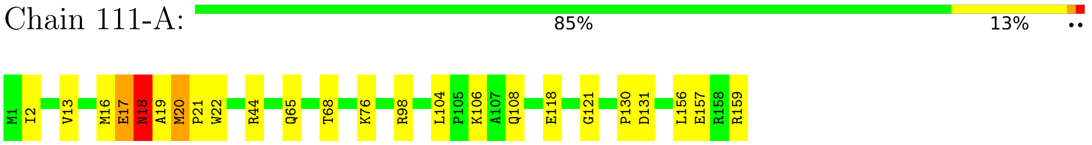


• Molecule 1: Dihydrofolate reductase



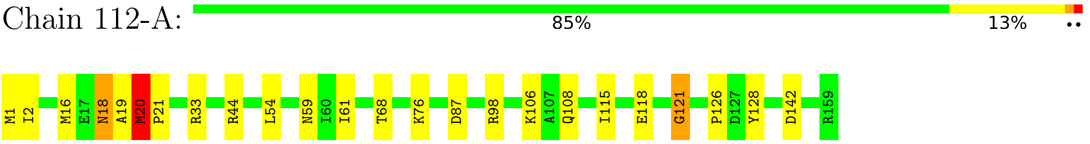
• Molecule 1: Dihydrofolate reductase

Chain 111-A:



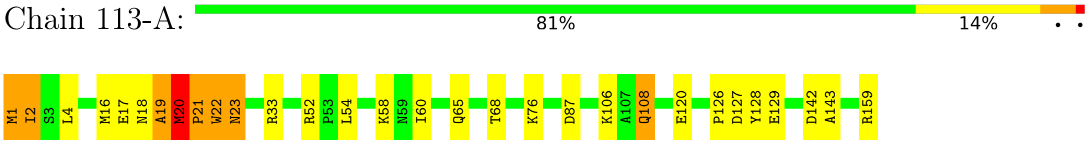
- Molecule 1: Dihydrofolate reductase

Chain 112-A:



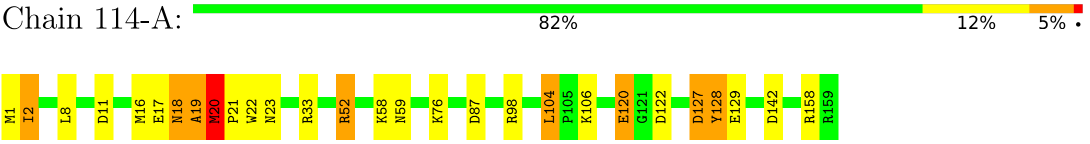
- Molecule 1: Dihydrofolate reductase

Chain 113-A:



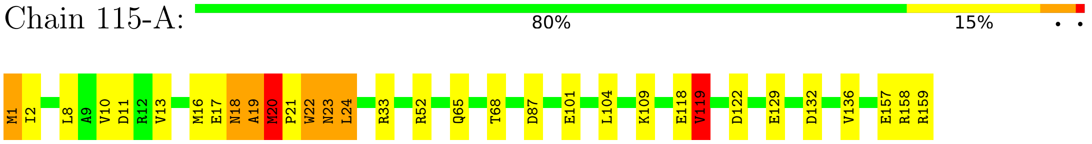
- Molecule 1: Dihydrofolate reductase

Chain 114-A:



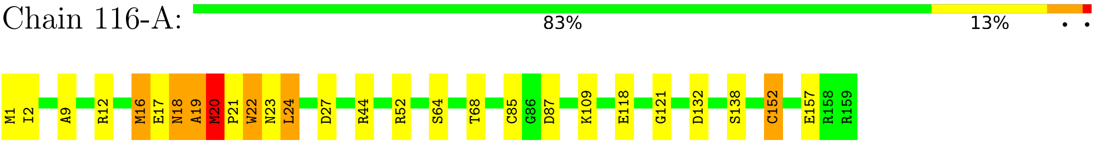
- Molecule 1: Dihydrofolate reductase

Chain 115-A:



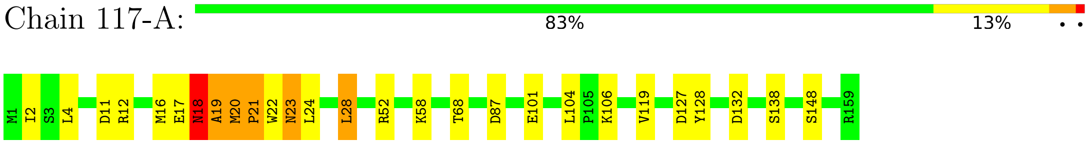
- Molecule 1: Dihydrofolate reductase

Chain 116-A:



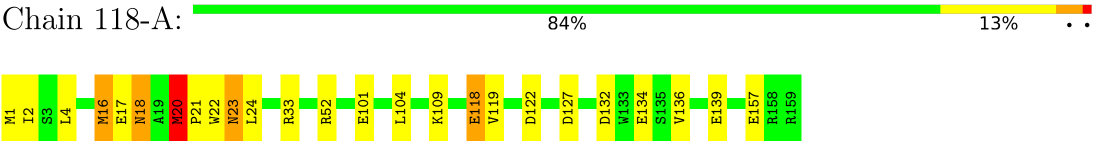
- Molecule 1: Dihydrofolate reductase

Chain 117-A:



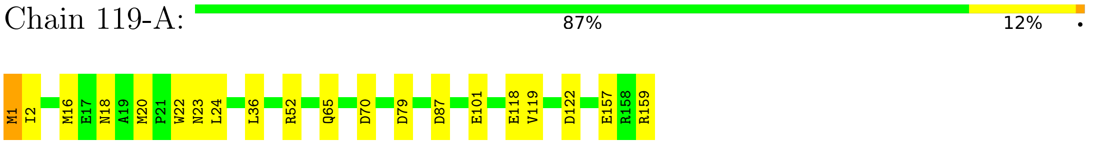
- Molecule 1: Dihydrofolate reductase

Chain 118-A:



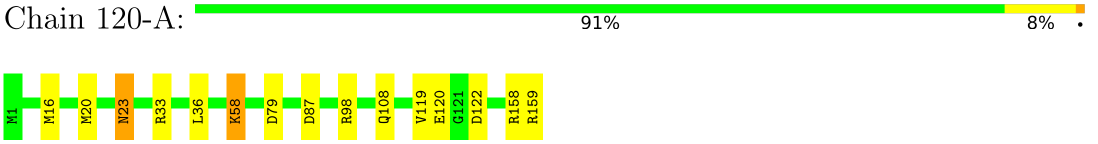
- Molecule 1: Dihydrofolate reductase

Chain 119-A:



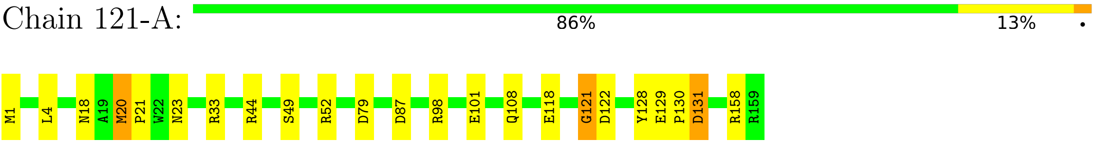
- Molecule 1: Dihydrofolate reductase

Chain 120-A:



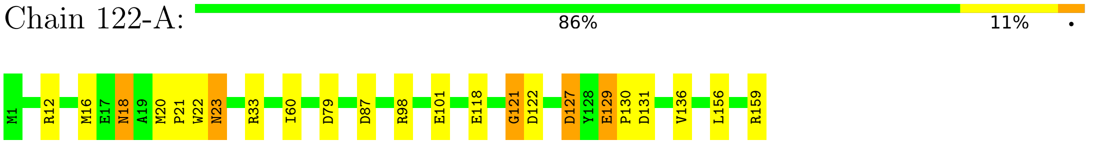
- Molecule 1: Dihydrofolate reductase

Chain 121-A:



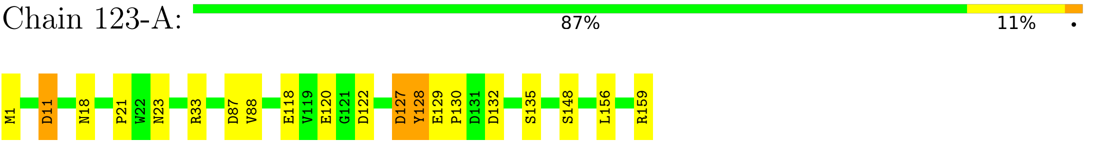
- Molecule 1: Dihydrofolate reductase

Chain 122-A:



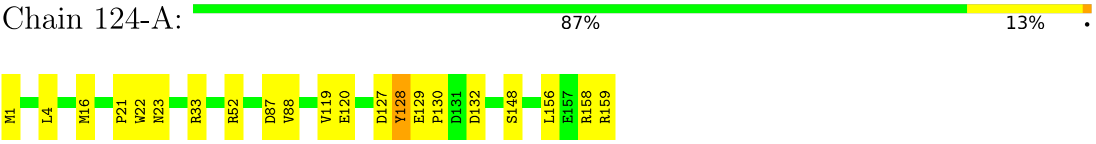
- Molecule 1: Dihydrofolate reductase

Chain 123-A:



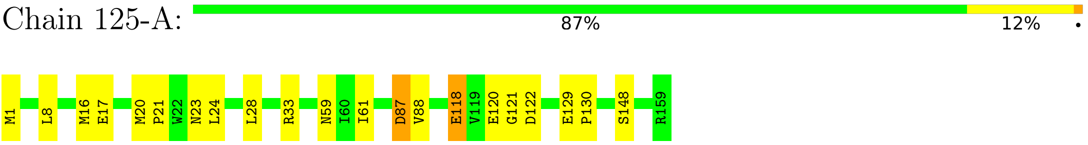
- Molecule 1: Dihydrofolate reductase

Chain 124-A:



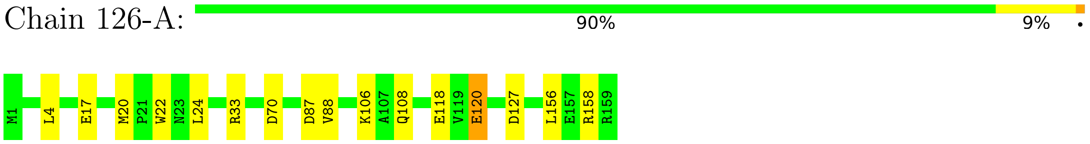
- Molecule 1: Dihydrofolate reductase

Chain 125-A:



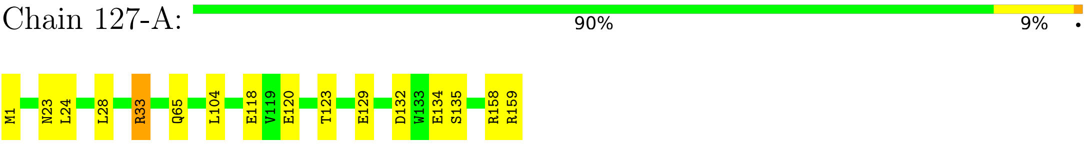
- Molecule 1: Dihydrofolate reductase

Chain 126-A:



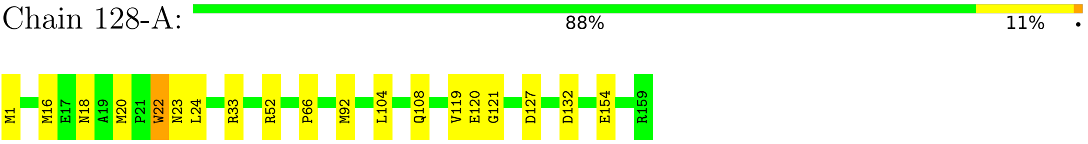
- Molecule 1: Dihydrofolate reductase

Chain 127-A:



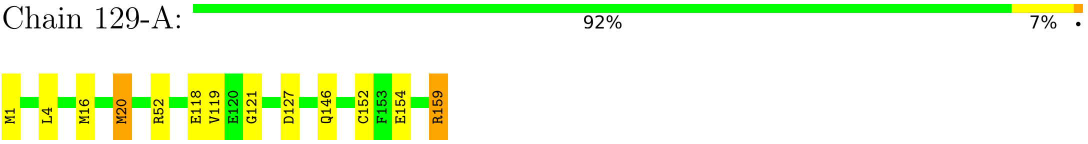
- Molecule 1: Dihydrofolate reductase

Chain 128-A:



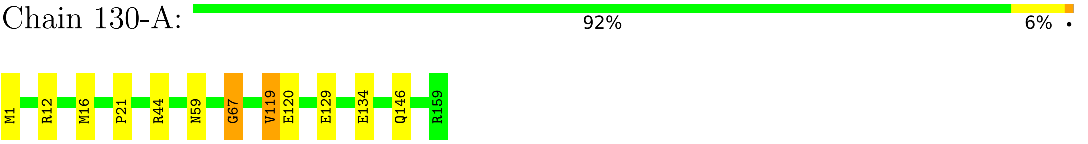
- Molecule 1: Dihydrofolate reductase

Chain 129-A:



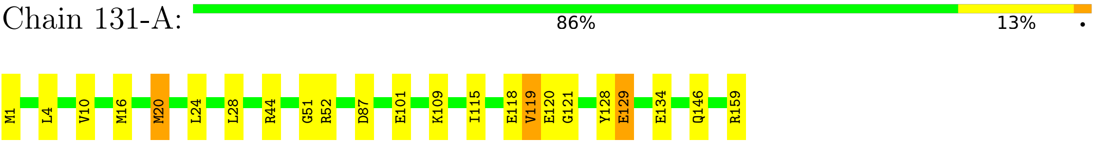
- Molecule 1: Dihydrofolate reductase

Chain 130-A:



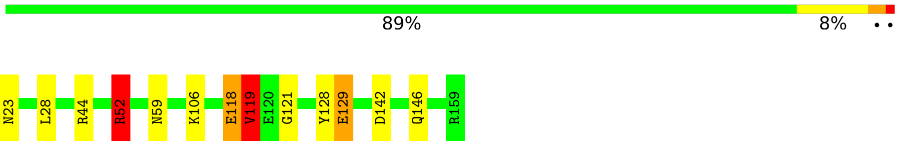
- Molecule 1: Dihydrofolate reductase

Chain 131-A:



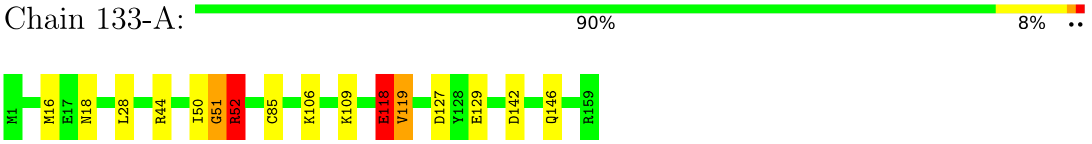
- Molecule 1: Dihydrofolate reductase

Chain 132-A:



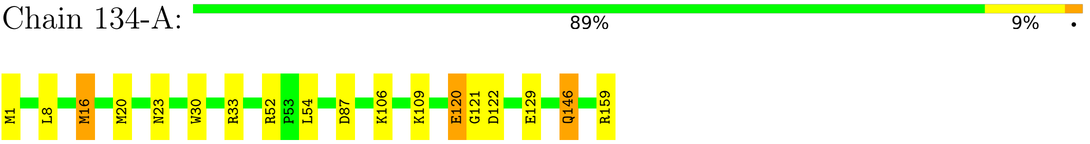
- Molecule 1: Dihydrofolate reductase

Chain 133-A:



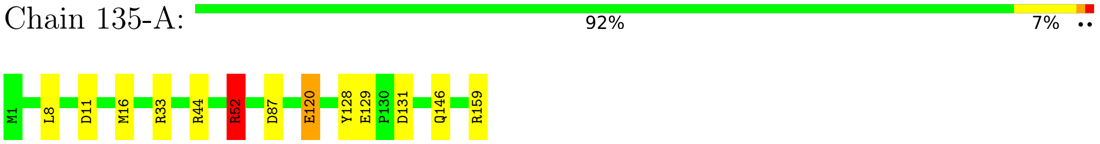
- Molecule 1: Dihydrofolate reductase

Chain 134-A:



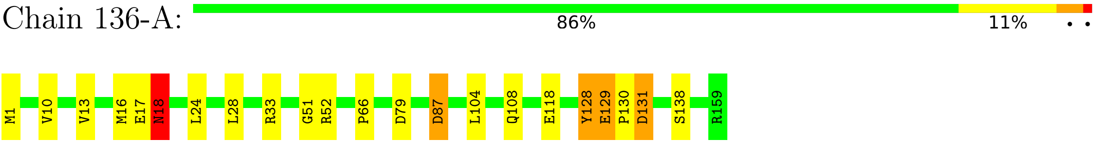
- Molecule 1: Dihydrofolate reductase

Chain 135-A:



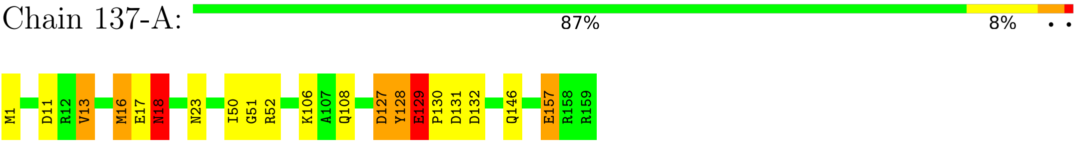
- Molecule 1: Dihydrofolate reductase

Chain 136-A:



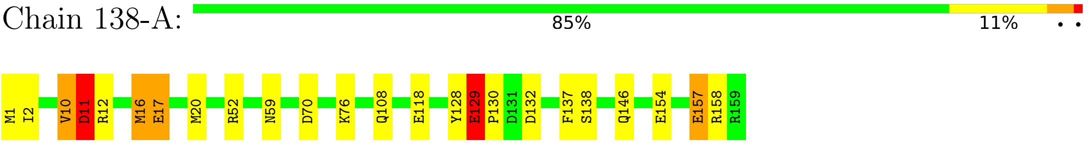
- Molecule 1: Dihydrofolate reductase

Chain 137-A:



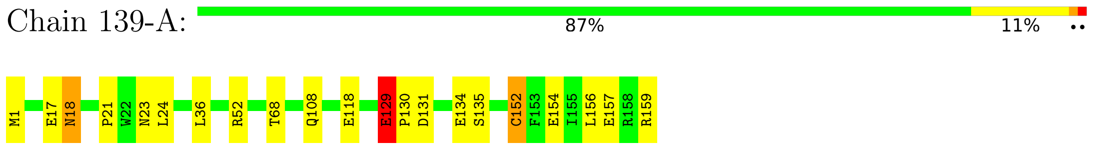
- Molecule 1: Dihydrofolate reductase

Chain 138-A:



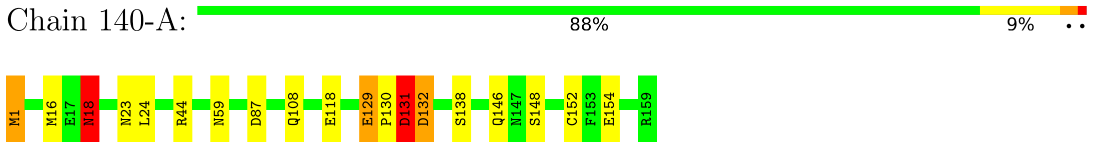
- Molecule 1: Dihydrofolate reductase

Chain 139-A:



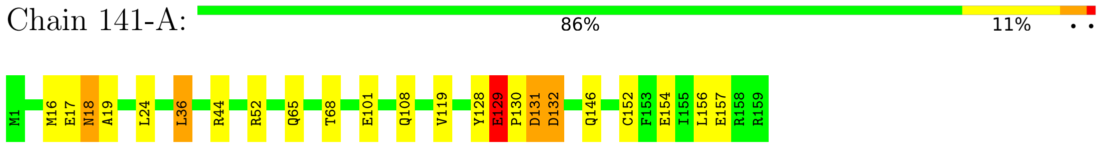
- Molecule 1: Dihydrofolate reductase

Chain 140-A:



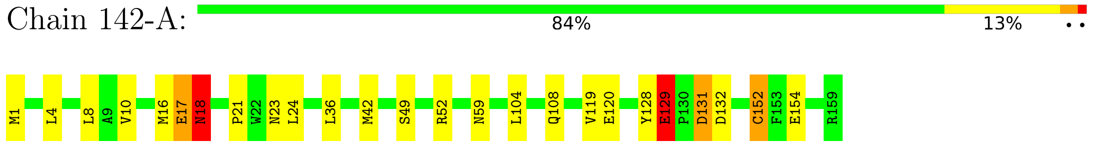
- Molecule 1: Dihydrofolate reductase

Chain 141-A:



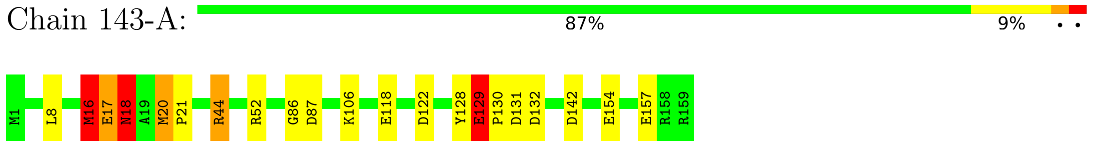
- Molecule 1: Dihydrofolate reductase

Chain 142-A:



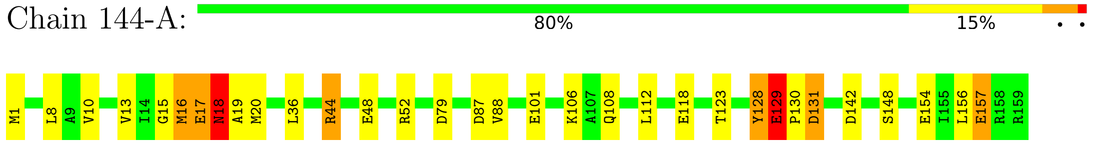
- Molecule 1: Dihydrofolate reductase

Chain 143-A:



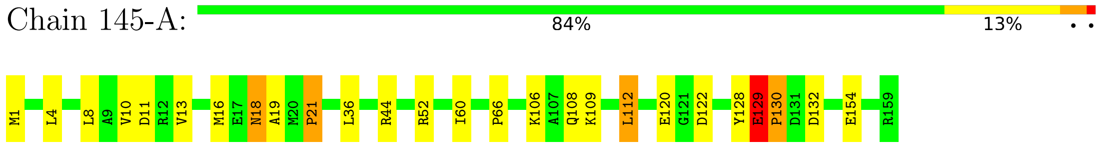
- Molecule 1: Dihydrofolate reductase

Chain 144-A:



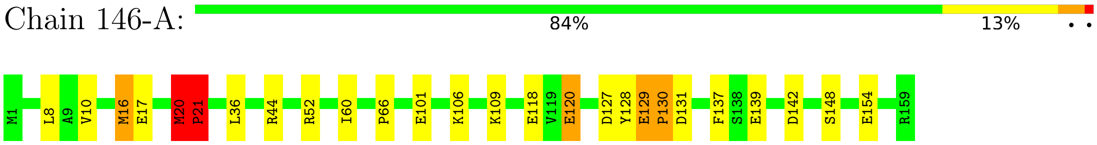
- Molecule 1: Dihydrofolate reductase

Chain 145-A:



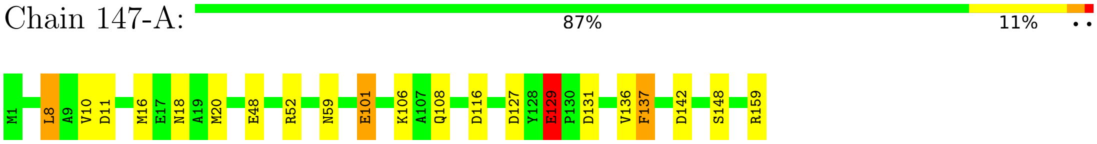
- Molecule 1: Dihydrofolate reductase

Chain 146-A:



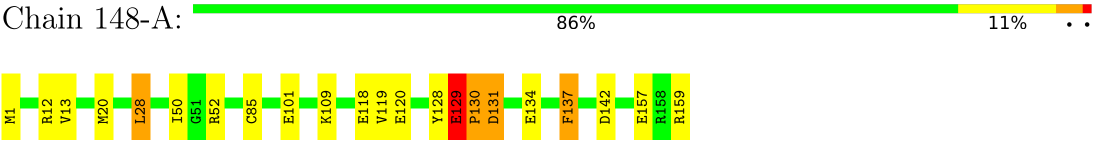
- Molecule 1: Dihydrofolate reductase

Chain 147-A:



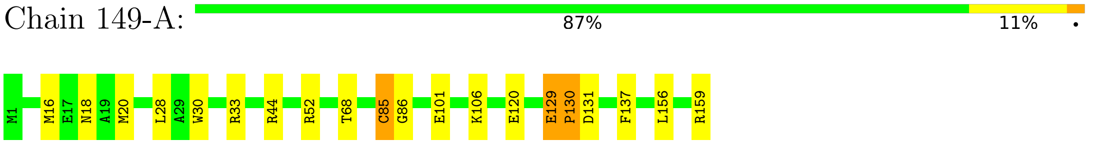
- Molecule 1: Dihydrofolate reductase

Chain 148-A:



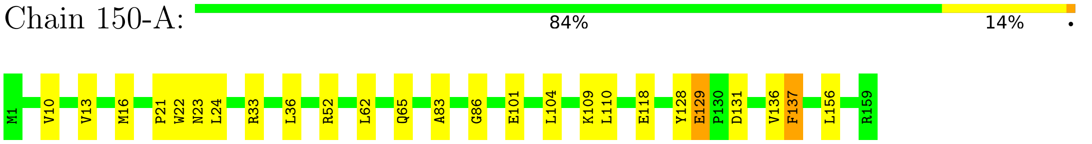
- Molecule 1: Dihydrofolate reductase

Chain 149-A:



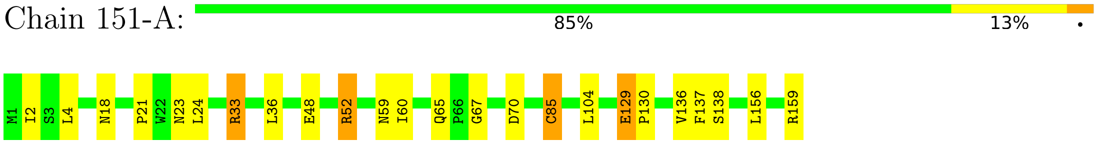
- Molecule 1: Dihydrofolate reductase

Chain 150-A:



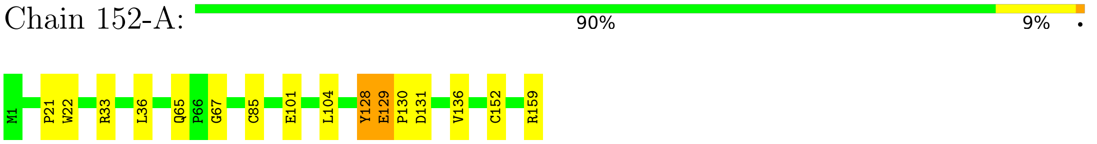
- Molecule 1: Dihydrofolate reductase

Chain 151-A:



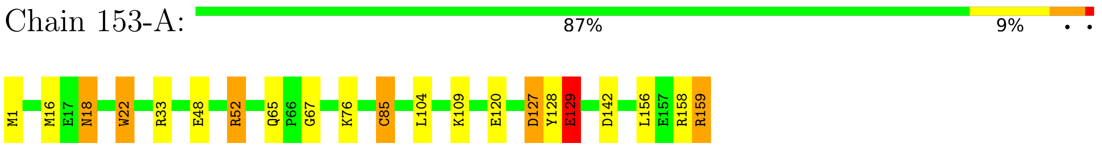
- Molecule 1: Dihydrofolate reductase

Chain 152-A:



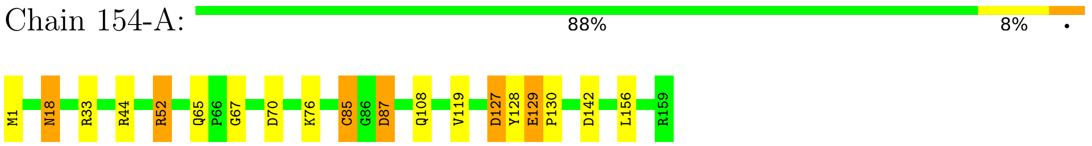
- Molecule 1: Dihydrofolate reductase

Chain 153-A:



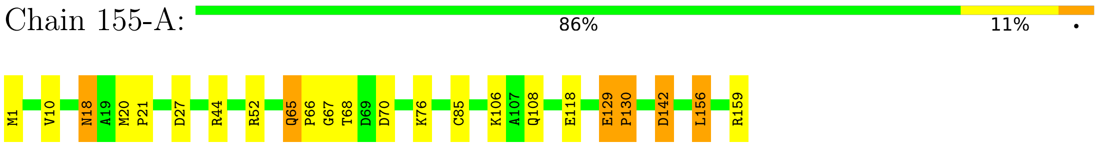
- Molecule 1: Dihydrofolate reductase

Chain 154-A:



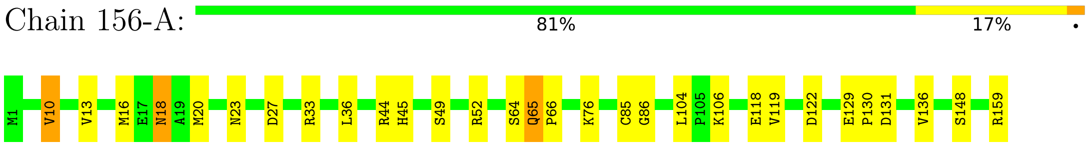
- Molecule 1: Dihydrofolate reductase

Chain 155-A:



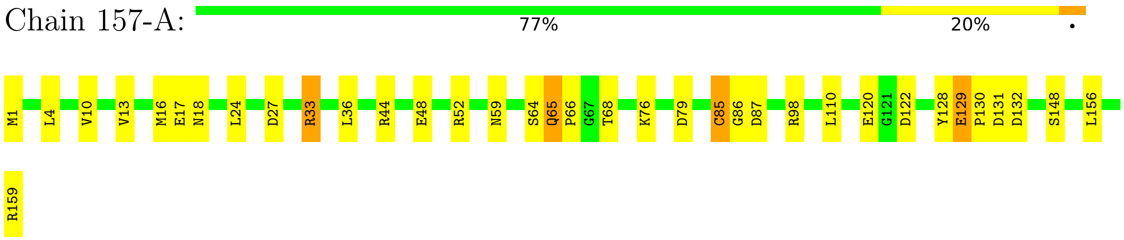
- Molecule 1: Dihydrofolate reductase

Chain 156-A:



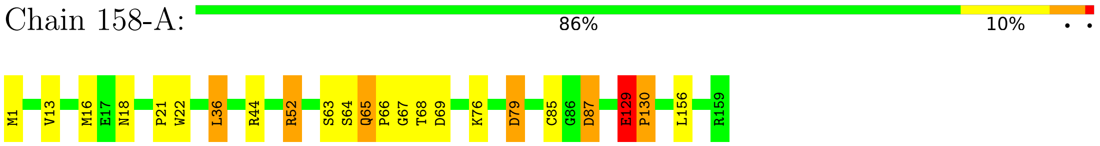
- Molecule 1: Dihydrofolate reductase

Chain 157-A:



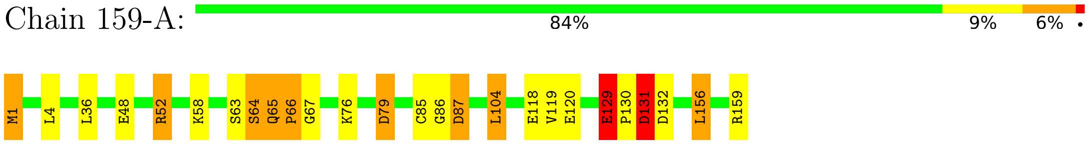
- Molecule 1: Dihydrofolate reductase

Chain 158-A:



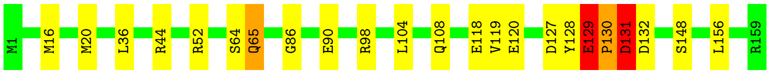
- Molecule 1: Dihydrofolate reductase

Chain 159-A:



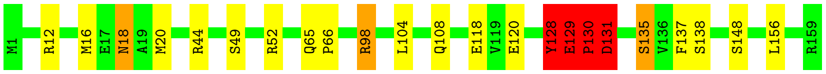
- Molecule 1: Dihydrofolate reductase

Chain 160-A:



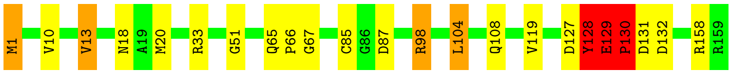
- Molecule 1: Dihydrofolate reductase

Chain 161-A:



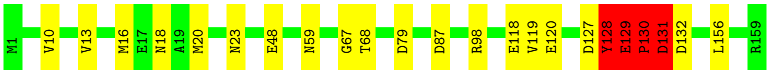
- Molecule 1: Dihydrofolate reductase

Chain 162-A:



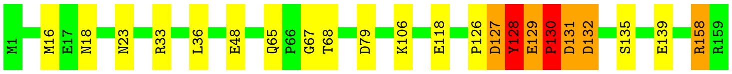
- Molecule 1: Dihydrofolate reductase

Chain 163-A:



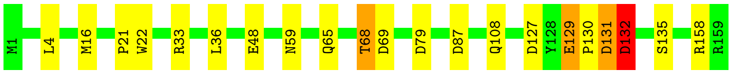
- Molecule 1: Dihydrofolate reductase

Chain 164-A:



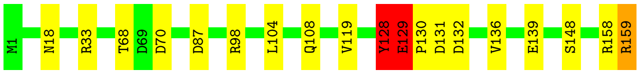
- Molecule 1: Dihydrofolate reductase

Chain 165-A:



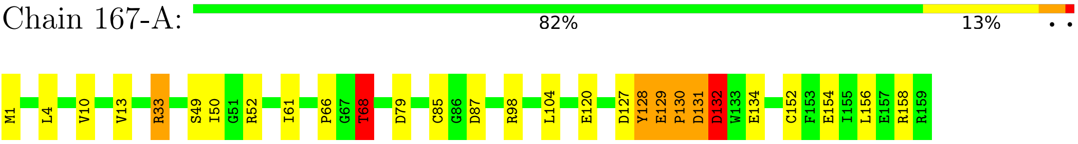
- Molecule 1: Dihydrofolate reductase

Chain 166-A:



- Molecule 1: Dihydrofolate reductase

Chain 167-A:


82%
13%
• •
M1
L4
V10
V13
R33
S49
I50
G51
R52
I61
P66
G67
I68
D79
C85
G86
D87
R98
L104
E120
D127
Y128
E129
P130
D131
D132
W133
E134
C152
F153
E154
I155
L156
E157
R158
R159

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.49, < L^2 > = 0.32$	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.*

---

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NAP, FOL, CA

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	157/159 (99%)	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	126-A	24	LEU
1	156-A	76	LYS
1	131-A	20	MET
1	125-A	148	SER
1	143-A	44	ARG

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FOL	16-A	201	-	34,34,34	1.08	4 (11%)	44,47,47	1.98	7 (15%)
4	NAP	138-A	204	-	45,52,52	1.76	10 (22%)	56,80,80	1.42	10 (17%)
2	FOL	24-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	2.12	13 (29%)
2	FOL	58-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	2.36	15 (34%)
2	FOL	143-A	201	-	34,34,34	1.14	3 (8%)	44,47,47	1.93	9 (20%)
4	NAP	63-A	204	-	45,52,52	1.75	9 (20%)	56,80,80	1.35	9 (16%)
2	FOL	32-A	201	-	34,34,34	1.08	4 (11%)	44,47,47	1.77	9 (20%)
2	FOL	63-A	201	-	34,34,34	1.15	3 (8%)	44,47,47	2.21	12 (27%)
4	NAP	80-A	204	-	45,52,52	1.83	10 (22%)	56,80,80	1.31	8 (14%)
2	FOL	132-A	201	-	34,34,34	1.29	5 (14%)	44,47,47	2.06	10 (22%)
4	NAP	117-A	204	-	45,52,52	1.81	11 (24%)	56,80,80	1.56	10 (17%)
4	NAP	107-A	204	-	45,52,52	1.86	10 (22%)	56,80,80	1.33	8 (14%)
2	FOL	51-A	201	-	34,34,34	1.16	3 (8%)	44,47,47	1.78	7 (15%)
4	NAP	46-A	204	-	45,52,52	1.77	10 (22%)	56,80,80	1.35	9 (16%)
4	NAP	59-A	204	-	45,52,52	1.70	9 (20%)	56,80,80	1.30	5 (8%)
2	FOL	37-A	201	-	34,34,34	1.23	4 (11%)	44,47,47	2.16	12 (27%)
2	FOL	18-A	201	-	34,34,34	1.08	3 (8%)	44,47,47	2.16	12 (27%)
2	FOL	153-A	201	-	34,34,34	1.07	3 (8%)	44,47,47	2.00	10 (22%)
2	FOL	34-A	201	-	34,34,34	1.08	3 (8%)	44,47,47	2.12	13 (29%)
2	FOL	28-A	201	-	34,34,34	1.25	3 (8%)	44,47,47	1.81	8 (18%)
4	NAP	64-A	204	-	45,52,52	1.82	10 (22%)	56,80,80	1.43	9 (16%)
4	NAP	92-A	204	-	45,52,52	1.77	10 (22%)	56,80,80	1.34	8 (14%)
2	FOL	47-A	201	-	34,34,34	1.20	4 (11%)	44,47,47	2.05	10 (22%)
4	NAP	17-A	204	-	45,52,52	1.83	9 (20%)	56,80,80	1.36	10 (17%)
4	NAP	30-A	204	-	45,52,52	1.89	9 (20%)	56,80,80	1.30	8 (14%)
2	FOL	45-A	201	-	34,34,34	1.14	3 (8%)	44,47,47	1.92	8 (18%)
4	NAP	61-A	204	-	45,52,52	1.80	11 (24%)	56,80,80	1.33	9 (16%)
2	FOL	11-A	201	-	34,34,34	1.04	3 (8%)	44,47,47	1.99	10 (22%)
2	FOL	149-A	201	-	34,34,34	1.05	3 (8%)	44,47,47	2.13	8 (18%)
4	NAP	89-A	204	-	45,52,52	1.77	10 (22%)	56,80,80	1.36	7 (12%)
2	FOL	92-A	201	-	34,34,34	1.22	4 (11%)	44,47,47	2.08	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	FOL	111-A	201	-	34,34,34	1.25	4 (11%)	44,47,47	1.92	11 (25%)
4	NAP	86-A	204	-	45,52,52	1.76	11 (24%)	56,80,80	1.30	10 (17%)
4	NAP	130-A	204	-	45,52,52	1.76	9 (20%)	56,80,80	1.45	10 (17%)
2	FOL	65-A	201	-	34,34,34	1.38	5 (14%)	44,47,47	2.04	13 (29%)
4	NAP	143-A	204	-	45,52,52	1.81	11 (24%)	56,80,80	1.28	9 (16%)
4	NAP	158-A	204	-	45,52,52	1.64	9 (20%)	56,80,80	1.37	5 (8%)
4	NAP	114-A	204	-	45,52,52	1.83	10 (22%)	56,80,80	1.32	9 (16%)
4	NAP	148-A	204	-	45,52,52	1.79	10 (22%)	56,80,80	1.42	10 (17%)
2	FOL	126-A	201	-	34,34,34	1.42	6 (17%)	44,47,47	2.77	16 (36%)
4	NAP	10-A	204	-	45,52,52	1.82	9 (20%)	56,80,80	1.33	9 (16%)
4	NAP	83-A	204	-	45,52,52	1.71	11 (24%)	56,80,80	1.36	6 (10%)
2	FOL	128-A	201	-	34,34,34	1.08	2 (5%)	44,47,47	2.28	12 (27%)
2	FOL	124-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	2.00	12 (27%)
2	FOL	19-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	1.81	9 (20%)
4	NAP	81-A	204	-	45,52,52	1.76	10 (22%)	56,80,80	1.46	6 (10%)
2	FOL	166-A	201	-	34,34,34	1.23	3 (8%)	44,47,47	1.56	5 (11%)
2	FOL	131-A	201	-	34,34,34	1.10	2 (5%)	44,47,47	2.07	10 (22%)
4	NAP	34-A	204	-	45,52,52	1.67	10 (22%)	56,80,80	1.15	6 (10%)
2	FOL	14-A	201	-	34,34,34	1.23	4 (11%)	44,47,47	2.47	14 (31%)
4	NAP	41-A	204	-	45,52,52	1.87	11 (24%)	56,80,80	1.37	9 (16%)
2	FOL	39-A	201	-	34,34,34	1.19	4 (11%)	44,47,47	2.19	13 (29%)
2	FOL	136-A	201	-	34,34,34	1.09	3 (8%)	44,47,47	2.09	14 (31%)
2	FOL	103-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	1.90	9 (20%)
4	NAP	120-A	204	-	45,52,52	1.80	10 (22%)	56,80,80	1.31	7 (12%)
4	NAP	18-A	204	-	45,52,52	1.85	10 (22%)	56,80,80	1.48	10 (17%)
2	FOL	60-A	201	-	34,34,34	1.22	4 (11%)	44,47,47	2.03	12 (27%)
4	NAP	78-A	204	-	45,52,52	1.78	11 (24%)	56,80,80	1.36	7 (12%)
4	NAP	106-A	204	-	45,52,52	1.90	9 (20%)	56,80,80	1.27	9 (16%)
2	FOL	64-A	201	-	34,34,34	1.11	3 (8%)	44,47,47	1.95	11 (25%)
4	NAP	14-A	204	-	45,52,52	1.80	10 (22%)	56,80,80	1.37	10 (17%)
2	FOL	107-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	1.95	9 (20%)
4	NAP	98-A	204	-	45,52,52	1.83	9 (20%)	56,80,80	1.30	9 (16%)
4	NAP	8-A	204	-	45,52,52	1.72	11 (24%)	56,80,80	1.32	6 (10%)
4	NAP	133-A	204	-	45,52,52	1.72	10 (22%)	56,80,80	1.31	5 (8%)
4	NAP	28-A	204	-	45,52,52	1.84	10 (22%)	56,80,80	1.34	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
4	NAP	137-A	204	-	45,52,52	1.79	10 (22%)	56,80,80	1.33	8 (14%)
2	FOL	109-A	201	-	34,34,34	1.16	4 (11%)	44,47,47	1.98	9 (20%)
4	NAP	88-A	204	-	45,52,52	1.76	11 (24%)	56,80,80	1.39	9 (16%)
4	NAP	19-A	204	-	45,52,52	1.86	10 (22%)	56,80,80	1.36	9 (16%)
4	NAP	53-A	204	-	45,52,52	1.83	9 (20%)	56,80,80	1.30	8 (14%)
2	FOL	114-A	201	-	34,34,34	1.18	4 (11%)	44,47,47	1.91	8 (18%)
4	NAP	139-A	204	-	45,52,52	1.76	10 (22%)	56,80,80	1.43	11 (19%)
4	NAP	111-A	204	-	45,52,52	1.83	11 (24%)	56,80,80	1.34	9 (16%)
2	FOL	20-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	1.70	6 (13%)
2	FOL	123-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	1.80	6 (13%)
4	NAP	157-A	204	-	45,52,52	1.69	9 (20%)	56,80,80	1.22	5 (8%)
2	FOL	2-A	201	-	34,34,34	1.16	3 (8%)	44,47,47	1.79	7 (15%)
2	FOL	119-A	201	-	34,34,34	1.17	3 (8%)	44,47,47	1.90	8 (18%)
4	NAP	153-A	204	-	45,52,52	1.76	11 (24%)	56,80,80	1.28	7 (12%)
4	NAP	29-A	204	-	45,52,52	1.83	11 (24%)	56,80,80	1.33	7 (12%)
2	FOL	68-A	201	-	34,34,34	1.21	4 (11%)	44,47,47	1.87	9 (20%)
2	FOL	127-A	201	-	34,34,34	1.14	2 (5%)	44,47,47	2.17	12 (27%)
4	NAP	13-A	204	-	45,52,52	1.79	10 (22%)	56,80,80	1.30	10 (17%)
4	NAP	9-A	204	-	45,52,52	1.73	11 (24%)	56,80,80	1.23	7 (12%)
2	FOL	155-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	1.95	12 (27%)
2	FOL	154-A	201	-	34,34,34	1.15	3 (8%)	44,47,47	1.87	7 (15%)
2	FOL	157-A	201	-	34,34,34	1.05	3 (8%)	44,47,47	1.70	8 (18%)
4	NAP	49-A	204	-	45,52,52	1.84	10 (22%)	56,80,80	1.53	11 (19%)
2	FOL	138-A	201	-	34,34,34	1.07	2 (5%)	44,47,47	2.23	12 (27%)
4	NAP	103-A	204	-	45,52,52	1.90	10 (22%)	56,80,80	1.36	7 (12%)
2	FOL	113-A	201	-	34,34,34	1.17	3 (8%)	44,47,47	1.99	13 (29%)
4	NAP	73-A	204	-	45,52,52	1.81	13 (28%)	56,80,80	1.45	11 (19%)
2	FOL	94-A	201	-	34,34,34	1.18	3 (8%)	44,47,47	1.96	12 (27%)
2	FOL	12-A	201	-	34,34,34	1.23	4 (11%)	44,47,47	1.85	7 (15%)
2	FOL	86-A	201	-	34,34,34	1.12	4 (11%)	44,47,47	1.92	9 (20%)
4	NAP	71-A	204	-	45,52,52	1.83	11 (24%)	56,80,80	1.31	10 (17%)
2	FOL	25-A	201	-	34,34,34	1.17	3 (8%)	44,47,47	2.27	13 (29%)
4	NAP	167-A	204	-	45,52,52	1.81	10 (22%)	56,80,80	1.32	9 (16%)
2	FOL	162-A	201	-	34,34,34	1.16	3 (8%)	44,47,47	1.69	7 (15%)
2	FOL	133-A	201	-	34,34,34	1.11	3 (8%)	44,47,47	2.20	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	FOL	22-A	201	-	34,34,34	1.12	3 (8%)	44,47,47	1.99	9 (20%)
2	FOL	48-A	201	-	34,34,34	1.18	3 (8%)	44,47,47	2.52	17 (38%)
4	NAP	25-A	204	-	45,52,52	1.88	10 (22%)	56,80,80	1.39	8 (14%)
4	NAP	6-A	204	-	45,52,52	1.73	10 (22%)	56,80,80	1.28	6 (10%)
2	FOL	104-A	201	-	34,34,34	1.05	2 (5%)	44,47,47	2.02	7 (15%)
2	FOL	118-A	201	-	34,34,34	1.22	3 (8%)	44,47,47	2.05	15 (34%)
2	FOL	75-A	201	-	34,34,34	1.05	3 (8%)	44,47,47	2.02	8 (18%)
4	NAP	1-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.32	10 (17%)
2	FOL	55-A	201	-	34,34,34	1.08	3 (8%)	44,47,47	1.89	9 (20%)
4	NAP	164-A	204	-	45,52,52	1.74	11 (24%)	56,80,80	1.37	10 (17%)
2	FOL	3-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	1.91	8 (18%)
2	FOL	108-A	201	-	34,34,34	1.06	3 (8%)	44,47,47	1.99	11 (25%)
2	FOL	106-A	201	-	34,34,34	1.17	2 (5%)	44,47,47	2.40	13 (29%)
4	NAP	33-A	204	-	45,52,52	1.88	11 (24%)	56,80,80	1.43	10 (17%)
4	NAP	2-A	204	-	45,52,52	1.76	9 (20%)	56,80,80	1.36	10 (17%)
4	NAP	91-A	204	-	45,52,52	1.76	10 (22%)	56,80,80	1.32	9 (16%)
2	FOL	29-A	201	-	34,34,34	1.08	2 (5%)	44,47,47	2.00	10 (22%)
2	FOL	80-A	201	-	34,34,34	1.27	4 (11%)	44,47,47	2.18	15 (34%)
4	NAP	90-A	204	-	45,52,52	1.74	11 (24%)	56,80,80	1.44	10 (17%)
2	FOL	165-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	1.94	11 (25%)
2	FOL	52-A	201	-	34,34,34	1.29	4 (11%)	44,47,47	2.19	13 (29%)
2	FOL	13-A	201	-	34,34,34	1.30	5 (14%)	44,47,47	2.60	16 (36%)
2	FOL	137-A	201	-	34,34,34	1.21	3 (8%)	44,47,47	1.82	8 (18%)
2	FOL	91-A	201	-	34,34,34	1.03	2 (5%)	44,47,47	1.96	9 (20%)
2	FOL	41-A	201	-	34,34,34	1.19	4 (11%)	44,47,47	2.15	9 (20%)
4	NAP	118-A	204	-	45,52,52	1.79	9 (20%)	56,80,80	2.13	9 (16%)
2	FOL	59-A	201	-	34,34,34	1.23	3 (8%)	44,47,47	2.02	10 (22%)
2	FOL	167-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	2.16	14 (31%)
2	FOL	44-A	201	-	34,34,34	1.21	3 (8%)	44,47,47	1.94	9 (20%)
2	FOL	27-A	201	-	34,34,34	1.23	3 (8%)	44,47,47	1.89	7 (15%)
2	FOL	99-A	201	-	34,34,34	1.11	3 (8%)	44,47,47	2.05	11 (25%)
4	NAP	100-A	204	-	45,52,52	1.86	9 (20%)	56,80,80	1.34	9 (16%)
2	FOL	145-A	201	-	34,34,34	1.03	4 (11%)	44,47,47	1.81	7 (15%)
4	NAP	102-A	204	-	45,52,52	1.87	10 (22%)	56,80,80	1.34	9 (16%)
4	NAP	39-A	204	-	45,52,52	1.89	10 (22%)	56,80,80	1.35	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
2	FOL	43-A	201	-	34,34,34	1.12	4 (11%)	44,47,47	2.27	12 (27%)
4	NAP	135-A	204	-	45,52,52	1.79	9 (20%)	56,80,80	1.42	11 (19%)
4	NAP	121-A	204	-	45,52,52	1.73	9 (20%)	56,80,80	1.30	8 (14%)
2	FOL	17-A	201	-	34,34,34	1.14	3 (8%)	44,47,47	1.73	6 (13%)
2	FOL	57-A	201	-	34,34,34	1.36	5 (14%)	44,47,47	2.22	18 (40%)
2	FOL	144-A	201	-	34,34,34	1.14	4 (11%)	44,47,47	2.22	15 (34%)
4	NAP	96-A	204	-	45,52,52	1.82	10 (22%)	56,80,80	1.28	7 (12%)
4	NAP	57-A	204	-	45,52,52	1.69	11 (24%)	56,80,80	2.14	4 (7%)
4	NAP	131-A	204	-	45,52,52	1.69	9 (20%)	56,80,80	1.20	5 (8%)
4	NAP	4-A	204	-	45,52,52	1.79	10 (22%)	56,80,80	1.35	9 (16%)
2	FOL	23-A	201	-	34,34,34	1.07	4 (11%)	44,47,47	1.99	10 (22%)
4	NAP	27-A	204	-	45,52,52	1.84	10 (22%)	56,80,80	1.34	8 (14%)
4	NAP	108-A	204	-	45,52,52	1.79	11 (24%)	56,80,80	1.53	7 (12%)
2	FOL	102-A	201	-	34,34,34	0.99	2 (5%)	44,47,47	1.90	8 (18%)
4	NAP	136-A	204	-	45,52,52	1.78	8 (17%)	56,80,80	1.30	9 (16%)
2	FOL	164-A	201	-	34,34,34	1.14	3 (8%)	44,47,47	1.84	8 (18%)
2	FOL	98-A	201	-	34,34,34	1.15	3 (8%)	44,47,47	2.03	9 (20%)
2	FOL	134-A	201	-	34,34,34	1.19	3 (8%)	44,47,47	2.23	15 (34%)
4	NAP	15-A	204	-	45,52,52	1.78	9 (20%)	56,80,80	1.44	11 (19%)
4	NAP	115-A	204	-	45,52,52	1.93	13 (28%)	56,80,80	1.56	11 (19%)
2	FOL	158-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	1.83	13 (29%)
4	NAP	50-A	204	-	45,52,52	1.86	11 (24%)	56,80,80	1.29	8 (14%)
4	NAP	129-A	204	-	45,52,52	1.78	9 (20%)	56,80,80	1.37	7 (12%)
4	NAP	62-A	204	-	45,52,52	1.84	12 (26%)	56,80,80	1.45	10 (17%)
4	NAP	94-A	204	-	45,52,52	1.80	11 (24%)	56,80,80	1.31	8 (14%)
4	NAP	134-A	204	-	45,52,52	1.64	8 (17%)	56,80,80	1.17	7 (12%)
2	FOL	54-A	201	-	34,34,34	1.05	3 (8%)	44,47,47	1.94	10 (22%)
2	FOL	56-A	201	-	34,34,34	1.17	4 (11%)	44,47,47	2.12	13 (29%)
2	FOL	6-A	201	-	34,34,34	1.34	4 (11%)	44,47,47	2.03	12 (27%)
4	NAP	144-A	204	-	45,52,52	1.79	9 (20%)	56,80,80	1.31	9 (16%)
4	NAP	79-A	204	-	45,52,52	1.84	11 (24%)	56,80,80	1.37	7 (12%)
4	NAP	48-A	204	-	45,52,52	1.83	9 (20%)	56,80,80	1.27	7 (12%)
4	NAP	84-A	204	-	45,52,52	1.72	9 (20%)	56,80,80	1.15	5 (8%)
2	FOL	4-A	201	-	34,34,34	1.19	4 (11%)	44,47,47	2.01	11 (25%)
4	NAP	109-A	204	-	45,52,52	1.75	11 (24%)	56,80,80	1.33	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAP	147-A	204	-	45,52,52	1.86	13 (28%)	56,80,80	1.37	9 (16%)
2	FOL	81-A	201	-	34,34,34	1.10	4 (11%)	44,47,47	2.16	11 (25%)
4	NAP	52-A	204	-	45,52,52	1.85	9 (20%)	56,80,80	1.38	6 (10%)
4	NAP	16-A	204	-	45,52,52	1.84	10 (22%)	56,80,80	1.29	9 (16%)
4	NAP	31-A	204	-	45,52,52	1.83	11 (24%)	56,80,80	1.25	6 (10%)
2	FOL	139-A	201	-	34,34,34	1.16	3 (8%)	44,47,47	2.32	12 (27%)
2	FOL	88-A	201	-	34,34,34	1.01	2 (5%)	44,47,47	1.92	8 (18%)
4	NAP	20-A	204	-	45,52,52	1.84	9 (20%)	56,80,80	1.31	8 (14%)
2	FOL	21-A	201	-	34,34,34	1.32	3 (8%)	44,47,47	2.14	13 (29%)
4	NAP	67-A	204	-	45,52,52	1.81	9 (20%)	56,80,80	1.32	8 (14%)
2	FOL	116-A	201	-	34,34,34	1.06	4 (11%)	44,47,47	1.90	8 (18%)
2	FOL	78-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	2.08	10 (22%)
2	FOL	146-A	201	-	34,34,34	1.09	3 (8%)	44,47,47	1.71	6 (13%)
4	NAP	127-A	204	-	45,52,52	1.75	9 (20%)	56,80,80	1.41	8 (14%)
2	FOL	125-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	2.03	10 (22%)
4	NAP	132-A	204	-	45,52,52	1.61	8 (17%)	56,80,80	1.22	4 (7%)
2	FOL	8-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	1.91	7 (15%)
4	NAP	43-A	204	-	45,52,52	1.80	9 (20%)	56,80,80	1.32	10 (17%)
4	NAP	51-A	204	-	45,52,52	1.85	11 (24%)	56,80,80	1.28	9 (16%)
4	NAP	156-A	204	-	45,52,52	1.77	9 (20%)	56,80,80	1.32	10 (17%)
4	NAP	101-A	204	-	45,52,52	1.83	11 (24%)	56,80,80	1.46	9 (16%)
2	FOL	160-A	201	-	34,34,34	1.23	3 (8%)	44,47,47	1.86	10 (22%)
2	FOL	101-A	201	-	34,34,34	1.10	4 (11%)	44,47,47	1.82	9 (20%)
4	NAP	87-A	204	-	45,52,52	1.78	9 (20%)	56,80,80	1.28	8 (14%)
4	NAP	151-A	204	-	45,52,52	1.73	10 (22%)	56,80,80	1.36	10 (17%)
2	FOL	151-A	201	-	34,34,34	1.15	3 (8%)	44,47,47	1.91	10 (22%)
2	FOL	53-A	201	-	34,34,34	1.31	3 (8%)	44,47,47	1.99	10 (22%)
4	NAP	72-A	204	-	45,52,52	1.84	11 (24%)	56,80,80	1.36	10 (17%)
2	FOL	130-A	201	-	34,34,34	1.12	3 (8%)	44,47,47	1.84	7 (15%)
4	NAP	32-A	204	-	45,52,52	1.74	11 (24%)	56,80,80	1.25	5 (8%)
4	NAP	110-A	204	-	45,52,52	1.86	10 (22%)	56,80,80	1.31	9 (16%)
4	NAP	5-A	204	-	45,52,52	1.76	10 (22%)	56,80,80	1.43	10 (17%)
4	NAP	113-A	204	-	45,52,52	1.84	9 (20%)	56,80,80	1.31	10 (17%)
2	FOL	110-A	201	-	34,34,34	1.07	3 (8%)	44,47,47	2.38	13 (29%)
4	NAP	99-A	204	-	45,52,52	1.88	10 (22%)	56,80,80	1.44	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|*Z*| > 2	Counts	RMSZ	#|*Z*| > 2
4	NAP	152-A	204	-	45,52,52	1.71	7 (15%)	56,80,80	1.26	7 (12%)
4	NAP	69-A	204	-	45,52,52	1.87	9 (20%)	56,80,80	1.27	8 (14%)
2	FOL	69-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	2.02	10 (22%)
2	FOL	142-A	201	-	34,34,34	1.01	2 (5%)	44,47,47	2.00	10 (22%)
4	NAP	47-A	204	-	45,52,52	1.84	10 (22%)	56,80,80	1.28	9 (16%)
4	NAP	146-A	204	-	45,52,52	1.82	10 (22%)	56,80,80	1.30	9 (16%)
4	NAP	142-A	204	-	45,52,52	1.76	11 (24%)	56,80,80	1.44	11 (19%)
2	FOL	140-A	201	-	34,34,34	0.99	2 (5%)	44,47,47	2.16	9 (20%)
4	NAP	112-A	204	-	45,52,52	1.83	9 (20%)	56,80,80	1.35	9 (16%)
2	FOL	71-A	201	-	34,34,34	1.07	3 (8%)	44,47,47	1.90	9 (20%)
2	FOL	156-A	201	-	34,34,34	1.11	3 (8%)	44,47,47	2.06	9 (20%)
4	NAP	54-A	204	-	45,52,52	1.79	10 (22%)	56,80,80	1.36	6 (10%)
4	NAP	93-A	204	-	45,52,52	1.76	10 (22%)	56,80,80	1.36	9 (16%)
4	NAP	76-A	204	-	45,52,52	1.84	11 (24%)	56,80,80	1.29	8 (14%)
2	FOL	93-A	201	-	34,34,34	1.09	3 (8%)	44,47,47	2.06	13 (29%)
4	NAP	11-A	204	-	45,52,52	1.82	10 (22%)	56,80,80	1.33	8 (14%)
4	NAP	140-A	204	-	45,52,52	1.81	11 (24%)	56,80,80	1.49	9 (16%)
2	FOL	9-A	201	-	34,34,34	1.12	3 (8%)	44,47,47	1.81	10 (22%)
4	NAP	160-A	204	-	45,52,52	1.80	12 (26%)	56,80,80	1.26	9 (16%)
2	FOL	70-A	201	-	34,34,34	1.16	3 (8%)	44,47,47	2.20	11 (25%)
4	NAP	149-A	204	-	45,52,52	1.79	10 (22%)	56,80,80	1.33	8 (14%)
2	FOL	7-A	201	-	34,34,34	1.09	3 (8%)	44,47,47	1.88	10 (22%)
4	NAP	74-A	204	-	45,52,52	1.82	10 (22%)	56,80,80	1.37	7 (12%)
2	FOL	74-A	201	-	34,34,34	1.31	4 (11%)	44,47,47	1.88	10 (22%)
2	FOL	49-A	201	-	34,34,34	1.04	2 (5%)	44,47,47	1.93	8 (18%)
2	FOL	73-A	201	-	34,34,34	1.22	4 (11%)	44,47,47	1.88	7 (15%)
4	NAP	3-A	204	-	45,52,52	1.82	10 (22%)	56,80,80	1.37	8 (14%)
4	NAP	97-A	204	-	45,52,52	1.86	11 (24%)	56,80,80	1.23	9 (16%)
2	FOL	117-A	201	-	34,34,34	1.14	3 (8%)	44,47,47	1.64	7 (15%)
4	NAP	159-A	204	-	45,52,52	1.62	7 (15%)	56,80,80	1.21	7 (12%)
2	FOL	97-A	201	-	34,34,34	1.10	2 (5%)	44,47,47	1.99	9 (20%)
2	FOL	79-A	201	-	34,34,34	1.06	3 (8%)	44,47,47	1.88	9 (20%)
4	NAP	40-A	204	-	45,52,52	1.86	10 (22%)	56,80,80	1.33	10 (17%)
2	FOL	33-A	201	-	34,34,34	1.16	3 (8%)	44,47,47	2.18	11 (25%)
2	FOL	76-A	201	-	34,34,34	1.29	3 (8%)	44,47,47	2.14	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	FOL	5-A	201	-	34,34,34	1.17	3 (8%)	44,47,47	1.96	12 (27%)
2	FOL	163-A	201	-	34,34,34	1.06	3 (8%)	44,47,47	1.94	11 (25%)
4	NAP	124-A	204	-	45,52,52	1.70	9 (20%)	56,80,80	1.35	9 (16%)
2	FOL	1-A	201	-	34,34,34	0.98	3 (8%)	44,47,47	1.89	11 (25%)
2	FOL	89-A	201	-	34,34,34	1.20	3 (8%)	44,47,47	1.87	12 (27%)
2	FOL	141-A	201	-	34,34,34	1.12	3 (8%)	44,47,47	1.93	12 (27%)
4	NAP	36-A	204	-	45,52,52	1.79	11 (24%)	56,80,80	1.31	9 (16%)
4	NAP	145-A	204	-	45,52,52	1.82	9 (20%)	56,80,80	1.35	8 (14%)
2	FOL	121-A	201	-	34,34,34	1.27	3 (8%)	44,47,47	1.78	9 (20%)
2	FOL	30-A	201	-	34,34,34	1.36	3 (8%)	44,47,47	1.97	8 (18%)
2	FOL	40-A	201	-	34,34,34	1.25	4 (11%)	44,47,47	1.92	10 (22%)
4	NAP	95-A	204	-	45,52,52	1.75	10 (22%)	56,80,80	1.35	8 (14%)
4	NAP	38-A	204	-	45,52,52	1.86	11 (24%)	56,80,80	1.39	13 (23%)
4	NAP	122-A	204	-	45,52,52	1.79	11 (24%)	56,80,80	1.31	9 (16%)
2	FOL	36-A	201	-	34,34,34	1.09	3 (8%)	44,47,47	1.79	8 (18%)
4	NAP	116-A	204	-	45,52,52	1.84	10 (22%)	56,80,80	1.36	10 (17%)
2	FOL	148-A	201	-	34,34,34	1.08	2 (5%)	44,47,47	1.96	9 (20%)
4	NAP	66-A	204	-	45,52,52	1.83	10 (22%)	56,80,80	1.26	8 (14%)
4	NAP	126-A	204	-	45,52,52	1.72	10 (22%)	56,80,80	1.26	8 (14%)
4	NAP	128-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.47	8 (14%)
2	FOL	90-A	201	-	34,34,34	1.09	4 (11%)	44,47,47	1.89	10 (22%)
2	FOL	10-A	201	-	34,34,34	1.09	3 (8%)	44,47,47	2.03	10 (22%)
2	FOL	96-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	1.91	8 (18%)
2	FOL	161-A	201	-	34,34,34	0.97	2 (5%)	44,47,47	1.91	9 (20%)
4	NAP	70-A	204	-	45,52,52	1.88	9 (20%)	56,80,80	1.31	9 (16%)
4	NAP	77-A	204	-	45,52,52	1.79	11 (24%)	56,80,80	1.55	8 (14%)
4	NAP	60-A	204	-	45,52,52	1.88	10 (22%)	56,80,80	1.33	9 (16%)
2	FOL	77-A	201	-	34,34,34	1.15	3 (8%)	44,47,47	1.97	8 (18%)
2	FOL	82-A	201	-	34,34,34	1.12	5 (14%)	44,47,47	2.16	12 (27%)
4	NAP	23-A	204	-	45,52,52	1.87	10 (22%)	56,80,80	1.53	10 (17%)
2	FOL	100-A	201	-	34,34,34	1.34	4 (11%)	44,47,47	2.05	12 (27%)
4	NAP	141-A	204	-	45,52,52	1.77	11 (24%)	56,80,80	1.31	8 (14%)
4	NAP	37-A	204	-	45,52,52	1.81	11 (24%)	56,80,80	1.32	8 (14%)
2	FOL	95-A	201	-	34,34,34	1.02	3 (8%)	44,47,47	2.02	11 (25%)
2	FOL	122-A	201	-	34,34,34	1.15	4 (11%)	44,47,47	1.79	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	FOL	31-A	201	-	34,34,34	1.14	3 (8%)	44,47,47	2.08	14 (31%)
4	NAP	55-A	204	-	45,52,52	1.81	11 (24%)	56,80,80	1.34	9 (16%)
2	FOL	159-A	201	-	34,34,34	1.02	1 (2%)	44,47,47	1.93	11 (25%)
2	FOL	62-A	201	-	34,34,34	1.14	3 (8%)	44,47,47	1.96	8 (18%)
2	FOL	66-A	201	-	34,34,34	1.06	3 (8%)	44,47,47	2.08	10 (22%)
4	NAP	58-A	204	-	45,52,52	1.75	10 (22%)	56,80,80	1.21	4 (7%)
2	FOL	135-A	201	-	34,34,34	1.16	3 (8%)	44,47,47	1.81	8 (18%)
2	FOL	61-A	201	-	34,34,34	1.13	3 (8%)	44,47,47	2.02	8 (18%)
2	FOL	15-A	201	-	34,34,34	1.23	3 (8%)	44,47,47	2.14	11 (25%)
2	FOL	84-A	201	-	34,34,34	1.01	2 (5%)	44,47,47	2.08	11 (25%)
4	NAP	85-A	204	-	45,52,52	1.80	10 (22%)	56,80,80	1.24	9 (16%)
4	NAP	65-A	204	-	45,52,52	1.84	11 (24%)	56,80,80	1.31	9 (16%)
4	NAP	125-A	204	-	45,52,52	1.70	9 (20%)	56,80,80	1.38	9 (16%)
4	NAP	35-A	204	-	45,52,52	1.82	10 (22%)	56,80,80	1.41	9 (16%)
4	NAP	162-A	204	-	45,52,52	1.77	11 (24%)	56,80,80	1.38	9 (16%)
2	FOL	42-A	201	-	34,34,34	1.28	4 (11%)	44,47,47	2.04	15 (34%)
2	FOL	35-A	201	-	34,34,34	1.08	3 (8%)	44,47,47	1.76	6 (13%)
4	NAP	150-A	204	-	45,52,52	1.74	9 (20%)	56,80,80	1.40	10 (17%)
4	NAP	82-A	204	-	45,52,52	1.75	10 (22%)	56,80,80	1.31	5 (8%)
2	FOL	67-A	201	-	34,34,34	1.10	3 (8%)	44,47,47	1.98	10 (22%)
2	FOL	152-A	201	-	34,34,34	1.22	3 (8%)	44,47,47	1.86	11 (25%)
4	NAP	154-A	204	-	45,52,52	1.73	11 (24%)	56,80,80	1.45	7 (12%)
4	NAP	163-A	204	-	45,52,52	1.77	11 (24%)	56,80,80	1.31	8 (14%)
2	FOL	105-A	201	-	34,34,34	1.21	3 (8%)	44,47,47	2.18	12 (27%)
4	NAP	12-A	204	-	45,52,52	1.78	10 (22%)	56,80,80	1.29	10 (17%)
4	NAP	44-A	204	-	45,52,52	1.83	10 (22%)	56,80,80	1.25	9 (16%)
4	NAP	26-A	204	-	45,52,52	1.83	10 (22%)	56,80,80	1.36	10 (17%)
4	NAP	7-A	204	-	45,52,52	1.68	11 (24%)	56,80,80	1.26	5 (8%)
4	NAP	119-A	204	-	45,52,52	1.93	12 (26%)	56,80,80	1.78	9 (16%)
2	FOL	26-A	201	-	34,34,34	1.33	4 (11%)	44,47,47	2.18	15 (34%)
4	NAP	105-A	204	-	45,52,52	1.86	11 (24%)	56,80,80	1.34	9 (16%)
4	NAP	68-A	204	-	45,52,52	1.83	11 (24%)	56,80,80	1.25	7 (12%)
2	FOL	150-A	201	-	34,34,34	1.08	3 (8%)	44,47,47	1.73	7 (15%)
4	NAP	22-A	204	-	45,52,52	1.87	11 (24%)	56,80,80	1.37	9 (16%)
2	FOL	85-A	201	-	34,34,34	1.17	3 (8%)	44,47,47	1.94	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	FOL	115-A	201	-	34,34,34	1.14	3 (8%)	44,47,47	2.10	13 (29%)
4	NAP	123-A	204	-	45,52,52	1.78	12 (26%)	56,80,80	1.41	9 (16%)
2	FOL	50-A	201	-	34,34,34	1.12	3 (8%)	44,47,47	1.88	9 (20%)
2	FOL	129-A	201	-	34,34,34	1.24	3 (8%)	44,47,47	2.21	16 (36%)
2	FOL	83-A	201	-	34,34,34	1.35	4 (11%)	44,47,47	2.04	14 (31%)
4	NAP	56-A	204	-	45,52,52	1.73	10 (22%)	56,80,80	1.92	9 (16%)
4	NAP	155-A	204	-	45,52,52	1.76	10 (22%)	56,80,80	1.30	9 (16%)
4	NAP	45-A	204	-	45,52,52	1.81	11 (24%)	56,80,80	1.40	9 (16%)
4	NAP	21-A	204	-	45,52,52	1.81	10 (22%)	56,80,80	1.30	8 (14%)
2	FOL	87-A	201	-	34,34,34	1.12	3 (8%)	44,47,47	1.87	8 (18%)
2	FOL	112-A	201	-	34,34,34	1.02	3 (8%)	44,47,47	1.97	8 (18%)
4	NAP	24-A	204	-	45,52,52	1.84	9 (20%)	56,80,80	1.29	8 (14%)
4	NAP	42-A	204	-	45,52,52	1.87	11 (24%)	56,80,80	1.48	10 (17%)
4	NAP	161-A	204	-	45,52,52	1.77	9 (20%)	56,80,80	1.29	8 (14%)
2	FOL	46-A	201	-	34,34,34	1.18	3 (8%)	44,47,47	2.15	11 (25%)
4	NAP	104-A	204	-	45,52,52	1.86	10 (22%)	56,80,80	1.48	10 (17%)
4	NAP	75-A	204	-	45,52,52	1.84	9 (20%)	56,80,80	1.33	9 (16%)
2	FOL	120-A	201	-	34,34,34	1.21	4 (11%)	44,47,47	1.85	10 (22%)
4	NAP	166-A	204	-	45,52,52	1.72	9 (20%)	56,80,80	1.30	8 (14%)
4	NAP	165-A	204	-	45,52,52	1.84	11 (24%)	56,80,80	1.36	7 (12%)
2	FOL	147-A	201	-	34,34,34	1.17	3 (8%)	44,47,47	1.82	9 (20%)
2	FOL	72-A	201	-	34,34,34	1.06	3 (8%)	44,47,47	2.17	9 (20%)
2	FOL	38-A	201	-	34,34,34	1.03	2 (5%)	44,47,47	2.01	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	16-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	138-A	204	-	-	3/31/67/67	0/5/5/5
2	FOL	24-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	58-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	143-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	63-A	204	-	-	7/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	32-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	63-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	80-A	204	-	-	0/31/67/67	0/5/5/5
2	FOL	132-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	117-A	204	-	-	3/31/67/67	0/5/5/5
4	NAP	107-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	51-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	46-A	204	-	-	4/31/67/67	0/5/5/5
4	NAP	59-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	37-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	18-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	153-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	34-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	28-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	64-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	92-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	47-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	17-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	30-A	204	-	-	0/31/67/67	0/5/5/5
2	FOL	45-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	61-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	11-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	149-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	89-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	92-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	111-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	86-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	130-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	65-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	143-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	158-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	148-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	126-A	201	-	-	8/22/22/22	0/3/3/3
4	NAP	10-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	83-A	204	-	-	0/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	128-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	124-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	19-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	81-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	166-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	131-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	34-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	14-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	41-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	39-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	136-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	103-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	120-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	18-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	60-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	78-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	106-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	64-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	14-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	107-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	98-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	8-A	204	-	-	0/31/67/67	0/5/5/5
4	NAP	133-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	28-A	204	-	-	4/31/67/67	0/5/5/5
4	NAP	137-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	109-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	88-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	19-A	204	-	-	3/31/67/67	0/5/5/5
4	NAP	53-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	114-A	201	-	-	9/22/22/22	0/3/3/3
4	NAP	139-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	111-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	20-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	123-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	157-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	2-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	119-A	201	-	-	3/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	153-A	204	-	-	3/31/67/67	0/5/5/5
4	NAP	29-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	68-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	127-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	13-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	9-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	155-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	154-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	157-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	49-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	138-A	201	-	-	6/22/22/22	0/3/3/3
4	NAP	103-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	113-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	73-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	94-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	12-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	86-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	71-A	204	-	-	0/31/67/67	0/5/5/5
2	FOL	25-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	167-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	162-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	133-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	22-A	201	-	-	8/22/22/22	0/3/3/3
2	FOL	48-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	25-A	204	-	-	0/31/67/67	0/5/5/5
4	NAP	6-A	204	-	-	0/31/67/67	0/5/5/5
2	FOL	104-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	118-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	75-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	1-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	55-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	164-A	204	-	-	3/31/67/67	0/5/5/5
2	FOL	3-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	108-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	106-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	33-A	204	-	-	5/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	2-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	91-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	29-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	80-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	90-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	165-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	52-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	13-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	137-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	91-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	41-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	118-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	59-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	167-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	44-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	27-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	99-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	100-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	145-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	102-A	204	-	-	3/31/67/67	0/5/5/5
4	NAP	39-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	43-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	135-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	121-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	17-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	57-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	144-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	96-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	57-A	204	-	-	4/31/67/67	0/5/5/5
4	NAP	131-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	4-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	23-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	27-A	204	-	-	4/31/67/67	0/5/5/5
4	NAP	108-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	102-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	136-A	204	-	-	3/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	164-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	98-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	134-A	201	-	-	8/22/22/22	0/3/3/3
4	NAP	15-A	204	-	-	6/31/67/67	0/5/5/5
4	NAP	115-A	204	-	-	0/31/67/67	0/5/5/5
2	FOL	158-A	201	-	-	7/22/22/22	0/3/3/3
4	NAP	50-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	129-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	94-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	134-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	54-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	56-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	6-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	144-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	79-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	48-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	84-A	204	-	-	5/31/67/67	0/5/5/5
2	FOL	4-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	109-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	147-A	204	-	-	0/31/67/67	0/5/5/5
2	FOL	81-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	52-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	16-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	31-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	139-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	88-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	20-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	21-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	67-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	116-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	78-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	146-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	127-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	125-A	201	-	-	8/22/22/22	0/3/3/3
4	NAP	132-A	204	-	-	4/31/67/67	0/5/5/5
2	FOL	8-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	43-A	204	-	-	2/31/67/67	0/5/5/5

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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	156-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	101-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	160-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	101-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	87-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	151-A	204	-	-	0/31/67/67	0/5/5/5
2	FOL	151-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	53-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	72-A	204	-	-	0/31/67/67	0/5/5/5
2	FOL	130-A	201	-	-	1/22/22/22	0/3/3/3
4	NAP	32-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	110-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	5-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	113-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	110-A	201	-	-	7/22/22/22	0/3/3/3
4	NAP	99-A	204	-	-	0/31/67/67	0/5/5/5
4	NAP	152-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	69-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	69-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	142-A	201	-	-	6/22/22/22	0/3/3/3
4	NAP	47-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	146-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	142-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	140-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	112-A	204	-	-	3/31/67/67	0/5/5/5
2	FOL	71-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	156-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	54-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	93-A	204	-	-	0/31/67/67	0/5/5/5
4	NAP	76-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	93-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	11-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	140-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	9-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	160-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	70-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	149-A	204	-	-	1/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	7-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	74-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	74-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	49-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	73-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	3-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	97-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	117-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	159-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	97-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	79-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	40-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	33-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	76-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	5-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	163-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	124-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	1-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	89-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	141-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	36-A	204	-	-	0/31/67/67	0/5/5/5
4	NAP	145-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	121-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	30-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	40-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	95-A	204	-	-	3/31/67/67	0/5/5/5
4	NAP	38-A	204	-	-	0/31/67/67	0/5/5/5
4	NAP	122-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	36-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	116-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	148-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	66-A	204	-	-	0/31/67/67	0/5/5/5
4	NAP	126-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	128-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	90-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	10-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	96-A	201	-	-	5/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	161-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	70-A	204	-	-	0/31/67/67	0/5/5/5
4	NAP	77-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	60-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	77-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	82-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	23-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	100-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	141-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	37-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	95-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	122-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	31-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	55-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	159-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	62-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	66-A	201	-	-	7/22/22/22	0/3/3/3
4	NAP	58-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	135-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	61-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	15-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	84-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	85-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	65-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	125-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	35-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	162-A	204	-	-	3/31/67/67	0/5/5/5
2	FOL	42-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	35-A	201	-	-	3/22/22/22	0/3/3/3
4	NAP	150-A	204	-	-	0/31/67/67	0/5/5/5
4	NAP	82-A	204	-	-	3/31/67/67	0/5/5/5
2	FOL	67-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	152-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	154-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	163-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	105-A	201	-	-	2/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAP	12-A	204	-	-	3/31/67/67	0/5/5/5
4	NAP	44-A	204	-	-	0/31/67/67	0/5/5/5
4	NAP	26-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	7-A	204	-	-	0/31/67/67	0/5/5/5
4	NAP	119-A	204	-	-	6/31/67/67	0/5/5/5
2	FOL	26-A	201	-	-	2/22/22/22	0/3/3/3
4	NAP	105-A	204	-	-	2/31/67/67	0/5/5/5
4	NAP	68-A	204	-	-	3/31/67/67	0/5/5/5
2	FOL	150-A	201	-	-	0/22/22/22	0/3/3/3
4	NAP	22-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	85-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	115-A	201	-	-	8/22/22/22	0/3/3/3
4	NAP	123-A	204	-	-	0/31/67/67	0/5/5/5
2	FOL	50-A	201	-	-	1/22/22/22	0/3/3/3
2	FOL	129-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	83-A	201	-	-	9/22/22/22	0/3/3/3
4	NAP	56-A	204	-	-	8/31/67/67	0/5/5/5
4	NAP	155-A	204	-	-	3/31/67/67	0/5/5/5
4	NAP	45-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	21-A	204	-	-	1/31/67/67	0/5/5/5
2	FOL	87-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	112-A	201	-	-	9/22/22/22	0/3/3/3
4	NAP	24-A	204	-	-	0/31/67/67	0/5/5/5
4	NAP	42-A	204	-	-	4/31/67/67	0/5/5/5
4	NAP	161-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	46-A	201	-	-	4/22/22/22	0/3/3/3
4	NAP	104-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	75-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	120-A	201	-	-	5/22/22/22	0/3/3/3
4	NAP	166-A	204	-	-	1/31/67/67	0/5/5/5
4	NAP	165-A	204	-	-	2/31/67/67	0/5/5/5
2	FOL	147-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	72-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	38-A	201	-	-	2/22/22/22	0/3/3/3

The worst 5 of 2215 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	69-A	204	NAP	O3B-C3B	-6.43	1.27	1.43
4	25-A	204	NAP	O3B-C3B	-6.42	1.27	1.43
4	75-A	204	NAP	O3B-C3B	-6.38	1.28	1.43
4	22-A	204	NAP	O3B-C3B	-6.37	1.28	1.43
4	116-A	204	NAP	O3B-C3B	-6.32	1.28	1.43

The worst 5 of 3114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	57-A	204	NAP	O2N-PN-O1N	12.37	173.38	112.24
4	118-A	204	NAP	O2N-PN-O1N	11.13	167.26	112.24
4	56-A	204	NAP	O2N-PN-O1N	8.90	156.26	112.24
2	139-A	201	FOL	C8A-C4A-C4	-7.94	114.69	119.95
2	106-A	201	FOL	CG-CB-CA	-7.59	98.96	113.16

There are no chirality outliers.

5 of 790 torsion outliers are listed below:

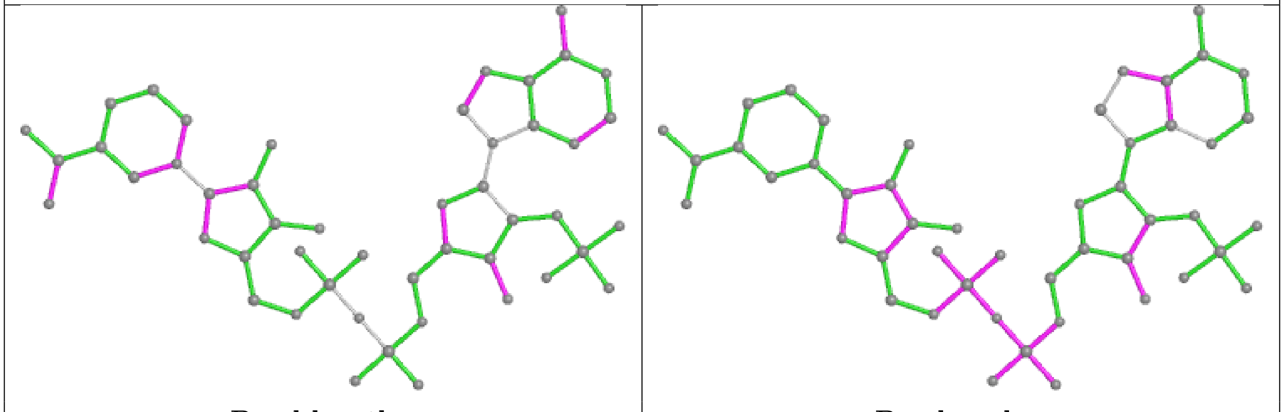
Mol	Chain	Res	Type	Atoms
2	7-A	201	FOL	CT-CA-CB-CG
2	14-A	201	FOL	CT-CA-CB-CG
2	22-A	201	FOL	N-CA-CB-CG
2	43-A	201	FOL	N-CA-CB-CG
2	53-A	201	FOL	CT-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

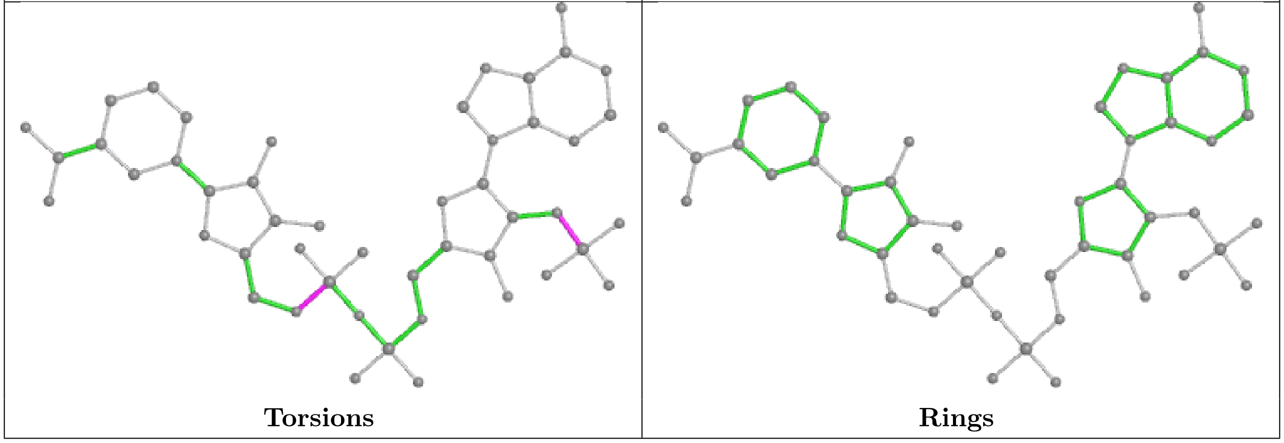
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand NAP A 204



Bond lengths

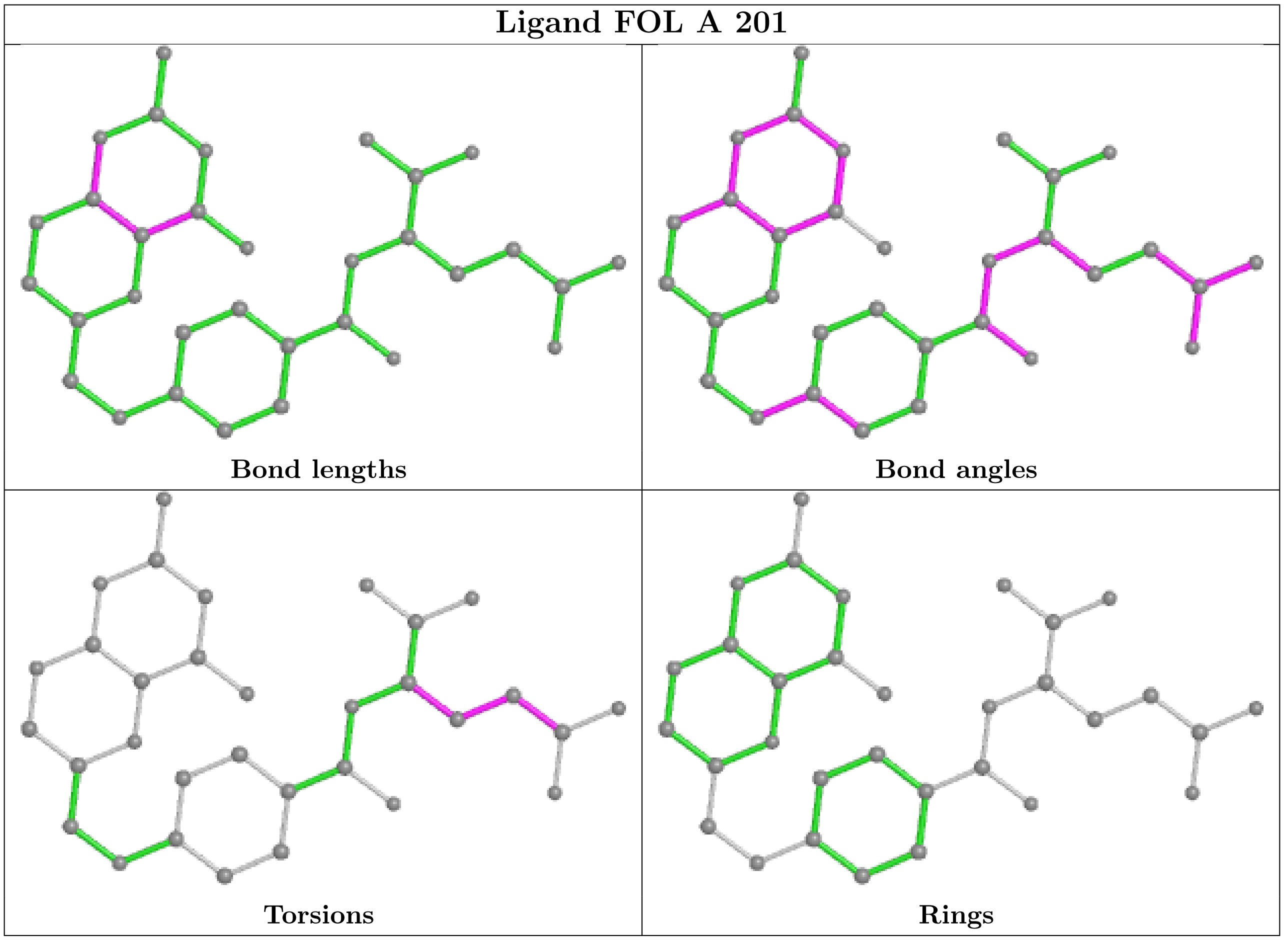
Bond angles



Torsions

Rings

Ligand FOL A 201



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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