



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2020 – 12:57 PM BST

PDB ID : 4PTJ
Title : Ensemble model for Escherichia coli dihydrofolate reductase at 277K
Authors : Keedy, D.A.; van den Bedem, H.; Sivak, D.A.; Petsko, G.A.; Ringe, D.; Wilson, M.A.; Fraser, J.S.
Deposited on : 2014-03-10
Resolution : 1.05 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

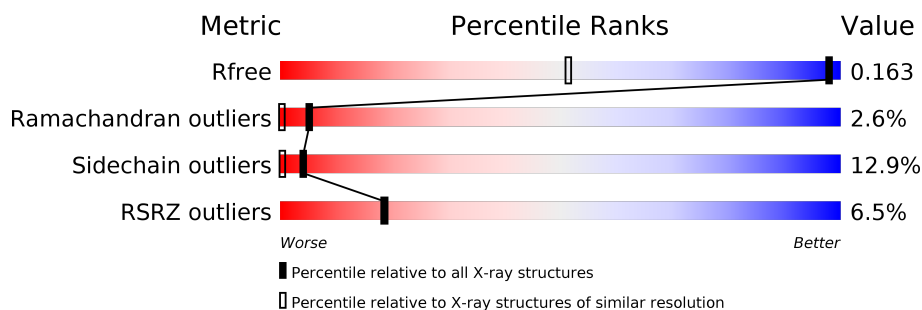
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1202 (1.10-1.02)
Ramachandran outliers	138981	1204 (1.10-1.02)
Sidechain outliers	138945	1202 (1.10-1.02)
RSRZ outliers	127900	1178 (1.10-1.02)

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

Mol	Chain	Length	Quality of chain
1	1-A	159	<div> <div>6%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	10-A	159	<div> <div>6%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
1	100-A	159	<div> <div>6%</div> <div>83%</div> <div>13%</div> <div>.</div> </div>
1	101-A	159	<div> <div>6%</div> <div>81%</div> <div>14%</div> <div>..</div> </div>
1	102-A	159	<div> <div>6%</div> <div>87%</div> <div>8%</div> <div>..</div> </div>
1	103-A	159	<div> <div>6%</div> <div>84%</div> <div>10%</div> <div>..</div> </div>
1	104-A	159	<div> <div>6%</div> <div>81%</div> <div>13%</div> <div>6%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	105-A	159	
1	106-A	159	
1	107-A	159	
1	108-A	159	
1	109-A	159	
1	11-A	159	
1	110-A	159	
1	111-A	159	
1	112-A	159	
1	113-A	159	
1	114-A	159	
1	115-A	159	
1	116-A	159	
1	117-A	159	
1	118-A	159	
1	119-A	159	
1	12-A	159	
1	120-A	159	
1	121-A	159	
1	122-A	159	
1	123-A	159	
1	124-A	159	
1	125-A	159	
1	13-A	159	
1	14-A	159	

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Mol	Chain	Length	Quality of chain
1	15-A	159	
1	16-A	159	
1	17-A	159	
1	18-A	159	
1	19-A	159	
1	2-A	159	
1	20-A	159	
1	21-A	159	
1	22-A	159	
1	23-A	159	
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	

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Mol	Chain	Length	Quality of chain
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	
1	47-A	159	
1	48-A	159	
1	49-A	159	
1	5-A	159	
1	50-A	159	
1	51-A	159	
1	52-A	159	
1	53-A	159	
1	54-A	159	
1	55-A	159	
1	56-A	159	
1	57-A	159	
1	58-A	159	
1	59-A	159	
1	6-A	159	

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Mol	Chain	Length	Quality of chain
1	60-A	159	
1	61-A	159	
1	62-A	159	
1	63-A	159	
1	64-A	159	
1	65-A	159	
1	66-A	159	
1	67-A	159	
1	68-A	159	
1	69-A	159	
1	7-A	159	
1	70-A	159	
1	71-A	159	
1	72-A	159	
1	73-A	159	
1	74-A	159	
1	75-A	159	
1	76-A	159	
1	77-A	159	
1	78-A	159	
1	79-A	159	
1	8-A	159	
1	80-A	159	
1	81-A	159	
1	82-A	159	

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Mol	Chain	Length	Quality of chain
1	83-A	159	
1	84-A	159	
1	85-A	159	
1	86-A	159	
1	87-A	159	
1	88-A	159	
1	89-A	159	
1	9-A	159	
1	90-A	159	
1	91-A	159	
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 339833 atoms, of which 157875 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Dihydrofolate reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	2-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	3-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	4-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	5-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	6-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	7-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	8-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	9-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	10-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	11-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	12-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	13-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	14-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	15-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	16-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	18-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	19-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	20-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	21-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	22-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	23-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	24-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	25-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	26-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	27-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	28-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	29-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	30-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	31-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	32-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	33-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	34-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	35-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	36-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	37-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 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	0	0	0
			2491	805	1221	217	241	7			
1	39-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	40-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	41-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	42-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	43-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	44-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	45-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	46-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	47-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	48-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	49-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	50-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	51-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	52-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	53-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	54-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	55-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	56-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	57-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	58-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	59-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	60-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	61-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	62-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	63-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	64-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	65-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	66-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	67-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	68-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	69-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	70-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	71-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	72-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	73-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	74-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	75-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	76-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	77-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	78-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	79-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	80-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	81-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	82-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	83-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	84-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	85-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	86-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	87-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	88-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	89-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	90-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	91-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	92-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	93-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	94-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	95-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	96-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	97-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	98-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	99-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	100-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	101-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	102-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	103-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	104-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	105-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	106-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	107-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	108-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	109-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	110-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	111-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	112-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	113-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	114-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	115-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	116-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	117-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	118-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	119-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	120-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			
1	121-A	159	Total	C	H	N	O	S	0	0	0
			2491	805	1221	217	241	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	122-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	123-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	124-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0
1	125-A	159	Total 2491	C 805	H 1221	N 217	O 241	S 7	0	0	0

-
- The chemical structure of FOL (Folic acid) is shown. It consists of a pteridine ring system (labeled with N1, N3, N9, N10, N11, N12, N13, N14, N15, N16, N17, N18, N19, N20, N21, N22, N23, N24, N25, N26, N27, N28, N29, N30, N31, N32, N33, N34, N35, N36, N37, N38, N39, N40, N41, N42, N43, N44, N45, N46, N47, N48, N49, N50, N51, N52, N53, N54, N55, N56, N57, N58, N59, N60, N61, N62, N63, N64, N65, N66, N67, N68, N69, N70, N71, N72, N73, N74, N75, N76, N77, N78, N79, N80, N81, N82, N83, N84, N85, N86, N87, N88, N89, N90, N91, N92, N93, N94, N95, N96, N97, N98, N99, N100, N101, N102, N103, N104, N105, N106, N107, N108, N109, N110, N111, N112, N113, N114, N115, N116, N117, N118, N119, N120, N121, N122, N123, N124, N125, N126, N127, N128, N129, N130, N131, N132, N133, N134, N135, N136, N137, N138, N139, N140, N141, N142, N143, N144, N145, N146, N147, N148, N149, N150, N151, N152, N153, N154, N155, N156, N157, N158, N159, N160, N161, N162, N163, N164, N165, N166, N167, N168, N169, N170, N171, N172, N173, N174, N175, N176, N177, N178, N179, N180, N181, N182, N183, N184, N185, N186, N187, N188, N189, N190, N191, N192, N193, N194, N195, N196, N197, N198, N199, N200, N201, N202, N203, N204, N205, N206, N207, N208, N209, N210, N211, N212, N213, N214, N215, N216, N217, N218, N219, N220, N221, N222, N223, N224, N225, N226, N227, N228, N229, N230, N231, N232, N233, N234, N235, N236, N237, N238, N239, N240, N241, N242, N243, N244, N245, N246, N247, N248, N249, N250, N251, N252, N253, N254, N255, N256, N257, N258, N259, N260, N261, N262, N263, N264, N265, N266, N267, N268, N269, N270, N271, N272, N273, N274, N275, N276, N277, N278, N279, N280, N281, N282, N283, N284, N285, N286, N287, N288, N289, N290, N291, N292, N293, N294, N295, N296, N297, N298, N299, N300, N301, N302, N303, N304, N305, N306, N307, N308, N309, N310, N311, N312, N313, N314, N315, N316, N317, N318, N319, N320, N321, N322, N323, N324, N325, N326, N327, N328, N329, N330, N331, N332, N333, N334, N335, N336, N337, N338, N339, N340, N341, N342, N343, N344, N345, N346, N347, N348, N349, N350, N351, N352, N353, N354, N355, N356, N357, N358, N359, N360, N361, N362, N363, N364, N365, N366, N367, N368, N369, N370, N371, N372, N373, N374, N375, N376, N377, N378, N379, N380, N381, N382, N383, N384, N385, N386, N387, N388, N389, N390, N391, N392, N393, N394, N395, N396, N397, N398, N399, N400, N401, N402, N403, N404, N405, N406, N407, N408, N409, N410, N411, N412, N413, N414, N415, N416, N417, N418, N419, N420, N421, N422, N423, N424, N425, N426, N427, N428, N429, N430, N431, N432, N433, N434, N435, N436, N437, N438, N439, N440, N441, N442, N443, N444, N445, N446, N447, N448, N449, N450, N451, N452, N453, N454, N455, N456, N457, N458, N459, N460, N461, N462, N463, N464, N465, N466, N467, N468, N469, N470, N471, N472, N473, N474, N475, N476, N477, N478, N479, N480, N481, N482, N483, N484, N485, N486, N487, N488, N489, N490, N491, N492, N493, N494, N495, N496, N497, N498, N499, N500, N501, N502, N503, N504, N505, N506, N507, N508, N509, N510, N511, N512, N513, N514, N515, N516, N517, N518, N519, N520, N521, N522, N523, N524, N525, N526, N527, N528, N529, N530, N531, N532, N533, N534, N535, N536, N537, N538, N539, N540, N541, N542, N543, N544, N545, N546, N547, N548, N549, N550, N551, N552, N553, N554, N555, N556, N557, N558, N559, N560, N561, N562, N563, N564, N565, N566, N567, N568, N569, N570, N571, N572, N573, N574, N575, N576, N577, N578, N579, N580, N581, N582, N583, N584, N585, N586, N587, N588, N589, N590, N591, N592, N593, N594, N595, N596, N597, N598, N599, N600, N601, N602, N603, N604, N605, N606, N607, N608, N609, N610, N611, N612, N613, N614, N615, N616, N617, N618, N619, N620, N621, N622, N623, N624, N625, N626, N627, N628, N629, N630, N631, N632, N633, N634, N635, N636, N637, N638, N639, N640, N641, N642, N643, N644, N645, N646, N647, N648, N649, N650, N651, N652, N653, N654, N655, N656, N657, N658, N659, N660, N661, N662, N663, N664, N665, N666, N667, N668, N669, N670, N671, N672, N673, N674, N675, N676, N677, N678, N679, N680, N681, N682, N683, N684, N685, N686, N687, N688, N689, N690, N691, N692, N693, N694, N695, N696, N697, N698, N699, N700, N701, N702, N703, N704, N705, N706, N707, N708, N709, N710, N711, N712, N713, N714, N715, N716, N717, N718, N719, N720, N721, N722, N723, N724, N725, N726, N727, N728, N729, N730, N731, N732, N733, N734, N735, N736, N737, N738, N739, N740, N741, N742, N743, N744, N745, N746, N747, N748, N749, N750, N751, N752, N753, N754, N755, N756, N757, N758, N759, N760, N761, N762, N763, N764, N765, N766, N767, N768, N769, N770, N771, N772, N773, N774, N775, N776, N777, N778, N779, N780, N781, N782, N783, N784, N785, N786, N787, N788, N789, N790, N791, N792, N793, N794, N795, N796, N797, N798, N799, N800, N801, N802, N803, N804, N805, N806, N807, N808, N809, N810, N811, N812, N813, N814, N815, N816, N817, N818, N819, N820, N821, N822, N823, N824, N825, N826, N827, N828, N829, N830, N83

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

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

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

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

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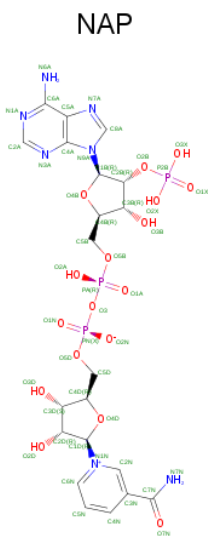
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	92-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	93-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	94-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	95-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	96-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	97-A	1	Total 49	C 19	H 17	N 7	O 6	0	0
2	98-A	1	Total 49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

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

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



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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	15-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	16-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	17-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	18-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	19-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	20-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	21-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	22-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	23-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	24-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	25-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	26-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	27-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	28-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	29-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	30-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	31-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	32-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	33-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	34-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	35-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	36-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	37-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	38-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	39-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	40-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	41-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	42-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	43-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	44-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	45-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	46-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	47-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	48-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	49-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	50-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	51-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	52-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	53-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	54-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	55-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	56-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	57-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	58-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	59-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	60-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	61-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	62-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	63-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	64-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	65-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	66-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	67-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	68-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	69-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	70-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	71-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	72-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	73-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	74-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	75-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	76-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	77-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	78-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	79-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	80-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	81-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	82-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	83-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	84-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	85-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	86-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	87-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	88-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	89-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	90-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	91-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	92-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	93-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	94-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	95-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	96-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	97-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	98-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	99-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	100-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	101-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	102-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	103-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	104-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	105-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	106-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	107-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	108-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	109-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	110-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	111-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	112-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	113-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	114-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	115-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	116-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	117-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	118-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0
3	119-A	1	Total 73	C 21	H 25	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	120-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	121-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	122-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	123-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	124-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		
3	125-A	1	Total	C	H	N	O	P	0	0
			73	21	25	7	17	3		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	122-A	2	Total	Mn	0	0
			2	2		
4	110-A	2	Total	Mn	0	0
			2	2		
4	37-A	2	Total	Mn	0	0
			2	2		
4	80-A	2	Total	Mn	0	0
			2	2		
4	94-A	2	Total	Mn	0	0
			2	2		
4	60-A	2	Total	Mn	0	0
			2	2		
4	123-A	2	Total	Mn	0	0
			2	2		
4	44-A	2	Total	Mn	0	0
			2	2		
4	50-A	2	Total	Mn	0	0
			2	2		
4	104-A	2	Total	Mn	0	0
			2	2		
4	12-A	2	Total	Mn	0	0
			2	2		
4	114-A	2	Total	Mn	0	0
			2	2		
4	19-A	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	73-A	2	Total 2	Mn 2	0	0
4	1-A	2	Total 2	Mn 2	0	0
4	53-A	2	Total 2	Mn 2	0	0
4	25-A	2	Total 2	Mn 2	0	0
4	32-A	2	Total 2	Mn 2	0	0
4	93-A	2	Total 2	Mn 2	0	0
4	77-A	2	Total 2	Mn 2	0	0
4	58-A	2	Total 2	Mn 2	0	0
4	57-A	2	Total 2	Mn 2	0	0
4	29-A	2	Total 2	Mn 2	0	0
4	101-A	2	Total 2	Mn 2	0	0
4	3-A	2	Total 2	Mn 2	0	0
4	11-A	2	Total 2	Mn 2	0	0
4	84-A	2	Total 2	Mn 2	0	0
4	98-A	2	Total 2	Mn 2	0	0
4	108-A	2	Total 2	Mn 2	0	0
4	16-A	2	Total 2	Mn 2	0	0
4	65-A	2	Total 2	Mn 2	0	0
4	117-A	2	Total 2	Mn 2	0	0
4	41-A	2	Total 2	Mn 2	0	0
4	5-A	2	Total 2	Mn 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	8-A	2	Total 2	Mn 2	0	0
4	21-A	2	Total 2	Mn 2	0	0
4	109-A	2	Total 2	Mn 2	0	0
4	102-A	2	Total 2	Mn 2	0	0
4	113-A	2	Total 2	Mn 2	0	0
4	36-A	2	Total 2	Mn 2	0	0
4	81-A	2	Total 2	Mn 2	0	0
4	97-A	2	Total 2	Mn 2	0	0
4	61-A	2	Total 2	Mn 2	0	0
4	48-A	2	Total 2	Mn 2	0	0
4	124-A	2	Total 2	Mn 2	0	0
4	45-A	2	Total 2	Mn 2	0	0
4	35-A	2	Total 2	Mn 2	0	0
4	105-A	2	Total 2	Mn 2	0	0
4	7-A	2	Total 2	Mn 2	0	0
4	15-A	2	Total 2	Mn 2	0	0
4	88-A	2	Total 2	Mn 2	0	0
4	18-A	2	Total 2	Mn 2	0	0
4	72-A	2	Total 2	Mn 2	0	0
4	52-A	2	Total 2	Mn 2	0	0
4	26-A	2	Total 2	Mn 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	120-A	2	Total 2	Mn 2	0	0
4	118-A	2	Total 2	Mn 2	0	0
4	89-A	2	Total 2	Mn 2	0	0
4	31-A	2	Total 2	Mn 2	0	0
4	82-A	2	Total 2	Mn 2	0	0
4	92-A	2	Total 2	Mn 2	0	0
4	76-A	2	Total 2	Mn 2	0	0
4	46-A	2	Total 2	Mn 2	0	0
4	56-A	2	Total 2	Mn 2	0	0
4	106-A	2	Total 2	Mn 2	0	0
4	10-A	2	Total 2	Mn 2	0	0
4	85-A	2	Total 2	Mn 2	0	0
4	39-A	2	Total 2	Mn 2	0	0
4	91-A	2	Total 2	Mn 2	0	0
4	66-A	2	Total 2	Mn 2	0	0
4	79-A	2	Total 2	Mn 2	0	0
4	55-A	2	Total 2	Mn 2	0	0
4	22-A	2	Total 2	Mn 2	0	0
4	103-A	2	Total 2	Mn 2	0	0
4	112-A	2	Total 2	Mn 2	0	0
4	86-A	2	Total 2	Mn 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	96-A	2	Total 2	Mn 2	0	0
4	62-A	2	Total 2	Mn 2	0	0
4	49-A	2	Total 2	Mn 2	0	0
4	125-A	2	Total 2	Mn 2	0	0
4	42-A	2	Total 2	Mn 2	0	0
4	119-A	2	Total 2	Mn 2	0	0
4	34-A	2	Total 2	Mn 2	0	0
4	14-A	2	Total 2	Mn 2	0	0
4	63-A	2	Total 2	Mn 2	0	0
4	68-A	2	Total 2	Mn 2	0	0
4	71-A	2	Total 2	Mn 2	0	0
4	27-A	2	Total 2	Mn 2	0	0
4	121-A	2	Total 2	Mn 2	0	0
4	111-A	2	Total 2	Mn 2	0	0
4	30-A	2	Total 2	Mn 2	0	0
4	83-A	2	Total 2	Mn 2	0	0
4	95-A	2	Total 2	Mn 2	0	0
4	2-A	2	Total 2	Mn 2	0	0
4	9-A	2	Total 2	Mn 2	0	0
4	75-A	2	Total 2	Mn 2	0	0
4	47-A	2	Total 2	Mn 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	51-A	2	Total 2	Mn 2	0	0
4	107-A	2	Total 2	Mn 2	0	0
4	13-A	2	Total 2	Mn 2	0	0
4	115-A	2	Total 2	Mn 2	0	0
4	74-A	2	Total 2	Mn 2	0	0
4	24-A	2	Total 2	Mn 2	0	0
4	4-A	2	Total 2	Mn 2	0	0
4	38-A	2	Total 2	Mn 2	0	0
4	33-A	2	Total 2	Mn 2	0	0
4	116-A	2	Total 2	Mn 2	0	0
4	90-A	2	Total 2	Mn 2	0	0
4	67-A	2	Total 2	Mn 2	0	0
4	78-A	2	Total 2	Mn 2	0	0
4	59-A	2	Total 2	Mn 2	0	0
4	54-A	2	Total 2	Mn 2	0	0
4	23-A	2	Total 2	Mn 2	0	0
4	28-A	2	Total 2	Mn 2	0	0
4	100-A	2	Total 2	Mn 2	0	0
4	87-A	2	Total 2	Mn 2	0	0
4	99-A	2	Total 2	Mn 2	0	0
4	6-A	2	Total 2	Mn 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	43-A	2	Total 2	Mn 2	0	0
4	17-A	2	Total 2	Mn 2	0	0
4	64-A	2	Total 2	Mn 2	0	0
4	69-A	2	Total 2	Mn 2	0	0
4	70-A	2	Total 2	Mn 2	0	0
4	40-A	2	Total 2	Mn 2	0	0
4	20-A	2	Total 2	Mn 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	1-A	89	Total 89	O 89	0	0
5	2-A	91	Total 91	O 91	0	0
5	3-A	82	Total 82	O 82	0	0
5	4-A	108	Total 108	O 108	0	0
5	5-A	105	Total 105	O 105	0	0
5	6-A	112	Total 112	O 112	0	0
5	7-A	107	Total 107	O 107	0	0
5	8-A	102	Total 102	O 102	0	0
5	9-A	96	Total 96	O 96	0	0
5	10-A	90	Total 90	O 90	0	0
5	11-A	110	Total 110	O 110	0	0
5	12-A	102	Total 102	O 102	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	13-A	117	Total 117	O 117	0	0
5	14-A	116	Total 116	O 116	0	0
5	15-A	113	Total 113	O 113	0	0
5	16-A	105	Total 105	O 105	0	0
5	17-A	95	Total 95	O 95	0	0
5	18-A	105	Total 105	O 105	0	0
5	19-A	108	Total 108	O 108	0	0
5	20-A	100	Total 100	O 100	0	0
5	21-A	103	Total 103	O 103	0	0
5	22-A	96	Total 96	O 96	0	0
5	23-A	110	Total 110	O 110	0	0
5	24-A	97	Total 97	O 97	0	0
5	25-A	106	Total 106	O 106	0	0
5	26-A	112	Total 112	O 112	0	0
5	27-A	102	Total 102	O 102	0	0
5	28-A	100	Total 100	O 100	0	0
5	29-A	95	Total 95	O 95	0	0
5	30-A	96	Total 96	O 96	0	0
5	31-A	93	Total 93	O 93	0	0
5	32-A	106	Total 106	O 106	0	0
5	33-A	105	Total 105	O 105	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	34-A	108	Total 108	O 108	0	0
5	35-A	100	Total 100	O 100	0	0
5	36-A	104	Total 104	O 104	0	0
5	37-A	108	Total 108	O 108	0	0
5	38-A	119	Total 119	O 119	0	0
5	39-A	118	Total 118	O 118	0	0
5	40-A	102	Total 102	O 102	0	0
5	41-A	98	Total 98	O 98	0	0
5	42-A	97	Total 97	O 97	0	0
5	43-A	102	Total 102	O 102	0	0
5	44-A	108	Total 108	O 108	0	0
5	45-A	107	Total 107	O 107	0	0
5	46-A	102	Total 102	O 102	0	0
5	47-A	102	Total 102	O 102	0	0
5	48-A	102	Total 102	O 102	0	0
5	49-A	105	Total 105	O 105	0	0
5	50-A	96	Total 96	O 96	0	0
5	51-A	104	Total 104	O 104	0	0
5	52-A	107	Total 107	O 107	0	0
5	53-A	105	Total 105	O 105	0	0
5	54-A	103	Total 103	O 103	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	55-A	106	Total 106	O 106	0	0
5	56-A	110	Total 110	O 110	0	0
5	57-A	108	Total 108	O 108	0	0
5	58-A	116	Total 116	O 116	0	0
5	59-A	108	Total 108	O 108	0	0
5	60-A	93	Total 93	O 93	0	0
5	61-A	109	Total 109	O 109	0	0
5	62-A	107	Total 107	O 107	0	0
5	63-A	110	Total 110	O 110	0	0
5	64-A	102	Total 102	O 102	0	0
5	65-A	96	Total 96	O 96	0	0
5	66-A	104	Total 104	O 104	0	0
5	67-A	99	Total 99	O 99	0	0
5	68-A	93	Total 93	O 93	0	0
5	69-A	95	Total 95	O 95	0	0
5	70-A	103	Total 103	O 103	0	0
5	71-A	103	Total 103	O 103	0	0
5	72-A	97	Total 97	O 97	0	0
5	73-A	108	Total 108	O 108	0	0
5	74-A	111	Total 111	O 111	0	0
5	75-A	109	Total 109	O 109	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	76-A	93	Total 93	O 93	0	0
5	77-A	87	Total 87	O 87	0	0
5	78-A	95	Total 95	O 95	0	0
5	79-A	115	Total 115	O 115	0	0
5	80-A	109	Total 109	O 109	0	0
5	81-A	106	Total 106	O 106	0	0
5	82-A	107	Total 107	O 107	0	0
5	83-A	116	Total 116	O 116	0	0
5	84-A	111	Total 111	O 111	0	0
5	85-A	118	Total 118	O 118	0	0
5	86-A	109	Total 109	O 109	0	0
5	87-A	113	Total 113	O 113	0	0
5	88-A	103	Total 103	O 103	0	0
5	89-A	109	Total 109	O 109	0	0
5	90-A	103	Total 103	O 103	0	0
5	91-A	93	Total 93	O 93	0	0
5	92-A	98	Total 98	O 98	0	0
5	93-A	117	Total 117	O 117	0	0
5	94-A	121	Total 121	O 121	0	0
5	95-A	111	Total 111	O 111	0	0
5	96-A	104	Total 104	O 104	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	97-A	93	Total 93	O 93	0	0
5	98-A	98	Total 98	O 98	0	0
5	99-A	99	Total 99	O 99	0	0
5	100-A	107	Total 107	O 107	0	0
5	101-A	107	Total 107	O 107	0	0
5	102-A	100	Total 100	O 100	0	0
5	103-A	105	Total 105	O 105	0	0
5	104-A	94	Total 94	O 94	0	0
5	105-A	90	Total 90	O 90	0	0
5	106-A	91	Total 91	O 91	0	0
5	107-A	113	Total 113	O 113	0	0
5	108-A	108	Total 108	O 108	0	0
5	109-A	111	Total 111	O 111	0	0
5	110-A	113	Total 113	O 113	0	0
5	111-A	109	Total 109	O 109	0	0
5	112-A	92	Total 92	O 92	0	0
5	113-A	101	Total 101	O 101	0	0
5	114-A	103	Total 103	O 103	0	0
5	115-A	102	Total 102	O 102	0	0
5	116-A	101	Total 101	O 101	0	0
5	117-A	95	Total 95	O 95	0	0

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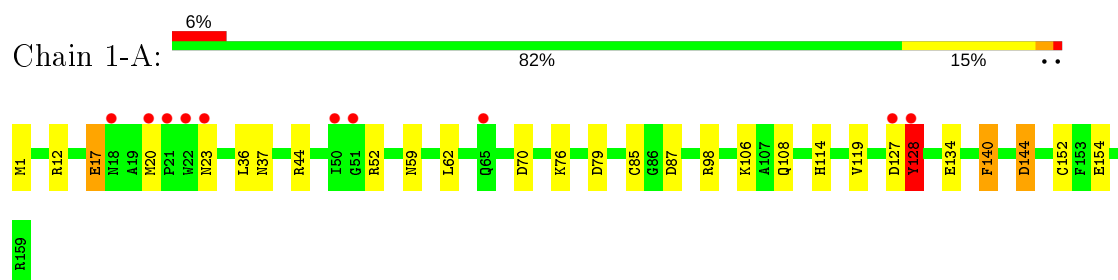
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	118-A	107	Total 107	O 107	0	0
5	119-A	106	Total 106	O 106	0	0
5	120-A	105	Total 105	O 105	0	0
5	121-A	115	Total 115	O 115	0	0
5	122-A	97	Total 97	O 97	0	0
5	123-A	105	Total 105	O 105	0	0
5	124-A	93	Total 93	O 93	0	0
5	125-A	102	Total 102	O 102	0	0

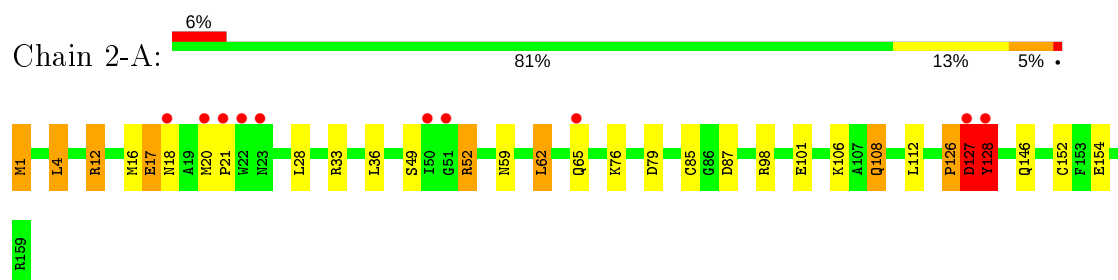
3 Residue-property plots [i](#)

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

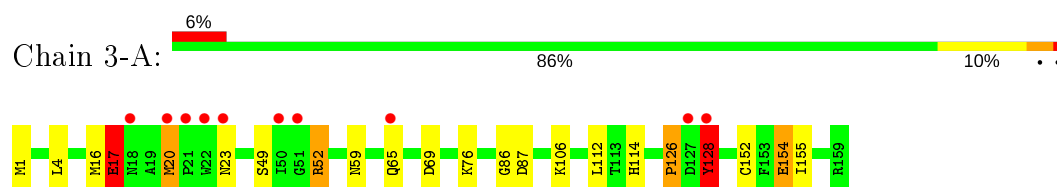
- Molecule 1: Dihydrofolate reductase



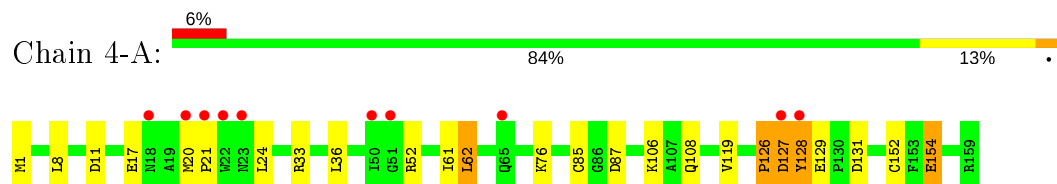
- Molecule 1: Dihydrofolate reductase



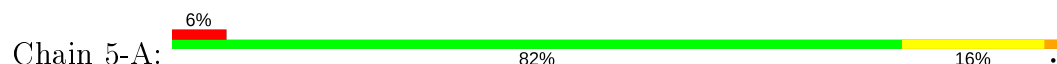
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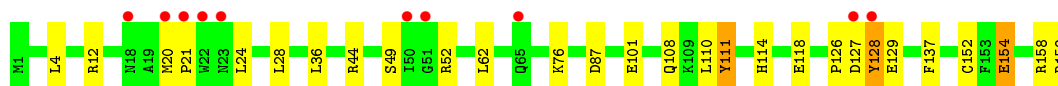


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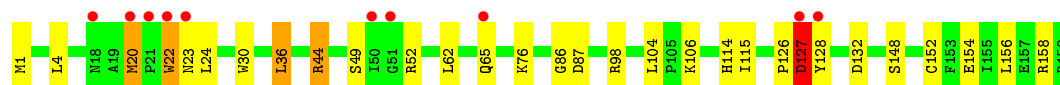
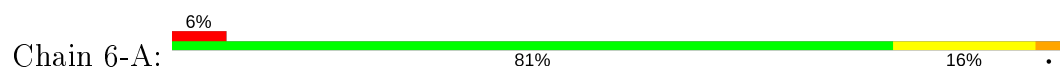


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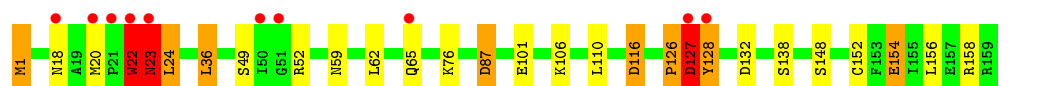
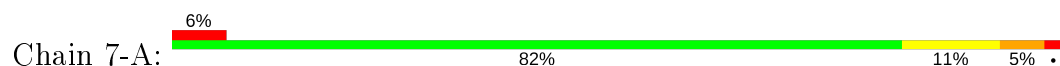




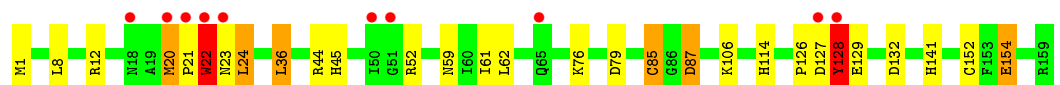
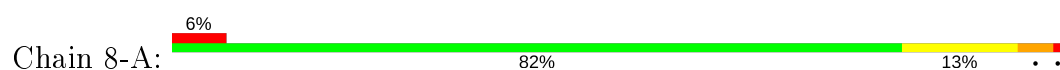
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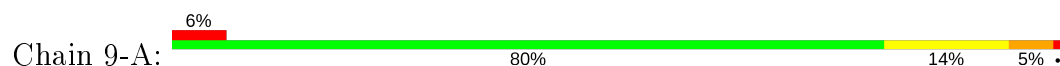
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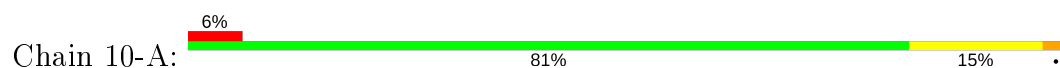
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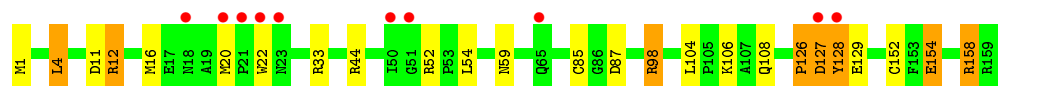
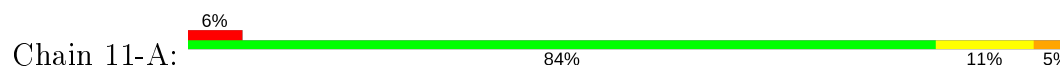
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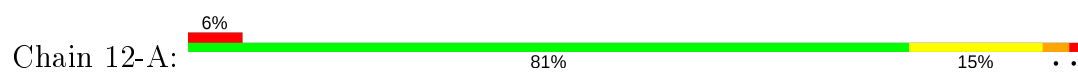
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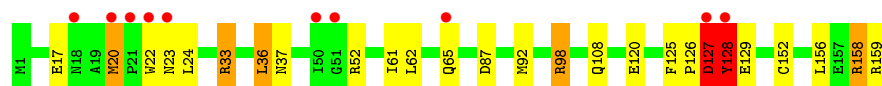
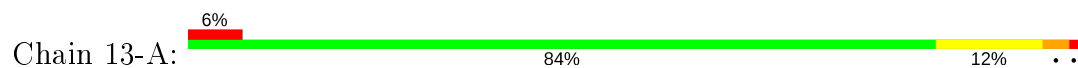
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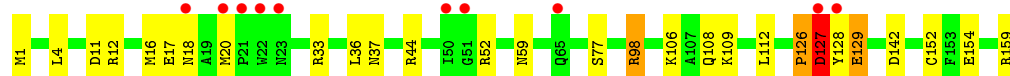
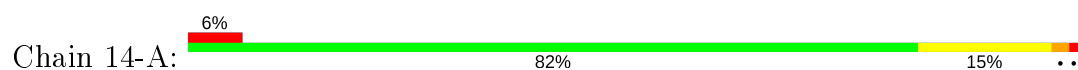
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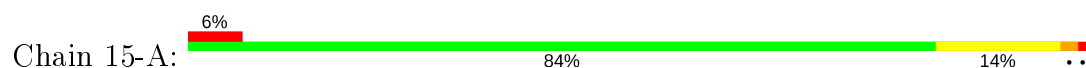
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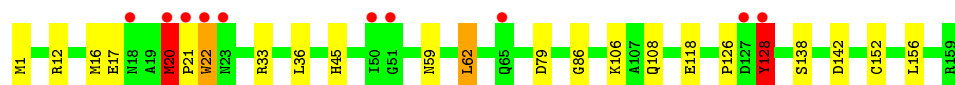
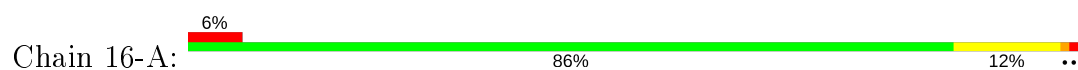
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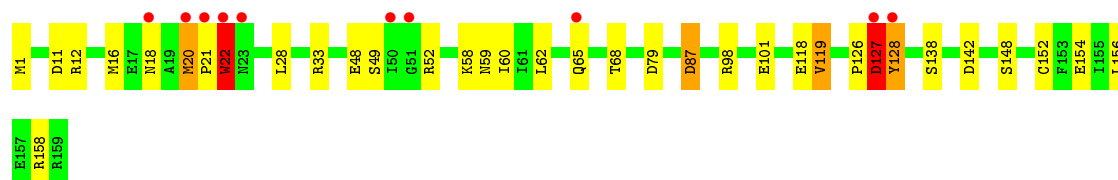
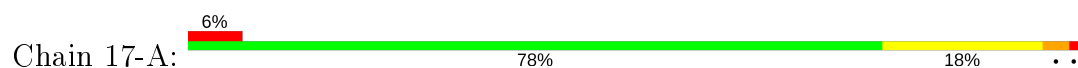
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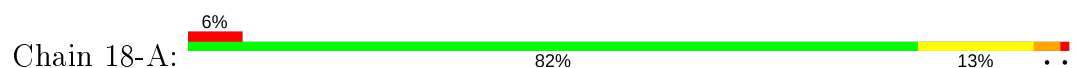
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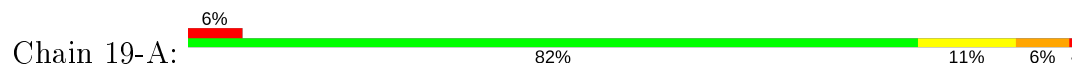


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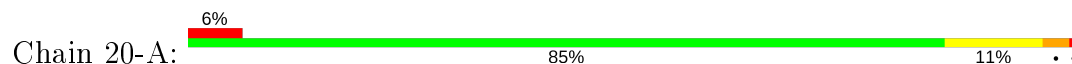




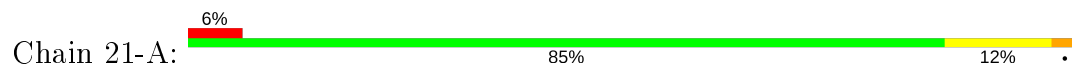
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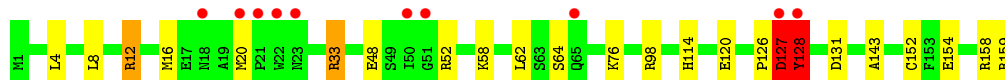
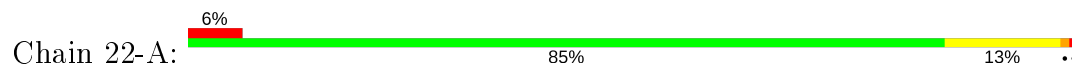
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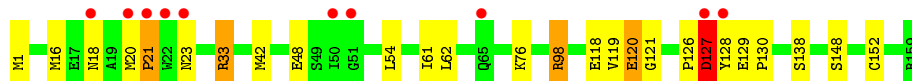
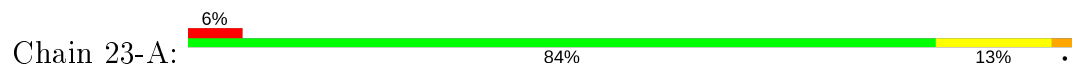
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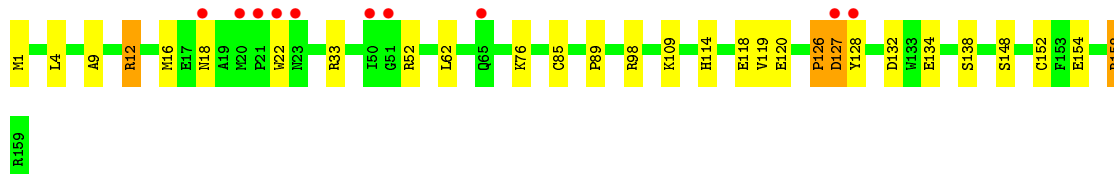
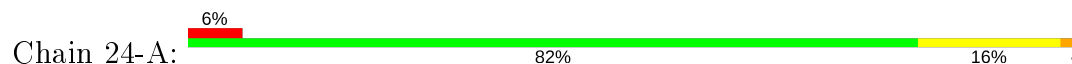
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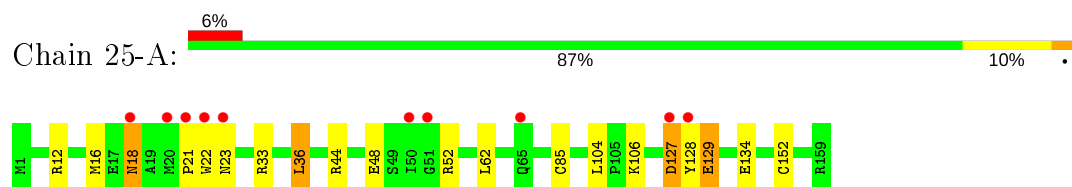
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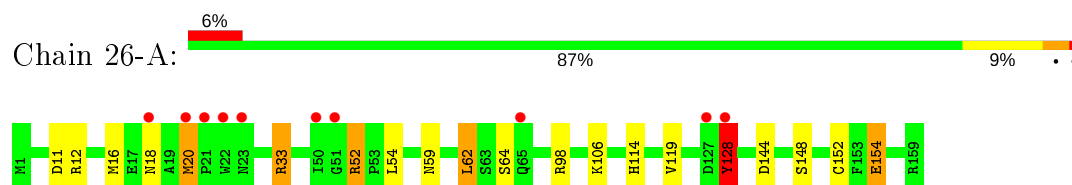
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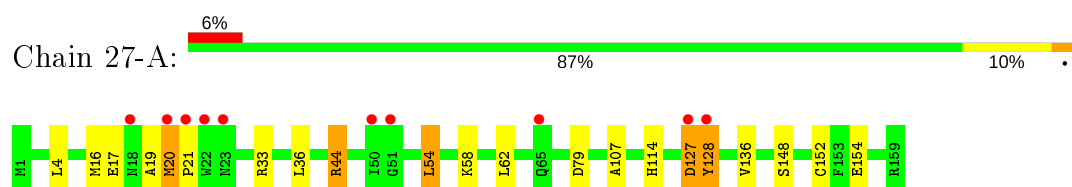
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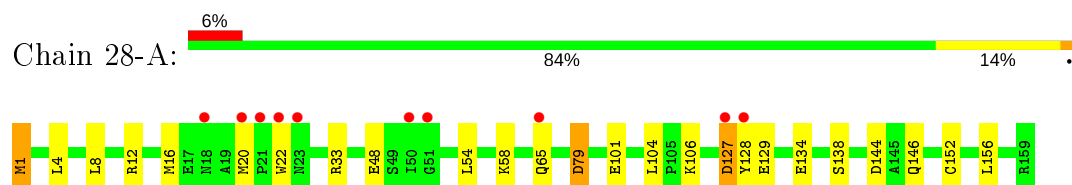
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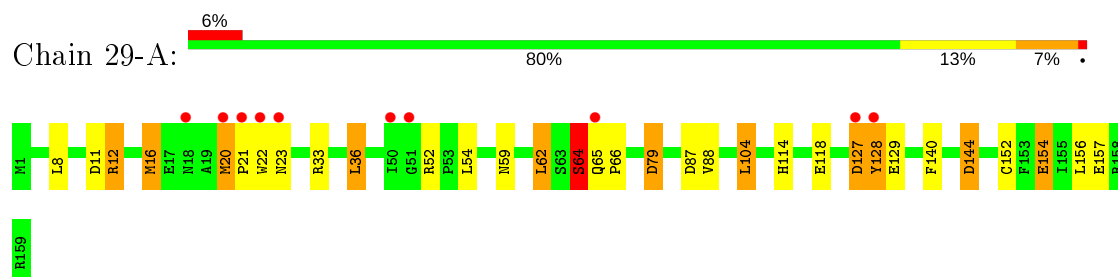
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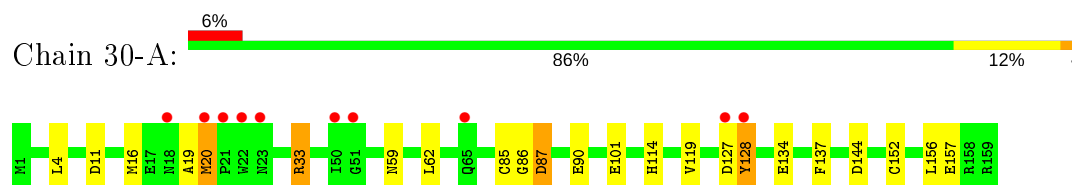
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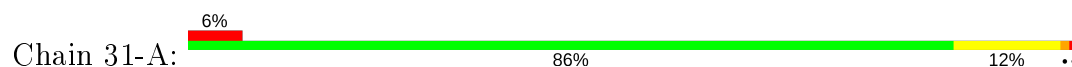
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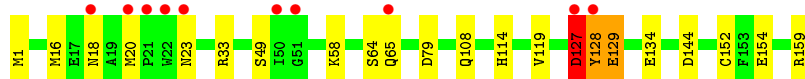


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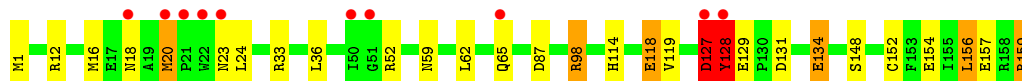
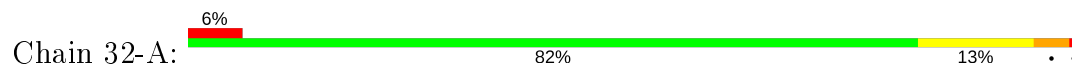


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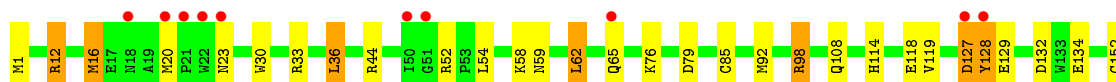
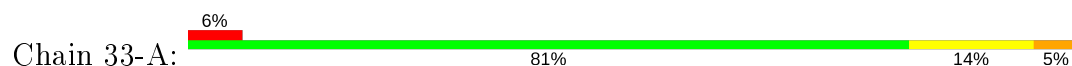




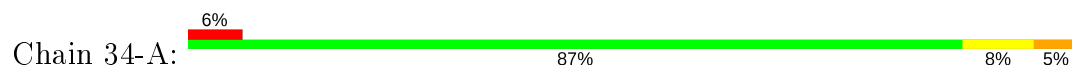
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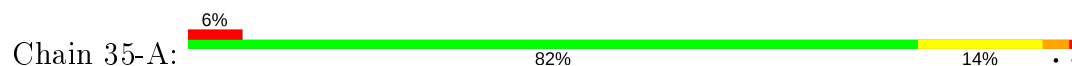
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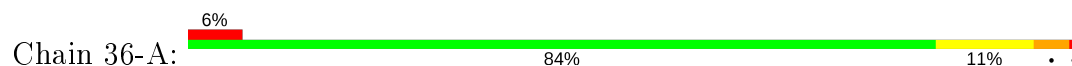
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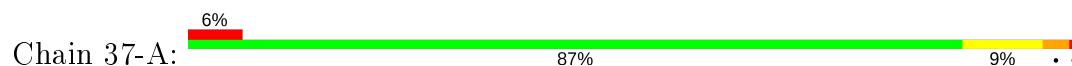
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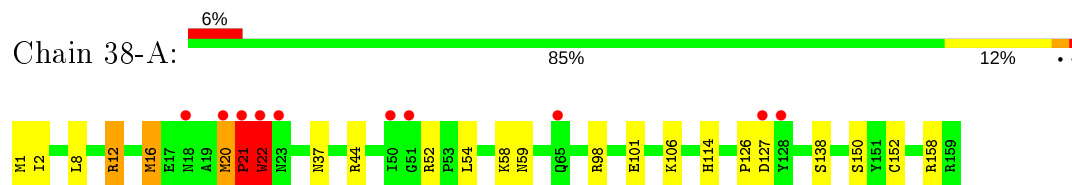
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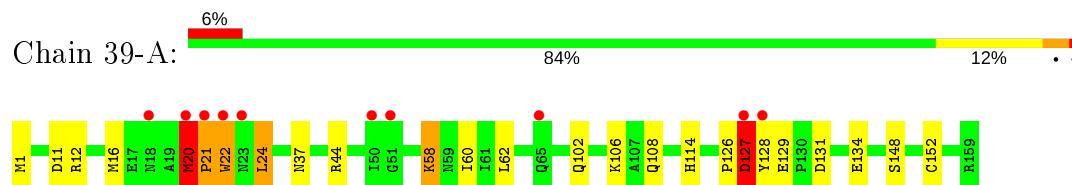
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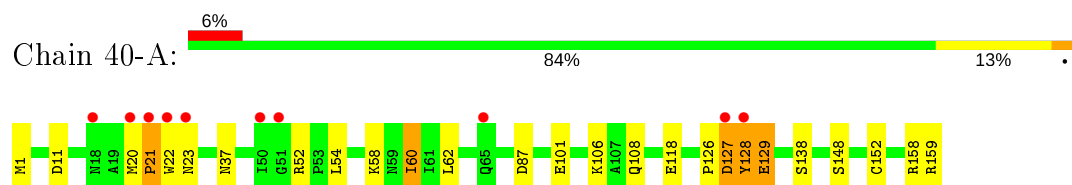
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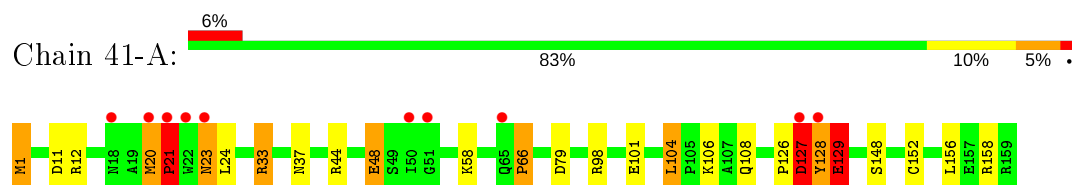
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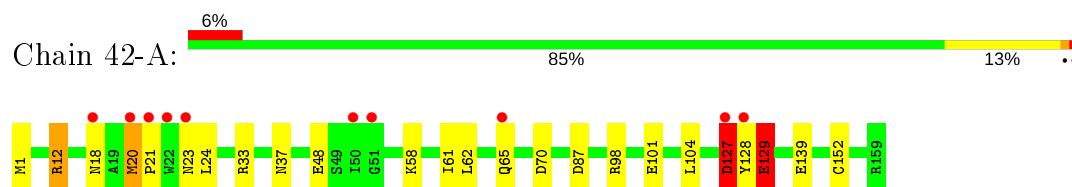
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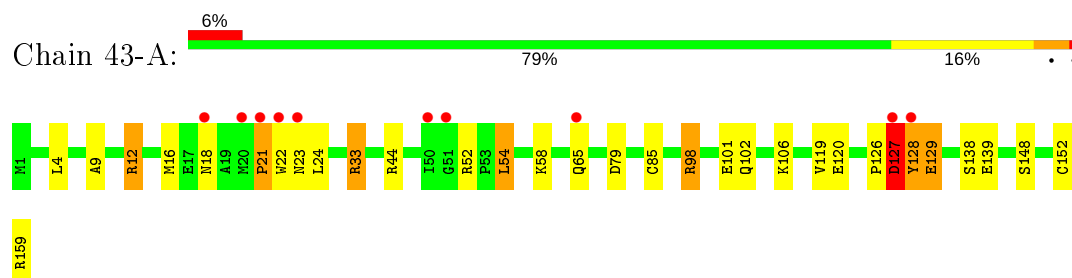
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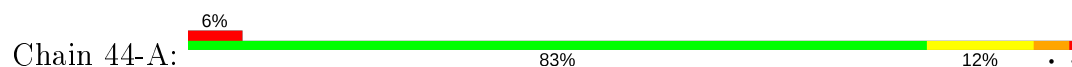
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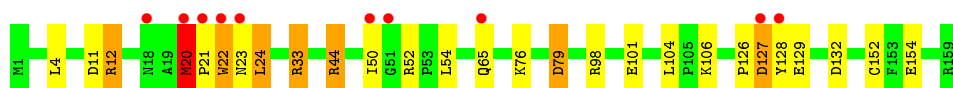


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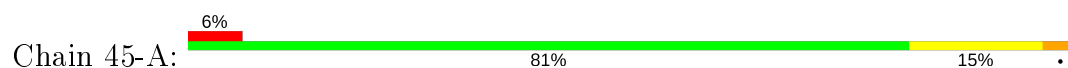


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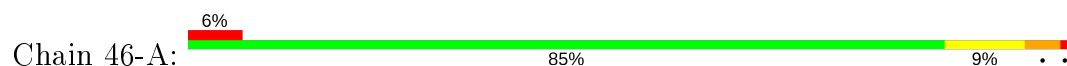




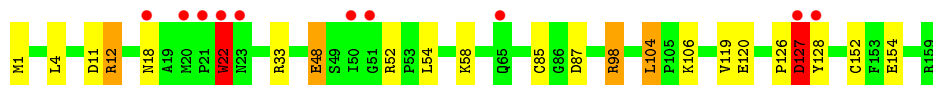
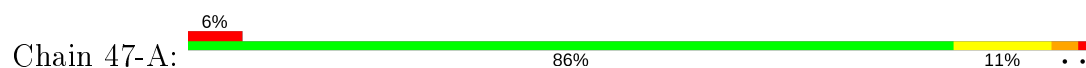
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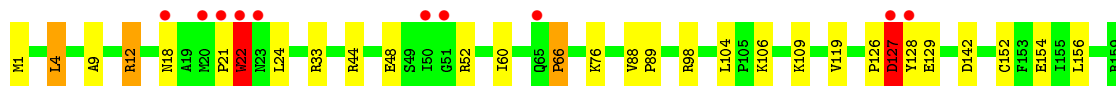
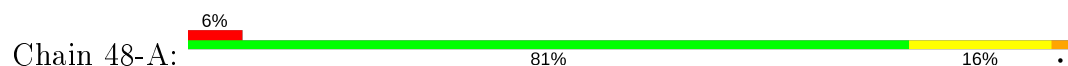
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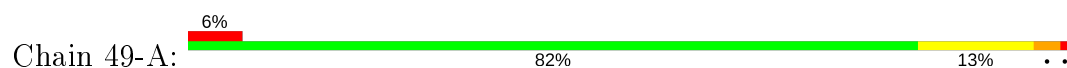
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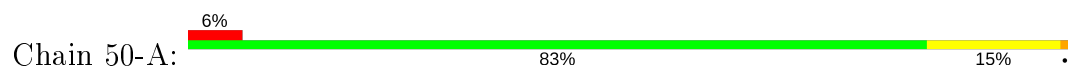
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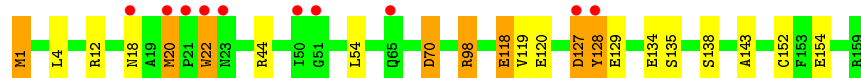
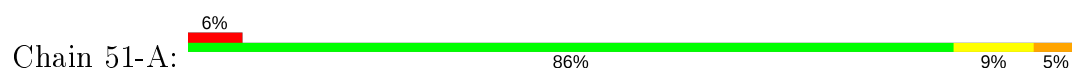
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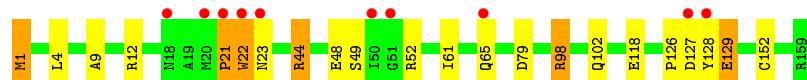
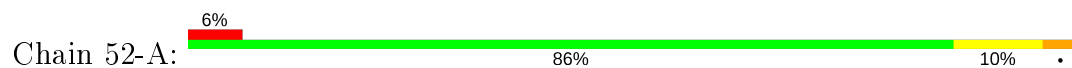
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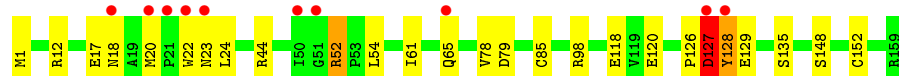
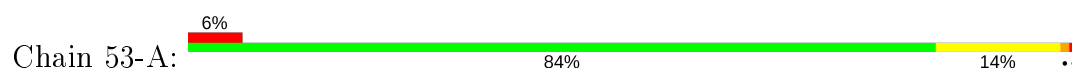
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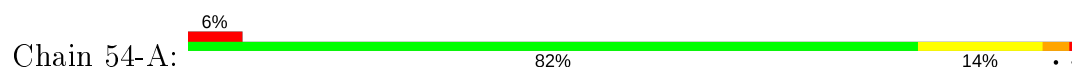
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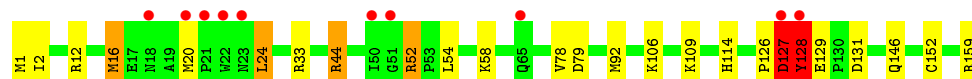
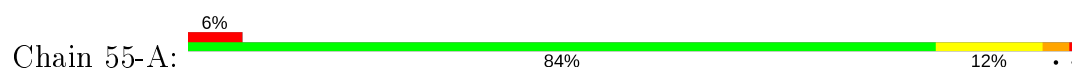
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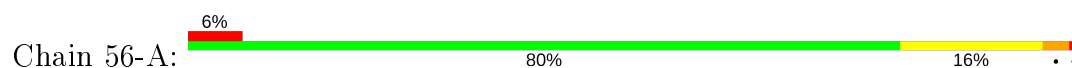
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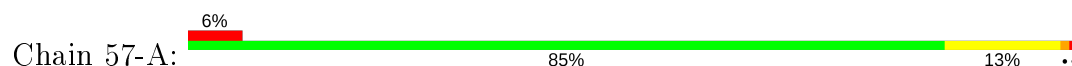
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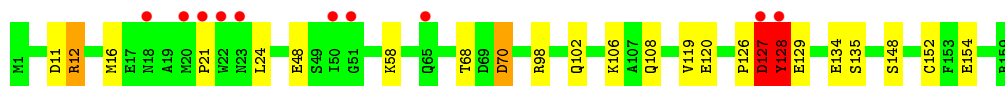


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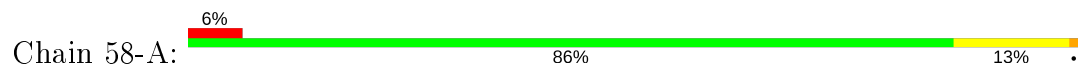


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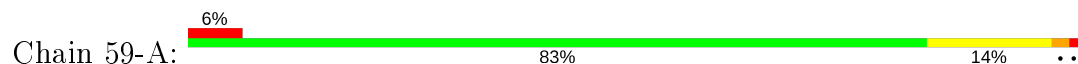




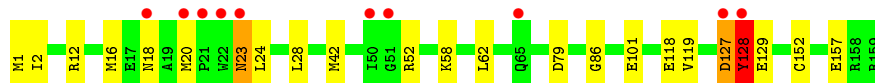
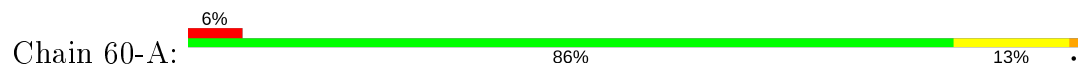
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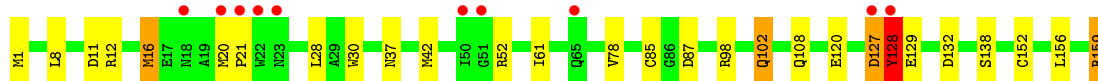
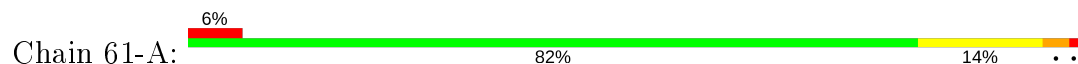
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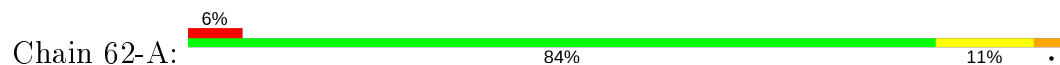
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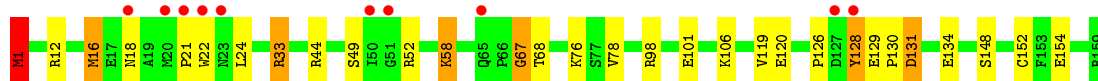
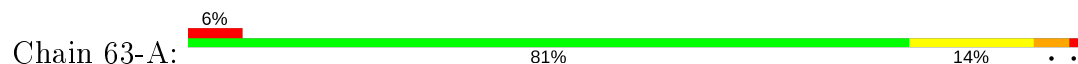
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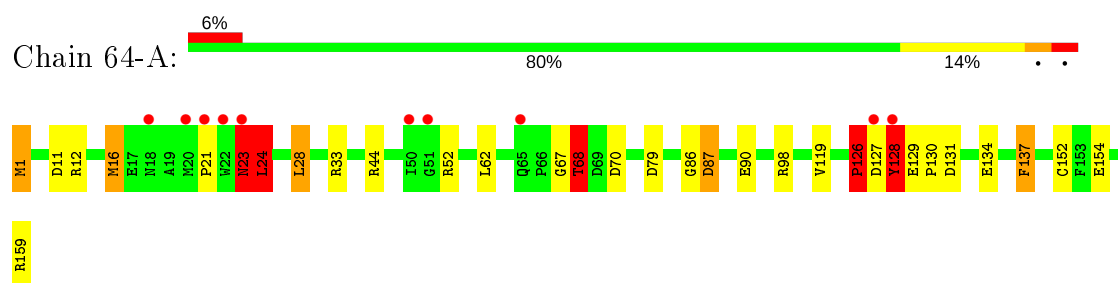
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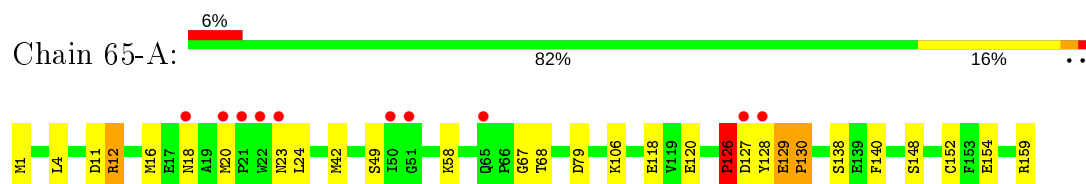
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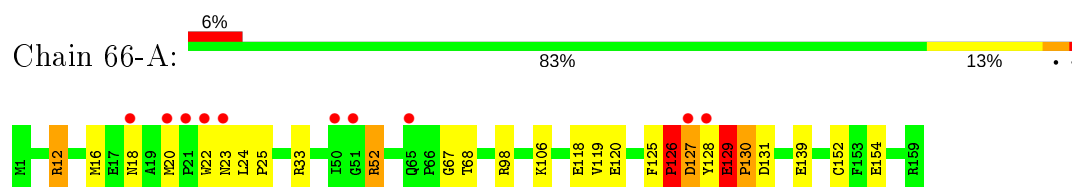
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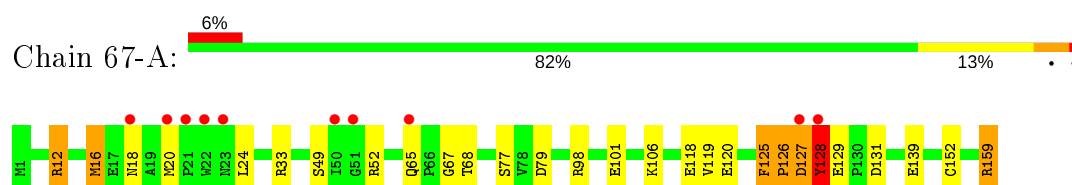
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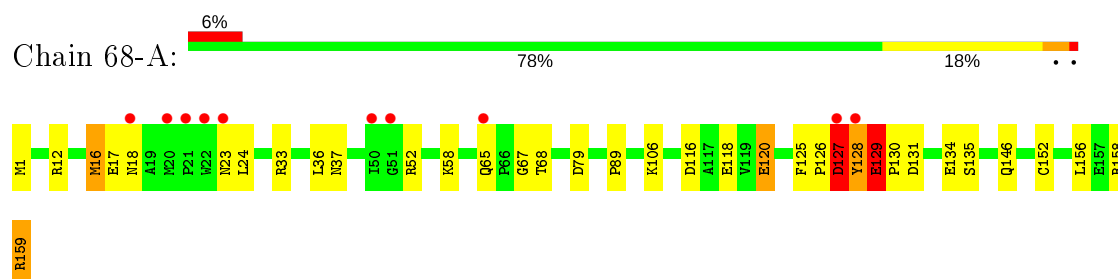
- Molecule 1: Dihydrofolate reductase



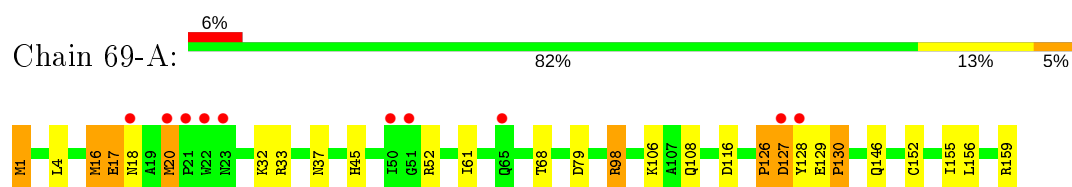
- Molecule 1: Dihydrofolate reductase



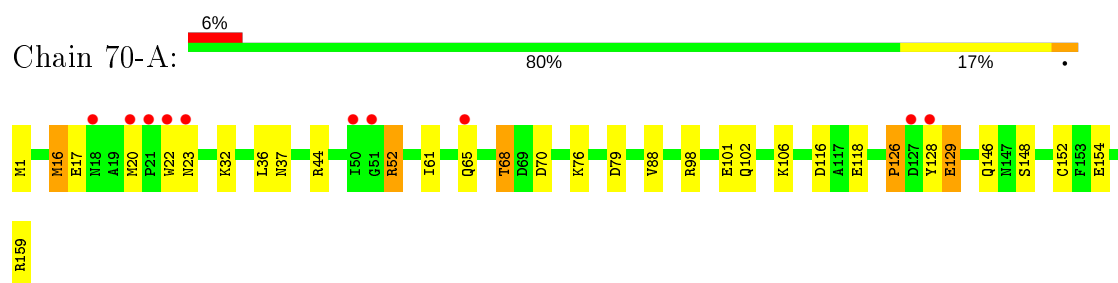
- Molecule 1: Dihydrofolate reductase



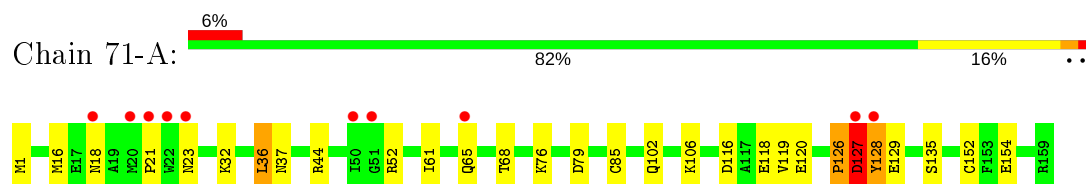
- Molecule 1: Dihydrofolate reductase



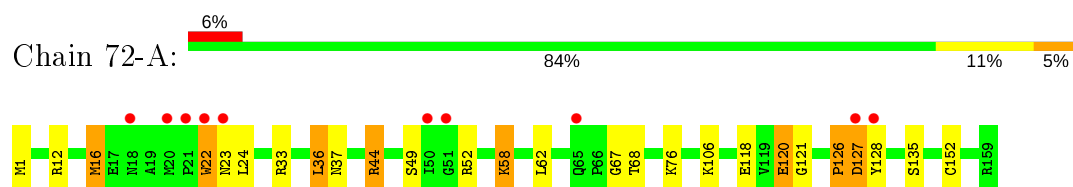
- Molecule 1: Dihydrofolate reductase



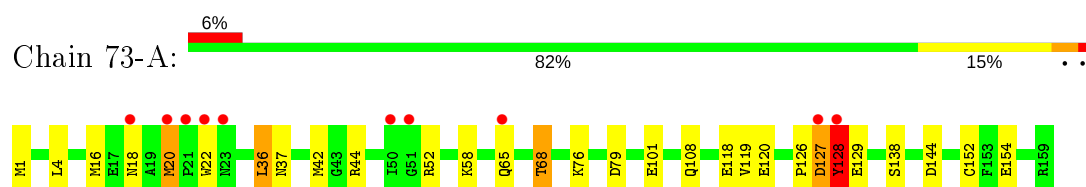
- Molecule 1: Dihydrofolate reductase



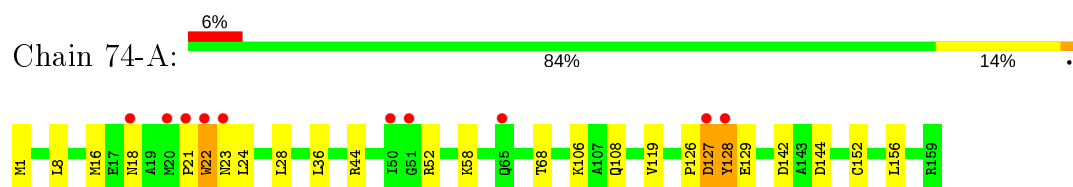
- Molecule 1: Dihydrofolate reductase



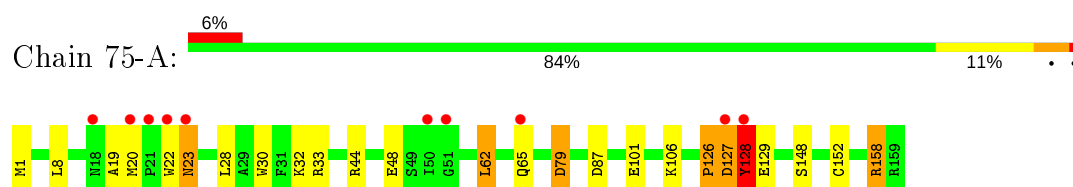
- Molecule 1: Dihydrofolate reductase



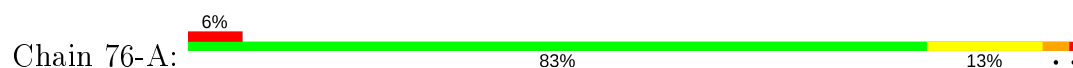
- Molecule 1: Dihydrofolate reductase

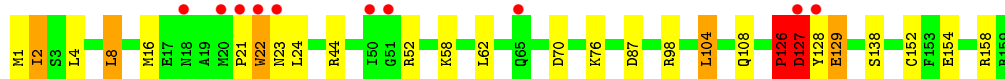


- Molecule 1: Dihydrofolate reductase

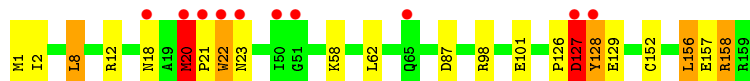
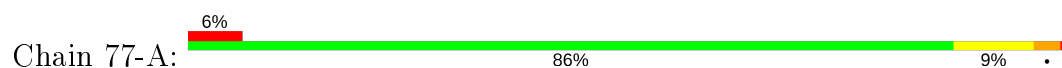


- Molecule 1: Dihydrofolate reductase





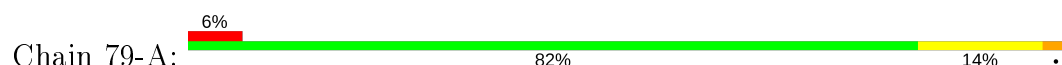
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



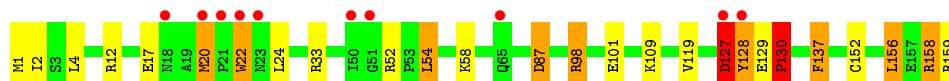
- Molecule 1: Dihydrofolate reductase



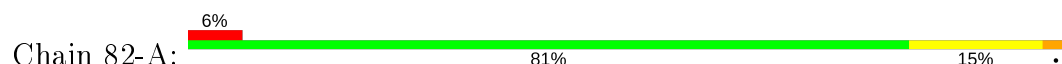
- Molecule 1: Dihydrofolate reductase



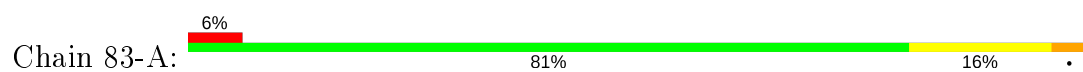
- Molecule 1: Dihydrofolate reductase



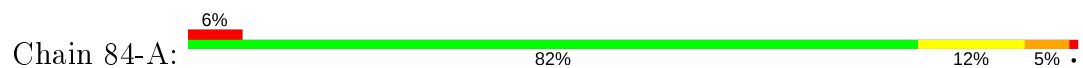
- Molecule 1: Dihydrofolate reductase



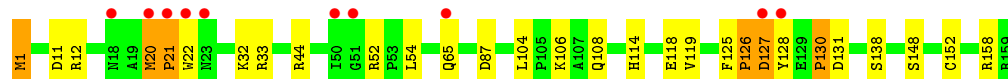
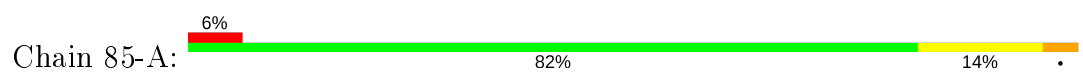
- Molecule 1: Dihydrofolate reductase



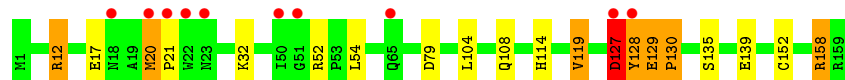
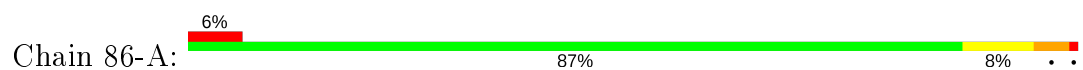
- Molecule 1: Dihydrofolate reductase



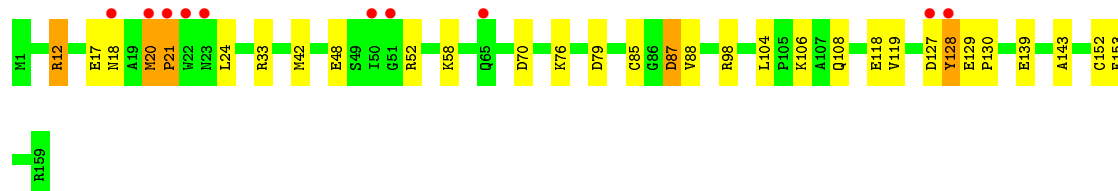
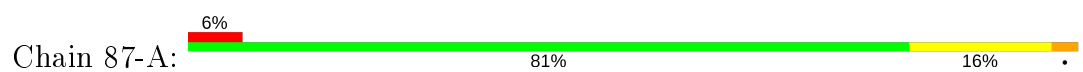
- Molecule 1: Dihydrofolate reductase



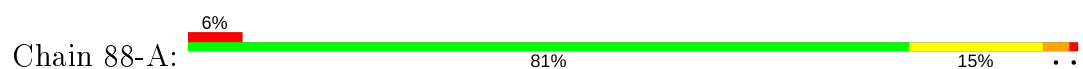
- Molecule 1: Dihydrofolate reductase



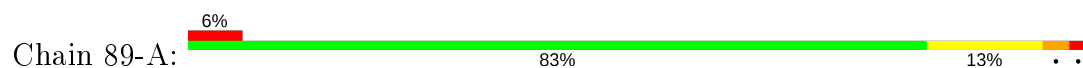
- Molecule 1: Dihydrofolate reductase

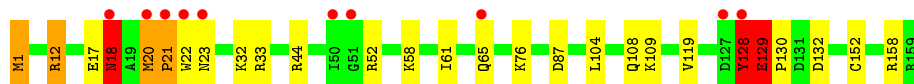


- Molecule 1: Dihydrofolate reductase

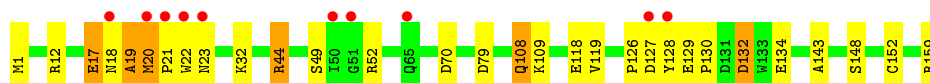
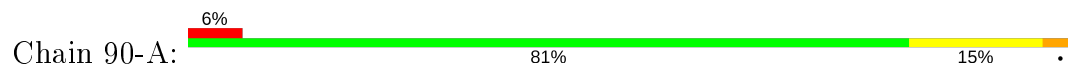


- Molecule 1: Dihydrofolate reductase

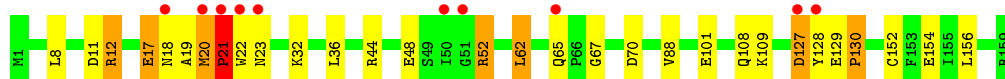
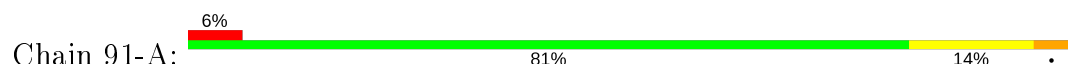




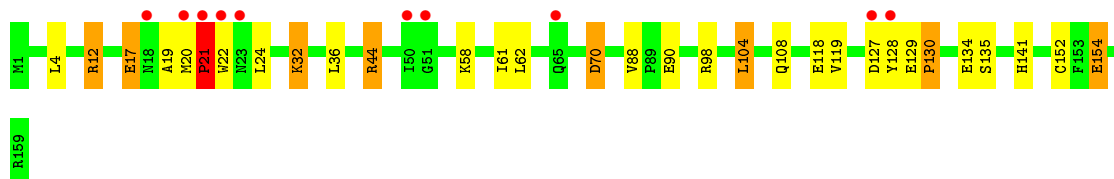
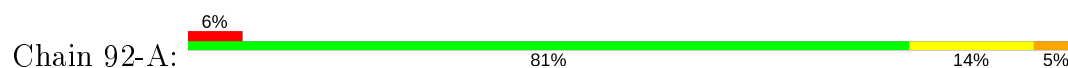
- Molecule 1: Dihydrofolate reductase



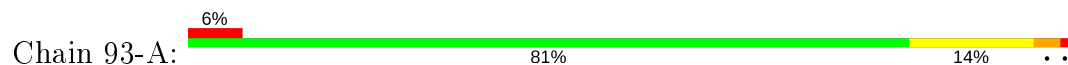
- Molecule 1: Dihydrofolate reductase



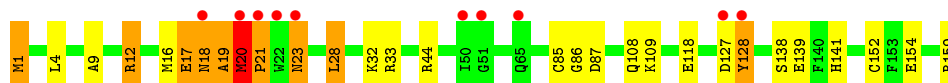
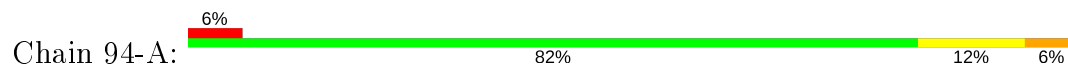
- Molecule 1: Dihydrofolate reductase



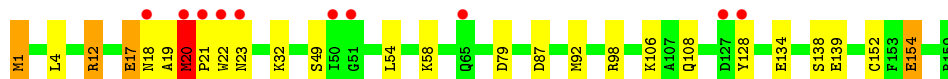
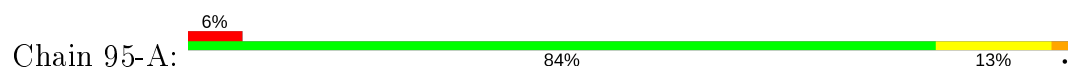
- Molecule 1: Dihydrofolate reductase



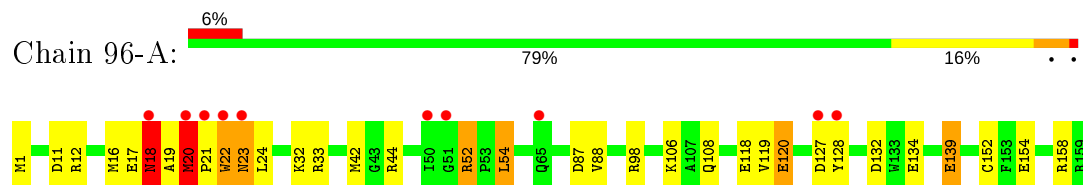
- Molecule 1: Dihydrofolate reductase



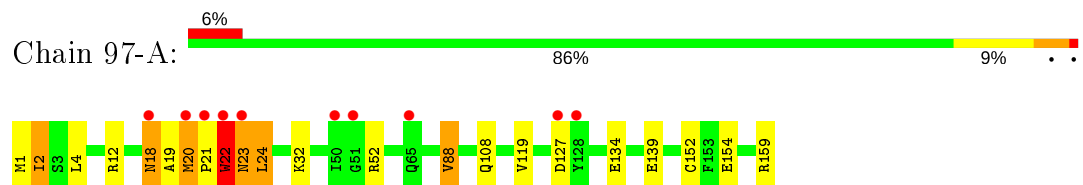
- Molecule 1: Dihydrofolate reductase



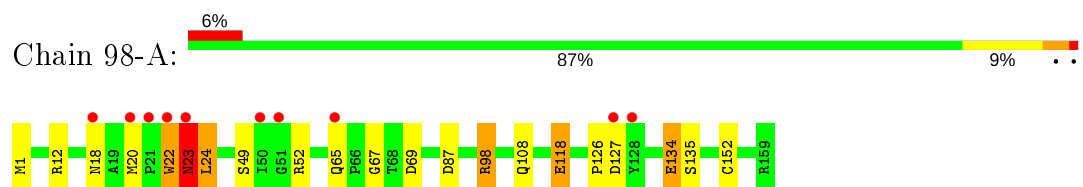
- Molecule 1: Dihydrofolate reductase



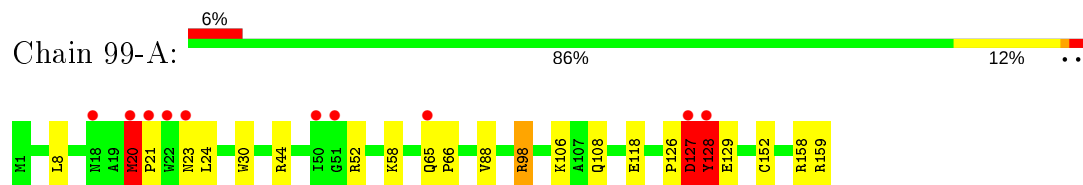
- Molecule 1: Dihydrofolate reductase



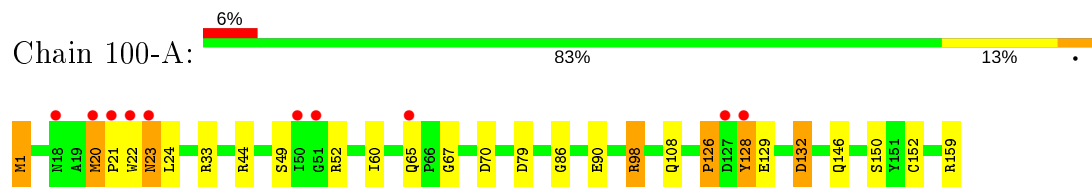
- Molecule 1: Dihydrofolate reductase



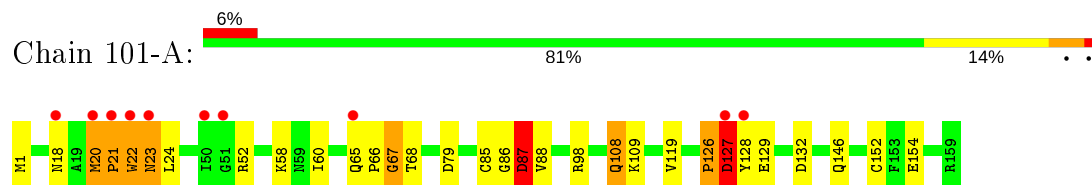
- Molecule 1: Dihydrofolate reductase



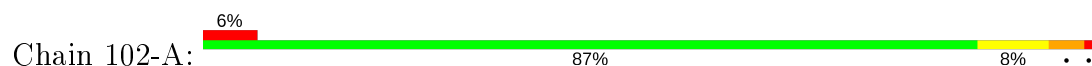
- Molecule 1: Dihydrofolate reductase

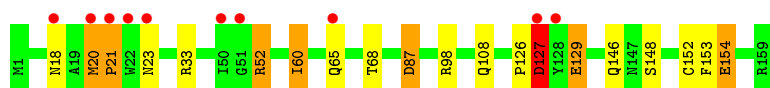


- Molecule 1: Dihydrofolate reductase

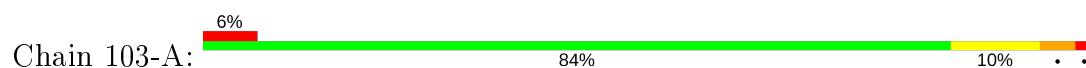


- Molecule 1: Dihydrofolate reductase

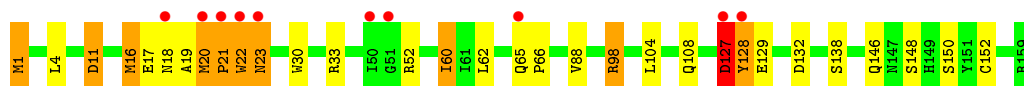
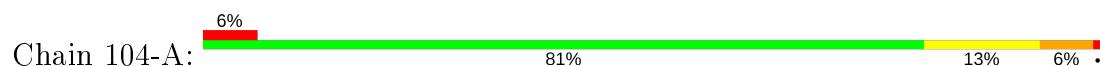




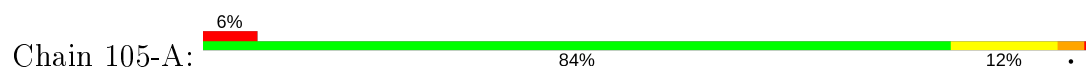
- Molecule 1: Dihydrofolate reductase



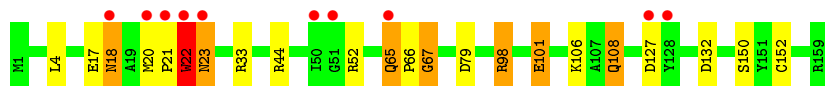
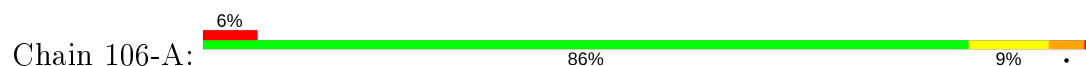
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



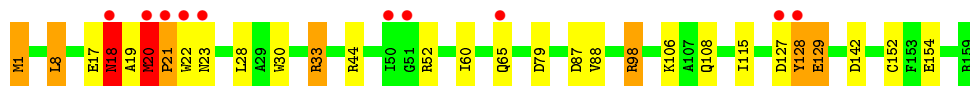
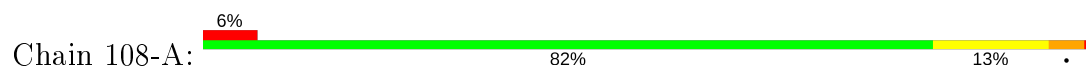
- Molecule 1: Dihydrofolate reductase



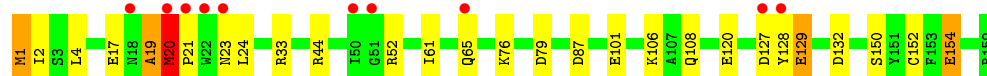
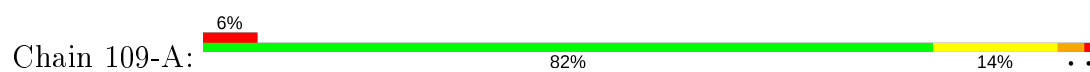
- Molecule 1: Dihydrofolate reductase



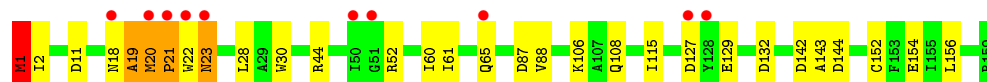
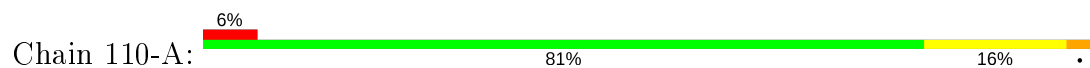
- Molecule 1: Dihydrofolate reductase



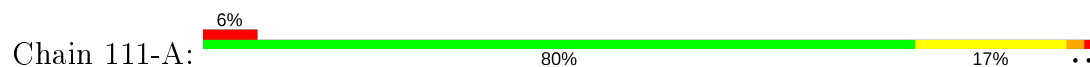
- Molecule 1: Dihydrofolate reductase



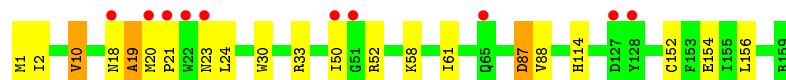
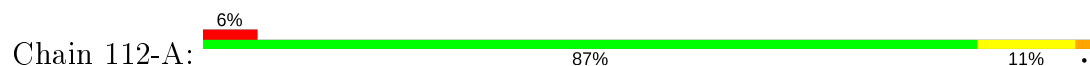
• Molecule 1: Dihydrofolate reductase



• Molecule 1: Dihydrofolate reductase



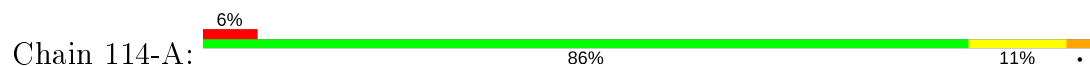
• Molecule 1: Dihydrofolate reductase



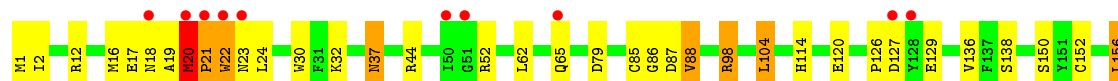
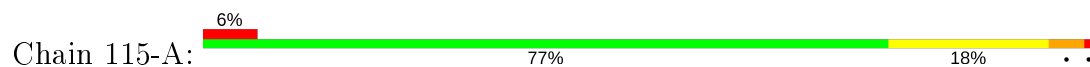
• Molecule 1: Dihydrofolate reductase



• Molecule 1: Dihydrofolate reductase

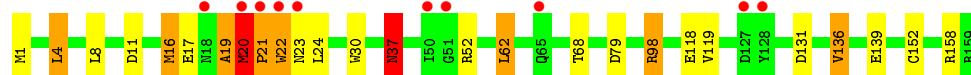
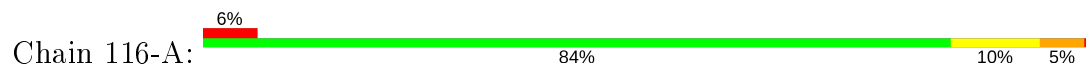


• Molecule 1: Dihydrofolate reductase

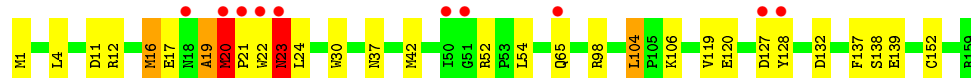
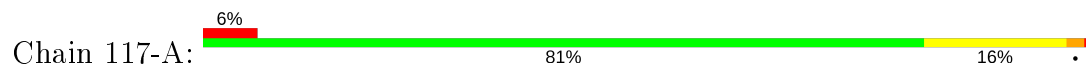




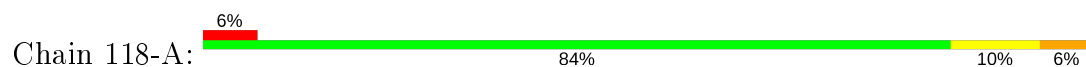
- Molecule 1: Dihydrofolate reductase



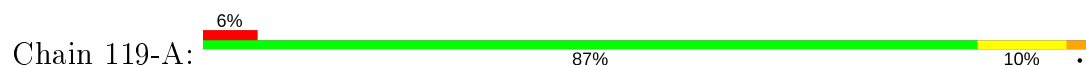
- Molecule 1: Dihydrofolate reductase



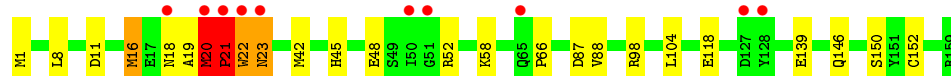
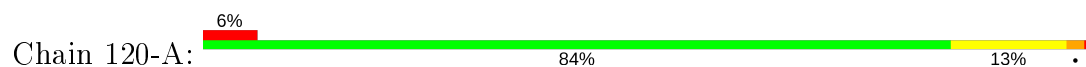
- Molecule 1: Dihydrofolate reductase



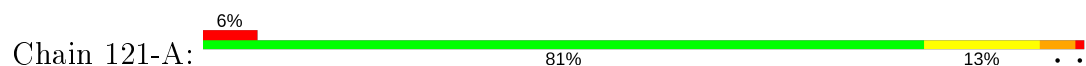
- Molecule 1: Dihydrofolate reductase




- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase

Chain 122-A:  6% 81% 14% . .




• Molecule 1: Dihydrofolate reductase

Chain 123-A:  6% 89% 6% . .




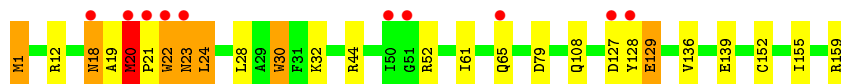
• Molecule 1: Dihydrofolate reductase

Chain 124-A:  6% 83% 13% . .



• Molecule 1: Dihydrofolate reductase

Chain 125-A:  6% 84% 11% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	34.30Å 45.52Å 98.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.40 – 1.05 49.36 – 1.05	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.40-1.05) 96.1 (49.36-1.05)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 1.05Å)	Xtriage
Refinement program	PHENIX 1.8.4-1496	Depositor
R, R_{free}	0.136 , 0.166 0.142 , 0.163	Depositor DCC
R_{free} test set	3666 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	10.4	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 999.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	339833	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.85	1/1296 (0.1%)	1.08	6/1762 (0.3%)
1	2-A	0.87	3/1296 (0.2%)	1.20	14/1762 (0.8%)
1	3-A	0.85	2/1296 (0.2%)	1.11	10/1762 (0.6%)
1	4-A	0.90	4/1296 (0.3%)	1.09	11/1762 (0.6%)
1	5-A	0.87	4/1296 (0.3%)	1.16	12/1762 (0.7%)
1	6-A	0.87	1/1296 (0.1%)	1.17	13/1762 (0.7%)
1	7-A	1.06	7/1296 (0.5%)	1.26	16/1762 (0.9%)
1	8-A	0.88	0/1296	1.18	10/1762 (0.6%)
1	9-A	0.97	3/1296 (0.2%)	1.22	15/1762 (0.9%)
1	10-A	0.91	2/1296 (0.2%)	1.17	15/1762 (0.9%)
1	11-A	0.99	6/1296 (0.5%)	1.19	17/1762 (1.0%)
1	12-A	0.88	2/1296 (0.2%)	1.14	10/1762 (0.6%)
1	13-A	0.92	3/1296 (0.2%)	1.23	12/1762 (0.7%)
1	14-A	0.96	3/1296 (0.2%)	1.25	11/1762 (0.6%)
1	15-A	0.91	2/1296 (0.2%)	1.14	7/1762 (0.4%)
1	16-A	0.81	0/1296	1.08	4/1762 (0.2%)
1	17-A	0.86	3/1296 (0.2%)	1.20	14/1762 (0.8%)
1	18-A	1.00	4/1296 (0.3%)	1.20	14/1762 (0.8%)
1	19-A	0.95	3/1296 (0.2%)	1.19	11/1762 (0.6%)
1	20-A	0.92	5/1296 (0.4%)	1.13	6/1762 (0.3%)
1	21-A	0.86	1/1296 (0.1%)	1.06	8/1762 (0.5%)
1	22-A	0.89	2/1296 (0.2%)	1.16	10/1762 (0.6%)
1	23-A	0.88	3/1296 (0.2%)	1.08	6/1762 (0.3%)
1	24-A	0.96	6/1296 (0.5%)	1.15	11/1762 (0.6%)
1	25-A	0.94	4/1296 (0.3%)	1.05	3/1762 (0.2%)
1	26-A	0.83	2/1296 (0.2%)	1.13	10/1762 (0.6%)
1	27-A	0.91	3/1296 (0.2%)	1.07	5/1762 (0.3%)
1	28-A	1.04	8/1296 (0.6%)	1.25	17/1762 (1.0%)
1	29-A	1.17	8/1296 (0.6%)	1.21	13/1762 (0.7%)
1	30-A	0.85	2/1296 (0.2%)	1.05	4/1762 (0.2%)
1	31-A	0.82	1/1296 (0.1%)	1.03	7/1762 (0.4%)
1	32-A	0.98	4/1296 (0.3%)	1.23	16/1762 (0.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	33-A	0.91	5/1296 (0.4%)	1.14	13/1762 (0.7%)
1	34-A	0.94	4/1296 (0.3%)	1.15	11/1762 (0.6%)
1	35-A	0.87	2/1296 (0.2%)	1.20	14/1762 (0.8%)
1	36-A	0.87	3/1296 (0.2%)	1.12	10/1762 (0.6%)
1	37-A	0.91	5/1296 (0.4%)	1.10	7/1762 (0.4%)
1	38-A	0.95	5/1296 (0.4%)	1.19	10/1762 (0.6%)
1	39-A	0.91	1/1296 (0.1%)	1.06	7/1762 (0.4%)
1	40-A	0.84	1/1296 (0.1%)	1.11	9/1762 (0.5%)
1	41-A	0.94	3/1296 (0.2%)	1.22	16/1762 (0.9%)
1	42-A	0.85	1/1296 (0.1%)	1.21	9/1762 (0.5%)
1	43-A	0.97	4/1296 (0.3%)	1.18	11/1762 (0.6%)
1	44-A	0.97	4/1296 (0.3%)	1.20	13/1762 (0.7%)
1	45-A	1.05	9/1296 (0.7%)	1.13	8/1762 (0.5%)
1	46-A	0.92	4/1296 (0.3%)	1.16	11/1762 (0.6%)
1	47-A	1.01	8/1296 (0.6%)	1.15	8/1762 (0.5%)
1	48-A	0.90	2/1296 (0.2%)	1.16	12/1762 (0.7%)
1	49-A	0.98	8/1296 (0.6%)	1.08	4/1762 (0.2%)
1	50-A	0.92	4/1296 (0.3%)	1.07	9/1762 (0.5%)
1	51-A	0.94	3/1296 (0.2%)	1.16	11/1762 (0.6%)
1	52-A	1.00	6/1296 (0.5%)	1.06	6/1762 (0.3%)
1	53-A	0.87	3/1296 (0.2%)	1.07	10/1762 (0.6%)
1	54-A	1.01	6/1296 (0.5%)	1.15	11/1762 (0.6%)
1	55-A	0.96	4/1296 (0.3%)	1.20	17/1762 (1.0%)
1	56-A	0.89	4/1296 (0.3%)	1.13	10/1762 (0.6%)
1	57-A	0.95	3/1296 (0.2%)	1.20	13/1762 (0.7%)
1	58-A	0.95	3/1296 (0.2%)	1.13	7/1762 (0.4%)
1	59-A	0.85	1/1296 (0.1%)	1.10	9/1762 (0.5%)
1	60-A	0.87	0/1296	1.12	7/1762 (0.4%)
1	61-A	0.98	7/1296 (0.5%)	1.15	11/1762 (0.6%)
1	62-A	0.94	3/1296 (0.2%)	1.14	7/1762 (0.4%)
1	63-A	1.05	4/1296 (0.3%)	1.23	16/1762 (0.9%)
1	64-A	1.32	8/1296 (0.6%)	1.36	22/1762 (1.2%)
1	65-A	0.90	2/1296 (0.2%)	1.09	7/1762 (0.4%)
1	66-A	1.03	3/1296 (0.2%)	1.23	12/1762 (0.7%)
1	67-A	0.91	4/1296 (0.3%)	1.17	15/1762 (0.9%)
1	68-A	1.01	7/1296 (0.5%)	1.30	15/1762 (0.9%)
1	69-A	0.90	1/1296 (0.1%)	1.13	8/1762 (0.5%)
1	70-A	0.89	1/1296 (0.1%)	1.23	17/1762 (1.0%)
1	71-A	0.93	5/1296 (0.4%)	1.06	5/1762 (0.3%)
1	72-A	0.93	4/1296 (0.3%)	1.22	13/1762 (0.7%)
1	73-A	0.94	3/1296 (0.2%)	1.16	12/1762 (0.7%)
1	74-A	0.94	3/1296 (0.2%)	1.08	5/1762 (0.3%)
1	75-A	0.94	1/1296 (0.1%)	1.15	7/1762 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	76-A	0.95	3/1296 (0.2%)	1.20	13/1762 (0.7%)
1	77-A	0.99	5/1296 (0.4%)	1.16	10/1762 (0.6%)
1	78-A	0.94	2/1296 (0.2%)	1.17	11/1762 (0.6%)
1	79-A	1.09	5/1296 (0.4%)	1.17	8/1762 (0.5%)
1	80-A	0.91	2/1296 (0.2%)	1.15	11/1762 (0.6%)
1	81-A	0.95	4/1296 (0.3%)	1.21	15/1762 (0.9%)
1	82-A	1.05	8/1296 (0.6%)	1.16	14/1762 (0.8%)
1	83-A	0.97	6/1296 (0.5%)	1.22	14/1762 (0.8%)
1	84-A	0.98	6/1296 (0.5%)	1.19	15/1762 (0.9%)
1	85-A	0.85	0/1296	1.25	13/1762 (0.7%)
1	86-A	0.93	3/1296 (0.2%)	1.11	6/1762 (0.3%)
1	87-A	0.89	2/1296 (0.2%)	1.10	6/1762 (0.3%)
1	88-A	0.92	0/1296	1.22	13/1762 (0.7%)
1	89-A	0.93	3/1296 (0.2%)	1.14	9/1762 (0.5%)
1	90-A	0.88	1/1296 (0.1%)	1.15	13/1762 (0.7%)
1	91-A	0.99	3/1296 (0.2%)	1.18	13/1762 (0.7%)
1	92-A	0.96	4/1296 (0.3%)	1.24	13/1762 (0.7%)
1	93-A	1.02	7/1296 (0.5%)	1.28	14/1762 (0.8%)
1	94-A	0.93	4/1296 (0.3%)	1.17	11/1762 (0.6%)
1	95-A	0.99	6/1296 (0.5%)	1.14	9/1762 (0.5%)
1	96-A	1.01	4/1296 (0.3%)	1.32	17/1762 (1.0%)
1	97-A	0.89	3/1296 (0.2%)	1.13	12/1762 (0.7%)
1	98-A	1.00	6/1296 (0.5%)	1.22	13/1762 (0.7%)
1	99-A	0.88	3/1296 (0.2%)	1.12	12/1762 (0.7%)
1	100-A	0.89	1/1296 (0.1%)	1.17	11/1762 (0.6%)
1	101-A	0.94	4/1296 (0.3%)	1.15	11/1762 (0.6%)
1	102-A	0.95	5/1296 (0.4%)	1.19	13/1762 (0.7%)
1	103-A	0.92	2/1296 (0.2%)	1.13	11/1762 (0.6%)
1	104-A	0.97	6/1296 (0.5%)	1.24	14/1762 (0.8%)
1	105-A	0.88	3/1296 (0.2%)	1.09	8/1762 (0.5%)
1	106-A	0.93	4/1296 (0.3%)	1.15	8/1762 (0.5%)
1	107-A	0.96	4/1296 (0.3%)	1.17	11/1762 (0.6%)
1	108-A	1.05	5/1296 (0.4%)	1.17	16/1762 (0.9%)
1	109-A	1.04	5/1296 (0.4%)	1.23	11/1762 (0.6%)
1	110-A	1.30	5/1296 (0.4%)	1.16	9/1762 (0.5%)
1	111-A	1.34	5/1296 (0.4%)	1.16	11/1762 (0.6%)
1	112-A	1.36	3/1296 (0.2%)	1.16	8/1762 (0.5%)
1	113-A	0.95	6/1296 (0.5%)	1.06	6/1762 (0.3%)
1	114-A	0.88	0/1296	1.11	8/1762 (0.5%)
1	115-A	0.93	5/1296 (0.4%)	1.22	14/1762 (0.8%)
1	116-A	0.93	3/1296 (0.2%)	1.17	11/1762 (0.6%)
1	117-A	0.99	4/1296 (0.3%)	1.12	12/1762 (0.7%)
1	118-A	0.96	4/1296 (0.3%)	1.18	9/1762 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	119-A	1.00	5/1296 (0.4%)	1.14	9/1762 (0.5%)
1	120-A	0.96	3/1296 (0.2%)	1.10	7/1762 (0.4%)
1	121-A	1.01	5/1296 (0.4%)	1.15	12/1762 (0.7%)
1	122-A	0.97	5/1296 (0.4%)	1.22	11/1762 (0.6%)
1	123-A	0.94	5/1296 (0.4%)	1.11	7/1762 (0.4%)
1	124-A	0.98	5/1296 (0.4%)	1.15	12/1762 (0.7%)
1	125-A	1.10	5/1296 (0.4%)	1.12	12/1762 (0.7%)
All	All	0.96	461/162000 (0.3%)	1.16	1350/220250 (0.6%)

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	3
1	3-A	0	3
1	4-A	0	3
1	5-A	0	2
1	6-A	0	2
1	7-A	0	5
1	8-A	0	4
1	9-A	0	4
1	10-A	0	4
1	11-A	0	3
1	12-A	0	3
1	13-A	0	3
1	14-A	0	2
1	15-A	0	3
1	16-A	0	4
1	17-A	0	4
1	18-A	0	2
1	19-A	0	2
1	21-A	0	1
1	22-A	0	3
1	23-A	0	3
1	24-A	0	2
1	26-A	0	1
1	27-A	0	1
1	29-A	0	2
1	30-A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	31-A	0	2
1	32-A	0	2
1	33-A	0	1
1	36-A	0	2
1	38-A	0	1
1	39-A	0	3
1	40-A	0	2
1	41-A	0	3
1	42-A	0	1
1	43-A	0	3
1	44-A	0	2
1	45-A	0	1
1	46-A	0	2
1	47-A	0	2
1	48-A	0	1
1	49-A	0	2
1	50-A	0	2
1	52-A	0	2
1	54-A	0	4
1	55-A	0	2
1	56-A	0	2
1	57-A	0	2
1	58-A	0	2
1	59-A	0	1
1	60-A	0	1
1	61-A	0	1
1	62-A	0	1
1	63-A	0	3
1	64-A	0	3
1	65-A	0	2
1	66-A	0	6
1	67-A	0	2
1	68-A	0	3
1	69-A	0	3
1	70-A	0	2
1	71-A	0	2
1	72-A	0	1
1	73-A	0	3
1	74-A	0	1
1	75-A	0	4
1	76-A	0	3
1	77-A	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	78-A	0	2
1	79-A	0	1
1	81-A	0	1
1	82-A	0	1
1	83-A	0	2
1	84-A	0	1
1	85-A	0	1
1	86-A	0	1
1	87-A	0	3
1	88-A	0	2
1	89-A	0	2
1	90-A	0	3
1	91-A	0	3
1	92-A	0	2
1	93-A	0	4
1	94-A	0	3
1	95-A	0	2
1	96-A	0	4
1	98-A	0	2
1	99-A	0	2
1	100-A	0	3
1	101-A	0	4
1	102-A	0	4
1	103-A	0	2
1	104-A	0	2
1	105-A	0	1
1	106-A	0	1
1	107-A	0	1
1	108-A	0	3
1	109-A	0	3
1	110-A	0	3
1	111-A	0	3
1	112-A	0	3
1	113-A	0	1
1	114-A	0	4
1	115-A	0	3
1	116-A	0	2
1	117-A	0	2
1	118-A	0	3
1	119-A	0	1
1	120-A	0	2
1	121-A	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	122-A	0	1
1	123-A	0	2
1	124-A	0	2
1	125-A	0	2
All	All	0	267

The worst 5 of 461 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	111-A	30	TRP	CB-CG	35.12	2.13	1.50
1	112-A	30	TRP	CB-CG	34.17	2.11	1.50
1	110-A	30	TRP	CB-CG	28.63	2.01	1.50
1	64-A	154	GLU	CB-CG	21.19	1.92	1.52
1	125-A	30	TRP	CB-CG	20.27	1.86	1.50

The worst 5 of 1350 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	68-A	16	MET	CG-SD-CE	-21.11	66.42	100.20
1	64-A	12	ARG	NE-CZ-NH2	20.89	130.75	120.30
1	85-A	125	PHE	C-N-CD	-19.27	78.22	120.60
1	98-A	12	ARG	NE-CZ-NH2	-17.49	111.56	120.30
1	19-A	52	ARG	NE-CZ-NH1	-15.53	112.53	120.30

There are no chirality outliers.

5 of 267 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	128	TYR	Peptide
1	2-A	126	PRO	Peptide
1	2-A	128	TYR	Peptide
1	2-A	16	MET	Peptide
1	3-A	16	MET	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1270	1221	1221	0	0
1	2-A	1270	1221	1221	0	0
1	3-A	1270	1221	1220	0	0
1	4-A	1270	1221	1221	0	0
1	5-A	1270	1221	1221	0	0
1	6-A	1270	1221	1221	0	0
1	7-A	1270	1221	1221	0	0
1	8-A	1270	1221	1221	0	0
1	9-A	1270	1221	1220	0	0
1	10-A	1270	1221	1221	0	0
1	11-A	1270	1221	1221	0	0
1	12-A	1270	1221	1220	0	0
1	13-A	1270	1221	1221	0	0
1	14-A	1270	1221	1221	0	0
1	15-A	1270	1221	1221	0	0
1	16-A	1270	1221	1221	0	0
1	17-A	1270	1221	1221	0	0
1	18-A	1270	1221	1221	0	0
1	19-A	1270	1221	1221	0	0
1	20-A	1270	1221	1221	0	0
1	21-A	1270	1221	1221	0	0
1	22-A	1270	1221	1221	0	0
1	23-A	1270	1221	1221	0	0
1	24-A	1270	1221	1221	0	0
1	25-A	1270	1221	1221	0	0
1	26-A	1270	1221	1221	0	0
1	27-A	1270	1221	1221	0	0
1	28-A	1270	1221	1221	0	0
1	29-A	1270	1221	1221	0	0
1	30-A	1270	1221	1221	0	0
1	31-A	1270	1221	1221	0	0
1	32-A	1270	1221	1221	0	0
1	33-A	1270	1221	1221	0	0
1	34-A	1270	1221	1221	0	0
1	35-A	1270	1221	1221	0	0
1	36-A	1270	1221	1221	0	0
1	37-A	1270	1221	1220	0	0
1	38-A	1270	1221	1221	0	0
1	39-A	1270	1221	1221	0	0
1	40-A	1270	1221	1221	0	0
1	41-A	1270	1221	1221	0	0
1	42-A	1270	1221	1221	0	0
1	43-A	1270	1221	1221	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	44-A	1270	1221	1221	0	0
1	45-A	1270	1221	1221	0	0
1	46-A	1270	1221	1221	0	0
1	47-A	1270	1221	1221	0	0
1	48-A	1270	1221	1221	0	0
1	49-A	1270	1221	1221	0	0
1	50-A	1270	1221	1221	0	0
1	51-A	1270	1221	1222	0	0
1	52-A	1270	1221	1221	0	0
1	53-A	1270	1221	1221	0	0
1	54-A	1270	1221	1221	0	0
1	55-A	1270	1221	1220	0	0
1	56-A	1270	1221	1221	0	0
1	57-A	1270	1221	1221	0	0
1	58-A	1270	1221	1221	0	0
1	59-A	1270	1221	1221	0	0
1	60-A	1270	1221	1220	0	0
1	61-A	1270	1221	1221	0	0
1	62-A	1270	1221	1221	0	0
1	63-A	1270	1221	1221	0	0
1	64-A	1270	1221	1221	0	0
1	65-A	1270	1221	1221	0	0
1	66-A	1270	1221	1221	0	0
1	67-A	1270	1221	1221	0	0
1	68-A	1270	1221	1221	0	0
1	69-A	1270	1221	1221	0	0
1	70-A	1270	1221	1221	0	0
1	71-A	1270	1221	1221	0	0
1	72-A	1270	1221	1221	0	0
1	73-A	1270	1221	1221	0	0
1	74-A	1270	1221	1221	0	0
1	75-A	1270	1221	1221	0	0
1	76-A	1270	1221	1221	0	0
1	77-A	1270	1221	1221	0	0
1	78-A	1270	1221	1221	0	0
1	79-A	1270	1221	1222	0	0
1	80-A	1270	1221	1222	0	0
1	81-A	1270	1221	1221	0	0
1	82-A	1270	1221	1222	0	0
1	83-A	1270	1221	1221	0	0
1	84-A	1270	1221	1221	0	0
1	85-A	1270	1221	1221	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	86-A	1270	1221	1221	0	0
1	87-A	1270	1221	1221	0	0
1	88-A	1270	1221	1220	0	0
1	89-A	1270	1221	1221	0	0
1	90-A	1270	1221	1221	0	0
1	91-A	1270	1221	1221	0	0
1	92-A	1270	1221	1221	0	0
1	93-A	1270	1221	1220	0	0
1	94-A	1270	1221	1221	0	0
1	95-A	1270	1221	1221	0	0
1	96-A	1270	1221	1221	0	0
1	97-A	1270	1221	1221	0	0
1	98-A	1270	1221	1221	0	0
1	99-A	1270	1221	1220	0	0
1	100-A	1270	1221	1221	0	0
1	101-A	1270	1221	1221	0	0
1	102-A	1270	1221	1221	0	0
1	103-A	1270	1221	1221	0	0
1	104-A	1270	1221	1221	0	0
1	105-A	1270	1221	1221	0	0
1	106-A	1270	1221	1221	0	0
1	107-A	1270	1221	1221	0	0
1	108-A	1270	1221	1221	0	0
1	109-A	1270	1221	1221	0	0
1	110-A	1270	1221	1221	0	0
1	111-A	1270	1221	1220	0	0
1	112-A	1270	1221	1220	0	0
1	113-A	1270	1221	1219	0	0
1	114-A	1270	1221	1221	0	0
1	115-A	1270	1221	1221	0	0
1	116-A	1270	1221	1221	0	0
1	117-A	1270	1221	1221	0	0
1	118-A	1270	1221	1221	0	0
1	119-A	1270	1221	1221	0	0
1	120-A	1270	1221	1221	0	0
1	121-A	1270	1221	1221	0	0
1	122-A	1270	1221	1221	0	0
1	123-A	1270	1221	1221	0	0
1	124-A	1270	1221	1221	0	0
1	125-A	1270	1221	1221	0	0
2	1-A	32	17	17	0	0
2	2-A	32	17	17	0	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	16	0	0
2	63-A	32	17	17	0	0
2	64-A	32	17	16	0	0
2	65-A	32	17	17	0	0
2	66-A	32	17	17	0	0
2	67-A	32	17	16	0	0
2	68-A	32	17	16	0	0
2	69-A	32	17	17	0	0
2	70-A	32	17	15	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	87-A	32	17	17	0	0
2	88-A	32	17	17	0	0
2	89-A	32	17	17	0	0
2	90-A	32	17	17	0	0
2	91-A	32	17	17	0	0
2	92-A	32	17	17	0	0
2	93-A	32	17	17	0	0
2	94-A	32	17	17	0	0
2	95-A	32	17	17	0	0
2	96-A	32	17	17	0	0
2	97-A	32	17	17	0	0
2	98-A	32	17	17	0	0
2	99-A	32	17	17	0	0
2	100-A	32	17	17	0	0
2	101-A	32	17	17	0	0
2	102-A	32	17	17	0	0
2	103-A	32	17	17	0	0
2	104-A	32	17	17	0	0
2	105-A	32	17	17	0	0
2	106-A	32	17	17	0	0
2	107-A	32	17	17	0	0
2	108-A	32	17	17	0	0
2	109-A	32	17	17	0	0
2	110-A	32	17	17	0	0
2	111-A	32	17	17	0	0
2	112-A	32	17	17	0	0
2	113-A	32	17	17	0	0
2	114-A	32	17	17	0	0
2	115-A	32	17	17	0	0
2	116-A	32	17	17	0	0
2	117-A	32	17	17	0	0
2	118-A	32	17	17	0	0
2	119-A	32	17	17	0	0
2	120-A	32	17	17	0	0
2	121-A	32	17	17	0	0
2	122-A	32	17	17	0	0
2	123-A	32	17	17	0	0
2	124-A	32	17	17	0	0
2	125-A	32	17	17	0	0
3	1-A	48	25	25	0	0
3	2-A	48	25	25	0	0
3	3-A	48	25	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	4-A	48	25	25	0	0
3	5-A	48	25	25	0	0
3	6-A	48	25	25	0	0
3	7-A	48	25	25	0	0
3	8-A	48	25	25	0	0
3	9-A	48	25	25	0	0
3	10-A	48	25	25	0	0
3	11-A	48	25	25	0	0
3	12-A	48	25	25	0	0
3	13-A	48	25	25	0	0
3	14-A	48	25	25	0	0
3	15-A	48	25	25	0	0
3	16-A	48	25	25	0	0
3	17-A	48	25	25	0	0
3	18-A	48	25	25	0	0
3	19-A	48	25	25	0	0
3	20-A	48	25	25	0	0
3	21-A	48	25	25	0	0
3	22-A	48	25	25	0	0
3	23-A	48	25	25	0	0
3	24-A	48	25	25	0	0
3	25-A	48	25	25	0	0
3	26-A	48	25	25	0	0
3	27-A	48	25	25	0	0
3	28-A	48	25	25	0	0
3	29-A	48	25	25	0	0
3	30-A	48	25	25	0	0
3	31-A	48	25	25	0	0
3	32-A	48	25	25	0	0
3	33-A	48	25	25	0	0
3	34-A	48	25	25	0	0
3	35-A	48	25	25	0	0
3	36-A	48	25	25	0	0
3	37-A	48	25	25	0	0
3	38-A	48	25	25	0	0
3	39-A	48	25	25	0	0
3	40-A	48	25	25	0	0
3	41-A	48	25	25	0	0
3	42-A	48	25	25	0	0
3	43-A	48	25	25	0	0
3	44-A	48	25	25	0	0
3	45-A	48	25	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	46-A	48	25	25	0	0
3	47-A	48	25	25	0	0
3	48-A	48	25	25	0	0
3	49-A	48	25	25	0	0
3	50-A	48	25	25	0	0
3	51-A	48	25	25	0	0
3	52-A	48	25	25	0	0
3	53-A	48	25	25	0	0
3	54-A	48	25	25	0	0
3	55-A	48	25	25	0	0
3	56-A	48	25	25	0	0
3	57-A	48	25	25	0	0
3	58-A	48	25	25	0	0
3	59-A	48	25	25	0	0
3	60-A	48	25	25	0	0
3	61-A	48	25	25	0	0
3	62-A	48	25	25	0	0
3	63-A	48	25	25	0	0
3	64-A	48	25	25	0	0
3	65-A	48	25	25	0	0
3	66-A	48	25	25	0	0
3	67-A	48	25	25	0	0
3	68-A	48	25	25	0	0
3	69-A	48	25	25	0	0
3	70-A	48	25	25	0	0
3	71-A	48	25	25	0	0
3	72-A	48	25	25	0	0
3	73-A	48	25	25	0	0
3	74-A	48	25	25	0	0
3	75-A	48	25	25	0	0
3	76-A	48	25	25	0	0
3	77-A	48	25	25	0	0
3	78-A	48	25	25	0	0
3	79-A	48	25	25	0	0
3	80-A	48	25	25	0	0
3	81-A	48	25	25	0	0
3	82-A	48	25	25	0	0
3	83-A	48	25	25	0	0
3	84-A	48	25	25	0	0
3	85-A	48	25	25	0	0
3	86-A	48	25	25	0	0
3	87-A	48	25	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	88-A	48	25	25	0	0
3	89-A	48	25	25	0	0
3	90-A	48	25	25	0	0
3	91-A	48	25	25	0	0
3	92-A	48	25	25	0	0
3	93-A	48	25	25	0	0
3	94-A	48	25	25	0	0
3	95-A	48	25	25	0	0
3	96-A	48	25	25	0	0
3	97-A	48	25	25	0	0
3	98-A	48	25	25	0	0
3	99-A	48	25	25	0	0
3	100-A	48	25	25	0	0
3	101-A	48	25	25	0	0
3	102-A	48	25	25	0	0
3	103-A	48	25	25	0	0
3	104-A	48	25	25	0	0
3	105-A	48	25	25	0	0
3	106-A	48	25	25	0	0
3	107-A	48	25	25	0	0
3	108-A	48	25	25	0	0
3	109-A	48	25	25	0	0
3	110-A	48	25	25	0	0
3	111-A	48	25	25	0	0
3	112-A	48	25	25	0	0
3	113-A	48	25	25	0	0
3	114-A	48	25	25	0	0
3	115-A	48	25	25	0	0
3	116-A	48	25	25	0	0
3	117-A	48	25	25	0	0
3	118-A	48	25	25	0	0
3	119-A	48	25	25	0	0
3	120-A	48	25	25	0	0
3	121-A	48	25	25	0	0
3	122-A	48	25	25	0	0
3	123-A	48	25	25	0	0
3	124-A	48	25	25	0	0
3	125-A	48	25	25	0	0
4	1-A	2	0	0	0	0
4	2-A	2	0	0	0	0
4	3-A	2	0	0	0	0
4	4-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	5-A	2	0	0	0	0
4	6-A	2	0	0	0	0
4	7-A	2	0	0	0	0
4	8-A	2	0	0	0	0
4	9-A	2	0	0	0	0
4	10-A	2	0	0	0	0
4	11-A	2	0	0	0	0
4	12-A	2	0	0	0	0
4	13-A	2	0	0	0	0
4	14-A	2	0	0	0	0
4	15-A	2	0	0	0	0
4	16-A	2	0	0	0	0
4	17-A	2	0	0	0	0
4	18-A	2	0	0	0	0
4	19-A	2	0	0	0	0
4	20-A	2	0	0	0	0
4	21-A	2	0	0	0	0
4	22-A	2	0	0	0	0
4	23-A	2	0	0	0	0
4	24-A	2	0	0	0	0
4	25-A	2	0	0	0	0
4	26-A	2	0	0	0	0
4	27-A	2	0	0	0	0
4	28-A	2	0	0	0	0
4	29-A	2	0	0	0	0
4	30-A	2	0	0	0	0
4	31-A	2	0	0	0	0
4	32-A	2	0	0	0	0
4	33-A	2	0	0	0	0
4	34-A	2	0	0	0	0
4	35-A	2	0	0	0	0
4	36-A	2	0	0	0	0
4	37-A	2	0	0	0	0
4	38-A	2	0	0	0	0
4	39-A	2	0	0	0	0
4	40-A	2	0	0	0	0
4	41-A	2	0	0	0	0
4	42-A	2	0	0	0	0
4	43-A	2	0	0	0	0
4	44-A	2	0	0	0	0
4	45-A	2	0	0	0	0
4	46-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	47-A	2	0	0	0	0
4	48-A	2	0	0	0	0
4	49-A	2	0	0	0	0
4	50-A	2	0	0	0	0
4	51-A	2	0	0	0	0
4	52-A	2	0	0	0	0
4	53-A	2	0	0	0	0
4	54-A	2	0	0	0	0
4	55-A	2	0	0	0	0
4	56-A	2	0	0	0	0
4	57-A	2	0	0	0	0
4	58-A	2	0	0	0	0
4	59-A	2	0	0	0	0
4	60-A	2	0	0	0	0
4	61-A	2	0	0	0	0
4	62-A	2	0	0	0	0
4	63-A	2	0	0	0	0
4	64-A	2	0	0	0	0
4	65-A	2	0	0	0	0
4	66-A	2	0	0	0	0
4	67-A	2	0	0	0	0
4	68-A	2	0	0	0	0
4	69-A	2	0	0	0	0
4	70-A	2	0	0	0	0
4	71-A	2	0	0	0	0
4	72-A	2	0	0	0	0
4	73-A	2	0	0	0	0
4	74-A	2	0	0	0	0
4	75-A	2	0	0	0	0
4	76-A	2	0	0	0	0
4	77-A	2	0	0	0	0
4	78-A	2	0	0	0	0
4	79-A	2	0	0	0	0
4	80-A	2	0	0	0	0
4	81-A	2	0	0	0	0
4	82-A	2	0	0	0	0
4	83-A	2	0	0	0	0
4	84-A	2	0	0	0	0
4	85-A	2	0	0	0	0
4	86-A	2	0	0	0	0
4	87-A	2	0	0	0	0
4	88-A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	89-A	2	0	0	0	0
4	90-A	2	0	0	0	0
4	91-A	2	0	0	0	0
4	92-A	2	0	0	0	0
4	93-A	2	0	0	0	0
4	94-A	2	0	0	0	0
4	95-A	2	0	0	0	0
4	96-A	2	0	0	0	0
4	97-A	2	0	0	0	0
4	98-A	2	0	0	0	0
4	99-A	2	0	0	0	0
4	100-A	2	0	0	0	0
4	101-A	2	0	0	0	0
4	102-A	2	0	0	0	0
4	103-A	2	0	0	0	0
4	104-A	2	0	0	0	0
4	105-A	2	0	0	0	0
4	106-A	2	0	0	0	0
4	107-A	2	0	0	0	0
4	108-A	2	0	0	0	0
4	109-A	2	0	0	0	0
4	110-A	2	0	0	0	0
4	111-A	2	0	0	0	0
4	112-A	2	0	0	0	0
4	113-A	2	0	0	0	0
4	114-A	2	0	0	0	0
4	115-A	2	0	0	0	0
4	116-A	2	0	0	0	0
4	117-A	2	0	0	0	0
4	118-A	2	0	0	0	0
4	119-A	2	0	0	0	0
4	120-A	2	0	0	0	0
4	121-A	2	0	0	0	0
4	122-A	2	0	0	0	0
4	123-A	2	0	0	0	0
4	124-A	2	0	0	0	0
4	125-A	2	0	0	0	0
5	1-A	89	0	0	0	0
5	2-A	91	0	0	0	0
5	3-A	82	0	0	0	0
5	4-A	108	0	0	0	0
5	5-A	105	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	6-A	112	0	0	0	0
5	7-A	107	0	0	0	0
5	8-A	102	0	0	0	0
5	9-A	96	0	0	0	0
5	10-A	90	0	0	0	0
5	11-A	110	0	0	0	0
5	12-A	102	0	0	0	0
5	13-A	117	0	0	0	0
5	14-A	116	0	0	0	0
5	15-A	113	0	0	0	0
5	16-A	105	0	0	0	0
5	17-A	95	0	0	0	0
5	18-A	105	0	0	0	0
5	19-A	108	0	0	0	0
5	20-A	100	0	0	0	0
5	21-A	103	0	0	0	0
5	22-A	96	0	0	0	0
5	23-A	110	0	0	0	0
5	24-A	97	0	0	0	0
5	25-A	106	0	0	0	0
5	26-A	112	0	0	0	0
5	27-A	102	0	0	0	0
5	28-A	100	0	0	0	0
5	29-A	95	0	0	0	0
5	30-A	96	0	0	0	0
5	31-A	93	0	0	0	0
5	32-A	106	0	0	0	0
5	33-A	105	0	0	0	0
5	34-A	108	0	0	0	0
5	35-A	100	0	0	0	0
5	36-A	104	0	0	0	0
5	37-A	108	0	0	0	0
5	38-A	119	0	0	0	0
5	39-A	118	0	0	0	0
5	40-A	102	0	0	0	0
5	41-A	98	0	0	0	0
5	42-A	97	0	0	0	0
5	43-A	102	0	0	0	0
5	44-A	108	0	0	0	0
5	45-A	107	0	0	0	0
5	46-A	102	0	0	0	0
5	47-A	102	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	48-A	102	0	0	0	0
5	49-A	105	0	0	0	0
5	50-A	96	0	0	0	0
5	51-A	104	0	0	0	0
5	52-A	107	0	0	0	0
5	53-A	105	0	0	0	0
5	54-A	103	0	0	0	0
5	55-A	106	0	0	0	0
5	56-A	110	0	0	0	0
5	57-A	108	0	0	0	0
5	58-A	116	0	0	0	0
5	59-A	108	0	0	0	0
5	60-A	93	0	0	0	0
5	61-A	109	0	0	0	0
5	62-A	107	0	0	0	0
5	63-A	110	0	0	0	0
5	64-A	102	0	0	0	0
5	65-A	96	0	0	0	0
5	66-A	104	0	0	0	0
5	67-A	99	0	0	0	0
5	68-A	93	0	0	0	0
5	69-A	95	0	0	0	0
5	70-A	103	0	0	0	0
5	71-A	103	0	0	0	0
5	72-A	97	0	0	0	0
5	73-A	108	0	0	0	0
5	74-A	111	0	0	0	0
5	75-A	109	0	0	0	0
5	76-A	93	0	0	0	0
5	77-A	87	0	0	0	0
5	78-A	95	0	0	0	0
5	79-A	115	0	0	0	0
5	80-A	109	0	0	0	0
5	81-A	106	0	0	0	0
5	82-A	107	0	0	0	0
5	83-A	116	0	0	0	0
5	84-A	111	0	0	0	0
5	85-A	118	0	0	0	0
5	86-A	109	0	0	0	0
5	87-A	113	0	0	0	0
5	88-A	103	0	0	0	0
5	89-A	109	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	90-A	103	0	0	0	0
5	91-A	93	0	0	0	0
5	92-A	98	0	0	0	0
5	93-A	117	0	0	0	0
5	94-A	121	0	0	0	0
5	95-A	111	0	0	0	0
5	96-A	104	0	0	0	0
5	97-A	93	0	0	0	0
5	98-A	98	0	0	0	0
5	99-A	99	0	0	0	0
5	100-A	107	0	0	0	0
5	101-A	107	0	0	0	0
5	102-A	100	0	0	0	0
5	103-A	105	0	0	0	0
5	104-A	94	0	0	0	0
5	105-A	90	0	0	0	0
5	106-A	91	0	0	0	0
5	107-A	113	0	0	0	0
5	108-A	108	0	0	0	0
5	109-A	111	0	0	0	0
5	110-A	113	0	0	0	0
5	111-A	109	0	0	0	0
5	112-A	92	0	0	0	0
5	113-A	101	0	0	0	0
5	114-A	103	0	0	0	0
5	115-A	102	0	0	0	0
5	116-A	101	0	0	0	0
5	117-A	95	0	0	0	0
5	118-A	107	0	0	0	0
5	119-A	106	0	0	0	0
5	120-A	105	0	0	0	0
5	121-A	115	0	0	0	0
5	122-A	97	0	0	0	0
5	123-A	105	0	0	0	0
5	124-A	93	0	0	0	0
5	125-A	102	0	0	0	0
All	All	181958	157875	157860	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	156/159 (98%)	145 (93%)	8 (5%)	3 (2%)	8	0
1	2-A	156/159 (98%)	146 (94%)	5 (3%)	5 (3%)	4	0
1	3-A	156/159 (98%)	147 (94%)	4 (3%)	5 (3%)	4	0
1	4-A	156/159 (98%)	147 (94%)	6 (4%)	3 (2%)	8	0
1	5-A	156/159 (98%)	148 (95%)	4 (3%)	4 (3%)	5	0
1	6-A	156/159 (98%)	147 (94%)	5 (3%)	4 (3%)	5	0
1	7-A	156/159 (98%)	148 (95%)	4 (3%)	4 (3%)	5	0
1	8-A	156/159 (98%)	146 (94%)	5 (3%)	5 (3%)	4	0
1	9-A	156/159 (98%)	146 (94%)	5 (3%)	5 (3%)	4	0
1	10-A	156/159 (98%)	145 (93%)	7 (4%)	4 (3%)	5	0
1	11-A	156/159 (98%)	144 (92%)	11 (7%)	1 (1%)	25	5
1	12-A	156/159 (98%)	141 (90%)	12 (8%)	3 (2%)	8	0
1	13-A	156/159 (98%)	147 (94%)	3 (2%)	6 (4%)	3	0
1	14-A	156/159 (98%)	148 (95%)	5 (3%)	3 (2%)	8	0
1	15-A	156/159 (98%)	144 (92%)	10 (6%)	2 (1%)	12	1
1	16-A	156/159 (98%)	150 (96%)	2 (1%)	4 (3%)	5	0
1	17-A	156/159 (98%)	149 (96%)	4 (3%)	3 (2%)	8	0
1	18-A	156/159 (98%)	146 (94%)	7 (4%)	3 (2%)	8	0
1	19-A	156/159 (98%)	149 (96%)	2 (1%)	5 (3%)	4	0
1	20-A	156/159 (98%)	146 (94%)	5 (3%)	5 (3%)	4	0
1	21-A	156/159 (98%)	150 (96%)	4 (3%)	2 (1%)	12	1
1	22-A	156/159 (98%)	143 (92%)	10 (6%)	3 (2%)	8	0
1	23-A	156/159 (98%)	146 (94%)	5 (3%)	5 (3%)	4	0
1	24-A	156/159 (98%)	145 (93%)	9 (6%)	2 (1%)	12	1
1	25-A	156/159 (98%)	147 (94%)	5 (3%)	4 (3%)	5	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	26-A	156/159 (98%)	148 (95%)	7 (4%)	1 (1%)	25	5
1	27-A	156/159 (98%)	149 (96%)	5 (3%)	2 (1%)	12	1
1	28-A	156/159 (98%)	145 (93%)	10 (6%)	1 (1%)	25	5
1	29-A	156/159 (98%)	145 (93%)	7 (4%)	4 (3%)	5	0
1	30-A	156/159 (98%)	144 (92%)	7 (4%)	5 (3%)	4	0
1	31-A	156/159 (98%)	148 (95%)	7 (4%)	1 (1%)	25	5
1	32-A	156/159 (98%)	151 (97%)	4 (3%)	1 (1%)	25	5
1	33-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	34-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	35-A	156/159 (98%)	144 (92%)	9 (6%)	3 (2%)	8	0
1	36-A	156/159 (98%)	145 (93%)	5 (3%)	6 (4%)	3	0
1	37-A	156/159 (98%)	145 (93%)	8 (5%)	3 (2%)	8	0
1	38-A	156/159 (98%)	143 (92%)	10 (6%)	3 (2%)	8	0
1	39-A	156/159 (98%)	146 (94%)	7 (4%)	3 (2%)	8	0
1	40-A	156/159 (98%)	148 (95%)	5 (3%)	3 (2%)	8	0
1	41-A	156/159 (98%)	142 (91%)	9 (6%)	5 (3%)	4	0
1	42-A	156/159 (98%)	147 (94%)	6 (4%)	3 (2%)	8	0
1	43-A	156/159 (98%)	145 (93%)	7 (4%)	4 (3%)	5	0
1	44-A	156/159 (98%)	148 (95%)	6 (4%)	2 (1%)	12	1
1	45-A	156/159 (98%)	144 (92%)	11 (7%)	1 (1%)	25	5
1	46-A	156/159 (98%)	149 (96%)	4 (3%)	3 (2%)	8	0
1	47-A	156/159 (98%)	150 (96%)	4 (3%)	2 (1%)	12	1
1	48-A	156/159 (98%)	144 (92%)	7 (4%)	5 (3%)	4	0
1	49-A	156/159 (98%)	149 (96%)	2 (1%)	5 (3%)	4	0
1	50-A	156/159 (98%)	151 (97%)	3 (2%)	2 (1%)	12	1
1	51-A	156/159 (98%)	148 (95%)	7 (4%)	1 (1%)	25	5
1	52-A	156/159 (98%)	149 (96%)	6 (4%)	1 (1%)	25	5
1	53-A	156/159 (98%)	148 (95%)	5 (3%)	3 (2%)	8	0
1	54-A	156/159 (98%)	146 (94%)	8 (5%)	2 (1%)	12	1
1	55-A	156/159 (98%)	146 (94%)	8 (5%)	2 (1%)	12	1
1	56-A	156/159 (98%)	148 (95%)	4 (3%)	4 (3%)	5	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	57-A	156/159 (98%)	148 (95%)	4 (3%)	4 (3%)	5	0
1	58-A	156/159 (98%)	148 (95%)	5 (3%)	3 (2%)	8	0
1	59-A	156/159 (98%)	149 (96%)	4 (3%)	3 (2%)	8	0
1	60-A	156/159 (98%)	148 (95%)	4 (3%)	4 (3%)	5	0
1	61-A	156/159 (98%)	149 (96%)	3 (2%)	4 (3%)	5	0
1	62-A	156/159 (98%)	148 (95%)	3 (2%)	5 (3%)	4	0
1	63-A	156/159 (98%)	144 (92%)	5 (3%)	7 (4%)	2	0
1	64-A	156/159 (98%)	136 (87%)	7 (4%)	13 (8%)	1	0
1	65-A	156/159 (98%)	140 (90%)	10 (6%)	6 (4%)	3	0
1	66-A	156/159 (98%)	146 (94%)	2 (1%)	8 (5%)	2	0
1	67-A	156/159 (98%)	143 (92%)	8 (5%)	5 (3%)	4	0
1	68-A	156/159 (98%)	146 (94%)	6 (4%)	4 (3%)	5	0
1	69-A	156/159 (98%)	147 (94%)	6 (4%)	3 (2%)	8	0
1	70-A	156/159 (98%)	149 (96%)	5 (3%)	2 (1%)	12	1
1	71-A	156/159 (98%)	145 (93%)	9 (6%)	2 (1%)	12	1
1	72-A	156/159 (98%)	147 (94%)	5 (3%)	4 (3%)	5	0
1	73-A	156/159 (98%)	148 (95%)	5 (3%)	3 (2%)	8	0
1	74-A	156/159 (98%)	147 (94%)	6 (4%)	3 (2%)	8	0
1	75-A	156/159 (98%)	151 (97%)	3 (2%)	2 (1%)	12	1
1	76-A	156/159 (98%)	143 (92%)	8 (5%)	5 (3%)	4	0
1	77-A	156/159 (98%)	149 (96%)	3 (2%)	4 (3%)	5	0
1	78-A	156/159 (98%)	148 (95%)	6 (4%)	2 (1%)	12	1
1	79-A	156/159 (98%)	143 (92%)	6 (4%)	7 (4%)	2	0
1	80-A	156/159 (98%)	146 (94%)	5 (3%)	5 (3%)	4	0
1	81-A	156/159 (98%)	146 (94%)	6 (4%)	4 (3%)	5	0
1	82-A	156/159 (98%)	141 (90%)	8 (5%)	7 (4%)	2	0
1	83-A	156/159 (98%)	147 (94%)	4 (3%)	5 (3%)	4	0
1	84-A	156/159 (98%)	144 (92%)	6 (4%)	6 (4%)	3	0
1	85-A	156/159 (98%)	145 (93%)	7 (4%)	4 (3%)	5	0
1	86-A	156/159 (98%)	147 (94%)	6 (4%)	3 (2%)	8	0
1	87-A	156/159 (98%)	145 (93%)	7 (4%)	4 (3%)	5	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	88-A	156/159 (98%)	148 (95%)	4 (3%)	4 (3%)	5	0
1	89-A	156/159 (98%)	148 (95%)	4 (3%)	4 (3%)	5	0
1	90-A	156/159 (98%)	144 (92%)	6 (4%)	6 (4%)	3	0
1	91-A	156/159 (98%)	145 (93%)	5 (3%)	6 (4%)	3	0
1	92-A	156/159 (98%)	145 (93%)	5 (3%)	6 (4%)	3	0
1	93-A	156/159 (98%)	145 (93%)	7 (4%)	4 (3%)	5	0
1	94-A	156/159 (98%)	147 (94%)	2 (1%)	7 (4%)	2	0
1	95-A	156/159 (98%)	148 (95%)	3 (2%)	5 (3%)	4	0
1	96-A	156/159 (98%)	142 (91%)	10 (6%)	4 (3%)	5	0
1	97-A	156/159 (98%)	140 (90%)	10 (6%)	6 (4%)	3	0
1	98-A	156/159 (98%)	145 (93%)	6 (4%)	5 (3%)	4	0
1	99-A	156/159 (98%)	148 (95%)	4 (3%)	4 (3%)	5	0
1	100-A	156/159 (98%)	145 (93%)	5 (3%)	6 (4%)	3	0
1	101-A	156/159 (98%)	146 (94%)	4 (3%)	6 (4%)	3	0
1	102-A	156/159 (98%)	148 (95%)	4 (3%)	4 (3%)	5	0
1	103-A	156/159 (98%)	147 (94%)	3 (2%)	6 (4%)	3	0
1	104-A	156/159 (98%)	144 (92%)	6 (4%)	6 (4%)	3	0
1	105-A	156/159 (98%)	141 (90%)	12 (8%)	3 (2%)	8	0
1	106-A	156/159 (98%)	144 (92%)	5 (3%)	7 (4%)	2	0
1	107-A	156/159 (98%)	146 (94%)	6 (4%)	4 (3%)	5	0
1	108-A	156/159 (98%)	145 (93%)	7 (4%)	4 (3%)	5	0
1	109-A	156/159 (98%)	145 (93%)	8 (5%)	3 (2%)	8	0
1	110-A	156/159 (98%)	143 (92%)	10 (6%)	3 (2%)	8	0
1	111-A	156/159 (98%)	147 (94%)	5 (3%)	4 (3%)	5	0
1	112-A	156/159 (98%)	143 (92%)	9 (6%)	4 (3%)	5	0
1	113-A	156/159 (98%)	146 (94%)	7 (4%)	3 (2%)	8	0
1	114-A	156/159 (98%)	145 (93%)	6 (4%)	5 (3%)	4	0
1	115-A	156/159 (98%)	146 (94%)	5 (3%)	5 (3%)	4	0
1	116-A	156/159 (98%)	147 (94%)	5 (3%)	4 (3%)	5	0
1	117-A	156/159 (98%)	143 (92%)	7 (4%)	6 (4%)	3	0
1	118-A	156/159 (98%)	143 (92%)	8 (5%)	5 (3%)	4	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	119-A	156/159 (98%)	143 (92%)	8 (5%)	5 (3%)	4	0
1	120-A	156/159 (98%)	144 (92%)	6 (4%)	6 (4%)	3	0
1	121-A	156/159 (98%)	140 (90%)	10 (6%)	6 (4%)	3	0
1	122-A	156/159 (98%)	143 (92%)	5 (3%)	8 (5%)	2	0
1	123-A	156/159 (98%)	146 (94%)	5 (3%)	5 (3%)	4	0
1	124-A	156/159 (98%)	145 (93%)	6 (4%)	5 (3%)	4	0
1	125-A	156/159 (98%)	142 (91%)	9 (6%)	5 (3%)	4	0
All	All	19500/19875 (98%)	18238 (94%)	756 (4%)	506 (3%)	5	0

5 of 506 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	17	GLU
1	1-A	127	ASP
1	2-A	17	GLU
1	2-A	18	ASN
1	3-A	17	GLU

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	135/135 (100%)	112 (83%)	23 (17%)	2	0
1	2-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	3-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	4-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	5-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	6-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	7-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	8-A	135/135 (100%)	115 (85%)	20 (15%)	3	0
1	9-A	135/135 (100%)	114 (84%)	21 (16%)	2	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	10-A	135/135 (100%)	114 (84%)	21 (16%)	2	0
1	11-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	12-A	135/135 (100%)	115 (85%)	20 (15%)	3	0
1	13-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	14-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	15-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	16-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	17-A	135/135 (100%)	112 (83%)	23 (17%)	2	0
1	18-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	19-A	135/135 (100%)	112 (83%)	23 (17%)	2	0
1	20-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	21-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	22-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	23-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	24-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	25-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	26-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	27-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	28-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	29-A	135/135 (100%)	111 (82%)	24 (18%)	2	0
1	30-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	31-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	32-A	135/135 (100%)	111 (82%)	24 (18%)	2	0
1	33-A	135/135 (100%)	112 (83%)	23 (17%)	2	0
1	34-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	35-A	135/135 (100%)	115 (85%)	20 (15%)	3	0
1	36-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	37-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	38-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	39-A	135/135 (100%)	114 (84%)	21 (16%)	2	0
1	40-A	135/135 (100%)	118 (87%)	17 (13%)	4	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	41-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	42-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	43-A	135/135 (100%)	112 (83%)	23 (17%)	2	0
1	44-A	135/135 (100%)	114 (84%)	21 (16%)	2	0
1	45-A	135/135 (100%)	112 (83%)	23 (17%)	2	0
1	46-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	47-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	48-A	135/135 (100%)	115 (85%)	20 (15%)	3	0
1	49-A	135/135 (100%)	114 (84%)	21 (16%)	2	0
1	50-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	51-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	52-A	135/135 (100%)	122 (90%)	13 (10%)	8	0
1	53-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	54-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	55-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	56-A	135/135 (100%)	111 (82%)	24 (18%)	2	0
1	57-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	58-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	59-A	135/135 (100%)	114 (84%)	21 (16%)	2	0
1	60-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	61-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	62-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	63-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	64-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	65-A	135/135 (100%)	115 (85%)	20 (15%)	3	0
1	66-A	135/135 (100%)	123 (91%)	12 (9%)	9	0
1	67-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	68-A	135/135 (100%)	113 (84%)	22 (16%)	2	0
1	69-A	135/135 (100%)	113 (84%)	22 (16%)	2	0
1	70-A	135/135 (100%)	113 (84%)	22 (16%)	2	0
1	71-A	135/135 (100%)	114 (84%)	21 (16%)	2	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	72-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	73-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	74-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	75-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	76-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	77-A	135/135 (100%)	123 (91%)	12 (9%)	9	0
1	78-A	135/135 (100%)	124 (92%)	11 (8%)	11	0
1	79-A	135/135 (100%)	114 (84%)	21 (16%)	2	0
1	80-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	81-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	82-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	83-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	84-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	85-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	86-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	87-A	135/135 (100%)	112 (83%)	23 (17%)	2	0
1	88-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	89-A	135/135 (100%)	113 (84%)	22 (16%)	2	0
1	90-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	91-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	92-A	135/135 (100%)	114 (84%)	21 (16%)	2	0
1	93-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	94-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
1	95-A	135/135 (100%)	120 (89%)	15 (11%)	6	0
1	96-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	97-A	135/135 (100%)	123 (91%)	12 (9%)	9	0
1	98-A	135/135 (100%)	123 (91%)	12 (9%)	9	0
1	99-A	135/135 (100%)	123 (91%)	12 (9%)	9	0
1	100-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	101-A	135/135 (100%)	115 (85%)	20 (15%)	3	0
1	102-A	135/135 (100%)	123 (91%)	12 (9%)	9	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	103-A	135/135 (100%)	114 (84%)	21 (16%)	2	0
1	104-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	105-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	106-A	135/135 (100%)	123 (91%)	12 (9%)	9	0
1	107-A	135/135 (100%)	123 (91%)	12 (9%)	9	0
1	108-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	109-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	110-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	111-A	135/135 (100%)	114 (84%)	21 (16%)	2	0
1	112-A	135/135 (100%)	127 (94%)	8 (6%)	19	2
1	113-A	135/135 (100%)	124 (92%)	11 (8%)	11	0
1	114-A	135/135 (100%)	123 (91%)	12 (9%)	9	0
1	115-A	135/135 (100%)	111 (82%)	24 (18%)	2	0
1	116-A	135/135 (100%)	116 (86%)	19 (14%)	3	0
1	117-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	118-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	119-A	135/135 (100%)	124 (92%)	11 (8%)	11	0
1	120-A	135/135 (100%)	121 (90%)	14 (10%)	7	0
1	121-A	135/135 (100%)	117 (87%)	18 (13%)	4	0
1	122-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	123-A	135/135 (100%)	125 (93%)	10 (7%)	13	1
1	124-A	135/135 (100%)	119 (88%)	16 (12%)	5	0
1	125-A	135/135 (100%)	118 (87%)	17 (13%)	4	0
All	All	16875/16875 (100%)	14694 (87%)	2181 (13%)	4	0

5 of 2181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	55-A	128	TYR
1	69-A	32	LYS
1	115-A	104	LEU
1	57-A	24	LEU
1	62-A	120	GLU

Some 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 ⓘ

125 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSD	52-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	48-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	70-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	58-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	63-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	121-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	85-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	37-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	8-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	19-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	65-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	5-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	107-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	30-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	88-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	40-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	2-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	103-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	16-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	38-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	41-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	114-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	105-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	50-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	28-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	125-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	106-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	75-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	6-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	35-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	20-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	92-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	49-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	97-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	64-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	31-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	89-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	76-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	24-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	51-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	33-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	110-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	60-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	56-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	15-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	4-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	124-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	10-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	109-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	11-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	42-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	72-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	120-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	45-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	18-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	68-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	53-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	117-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	101-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	104-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	111-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	57-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	14-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	98-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	93-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	29-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	71-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	26-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	55-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	115-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	86-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	47-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	91-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	73-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	44-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	1-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	119-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	3-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	67-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	123-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	116-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	80-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	78-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	87-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	66-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	13-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	46-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	77-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	32-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	108-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	82-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	7-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	69-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	27-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	25-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	34-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	22-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	9-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	100-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	43-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	94-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	62-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	102-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	59-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	81-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	90-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	84-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	12-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	17-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	112-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	21-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	74-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	61-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	96-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	36-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	113-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	39-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	99-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	118-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	95-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	54-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	122-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	83-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)
1	CSD	23-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	79-A	152	1	3,7,8	1.15	0	1,8,10	4.88	1 (100%)

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
1	CSD	52-A	152	1	-	2/2/6/8	-
1	CSD	48-A	152	1	-	2/2/6/8	-
1	CSD	70-A	152	1	-	2/2/6/8	-
1	CSD	58-A	152	1	-	2/2/6/8	-
1	CSD	63-A	152	1	-	2/2/6/8	-
1	CSD	121-A	152	1	-	2/2/6/8	-
1	CSD	85-A	152	1	-	2/2/6/8	-
1	CSD	37-A	152	1	-	2/2/6/8	-
1	CSD	8-A	152	1	-	2/2/6/8	-
1	CSD	19-A	152	1	-	2/2/6/8	-
1	CSD	65-A	152	1	-	2/2/6/8	-
1	CSD	5-A	152	1	-	2/2/6/8	-
1	CSD	107-A	152	1	-	2/2/6/8	-
1	CSD	30-A	152	1	-	2/2/6/8	-
1	CSD	88-A	152	1	-	2/2/6/8	-
1	CSD	40-A	152	1	-	2/2/6/8	-
1	CSD	2-A	152	1	-	2/2/6/8	-
1	CSD	103-A	152	1	-	2/2/6/8	-
1	CSD	16-A	152	1	-	2/2/6/8	-
1	CSD	38-A	152	1	-	2/2/6/8	-
1	CSD	41-A	152	1	-	2/2/6/8	-
1	CSD	114-A	152	1	-	2/2/6/8	-
1	CSD	105-A	152	1	-	2/2/6/8	-
1	CSD	50-A	152	1	-	2/2/6/8	-
1	CSD	28-A	152	1	-	2/2/6/8	-
1	CSD	125-A	152	1	-	2/2/6/8	-
1	CSD	106-A	152	1	-	2/2/6/8	-
1	CSD	75-A	152	1	-	2/2/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	6-A	152	1	-	2/2/6/8	-
1	CSD	35-A	152	1	-	2/2/6/8	-
1	CSD	20-A	152	1	-	2/2/6/8	-
1	CSD	92-A	152	1	-	2/2/6/8	-
1	CSD	49-A	152	1	-	2/2/6/8	-
1	CSD	97-A	152	1	-	2/2/6/8	-
1	CSD	64-A	152	1	-	2/2/6/8	-
1	CSD	31-A	152	1	-	2/2/6/8	-
1	CSD	89-A	152	1	-	2/2/6/8	-
1	CSD	76-A	152	1	-	2/2/6/8	-
1	CSD	24-A	152	1	-	2/2/6/8	-
1	CSD	51-A	152	1	-	2/2/6/8	-
1	CSD	33-A	152	1	-	2/2/6/8	-
1	CSD	110-A	152	1	-	2/2/6/8	-
1	CSD	60-A	152	1	-	2/2/6/8	-
1	CSD	56-A	152	1	-	2/2/6/8	-
1	CSD	15-A	152	1	-	2/2/6/8	-
1	CSD	4-A	152	1	-	2/2/6/8	-
1	CSD	124-A	152	1	-	2/2/6/8	-
1	CSD	10-A	152	1	-	2/2/6/8	-
1	CSD	109-A	152	1	-	2/2/6/8	-
1	CSD	11-A	152	1	-	2/2/6/8	-
1	CSD	42-A	152	1	-	2/2/6/8	-
1	CSD	72-A	152	1	-	2/2/6/8	-
1	CSD	120-A	152	1	-	2/2/6/8	-
1	CSD	45-A	152	1	-	2/2/6/8	-
1	CSD	18-A	152	1	-	2/2/6/8	-
1	CSD	68-A	152	1	-	2/2/6/8	-
1	CSD	53-A	152	1	-	2/2/6/8	-
1	CSD	117-A	152	1	-	2/2/6/8	-
1	CSD	101-A	152	1	-	2/2/6/8	-
1	CSD	104-A	152	1	-	2/2/6/8	-
1	CSD	111-A	152	1	-	2/2/6/8	-
1	CSD	57-A	152	1	-	2/2/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	14-A	152	1	-	2/2/6/8	-
1	CSD	98-A	152	1	-	2/2/6/8	-
1	CSD	93-A	152	1	-	2/2/6/8	-
1	CSD	29-A	152	1	-	2/2/6/8	-
1	CSD	71-A	152	1	-	2/2/6/8	-
1	CSD	26-A	152	1	-	2/2/6/8	-
1	CSD	55-A	152	1	-	2/2/6/8	-
1	CSD	115-A	152	1	-	2/2/6/8	-
1	CSD	86-A	152	1	-	2/2/6/8	-
1	CSD	47-A	152	1	-	2/2/6/8	-
1	CSD	91-A	152	1	-	2/2/6/8	-
1	CSD	73-A	152	1	-	2/2/6/8	-
1	CSD	44-A	152	1	-	2/2/6/8	-
1	CSD	1-A	152	1	-	2/2/6/8	-
1	CSD	119-A	152	1	-	2/2/6/8	-
1	CSD	3-A	152	1	-	2/2/6/8	-
1	CSD	67-A	152	1	-	2/2/6/8	-
1	CSD	123-A	152	1	-	2/2/6/8	-
1	CSD	116-A	152	1	-	2/2/6/8	-
1	CSD	80-A	152	1	-	2/2/6/8	-
1	CSD	78-A	152	1	-	2/2/6/8	-
1	CSD	87-A	152	1	-	2/2/6/8	-
1	CSD	66-A	152	1	-	2/2/6/8	-
1	CSD	13-A	152	1	-	2/2/6/8	-
1	CSD	46-A	152	1	-	2/2/6/8	-
1	CSD	77-A	152	1	-	2/2/6/8	-
1	CSD	32-A	152	1	-	2/2/6/8	-
1	CSD	108-A	152	1	-	2/2/6/8	-
1	CSD	82-A	152	1	-	2/2/6/8	-
1	CSD	7-A	152	1	-	2/2/6/8	-
1	CSD	69-A	152	1	-	2/2/6/8	-
1	CSD	27-A	152	1	-	2/2/6/8	-
1	CSD	25-A	152	1	-	2/2/6/8	-
1	CSD	34-A	152	1	-	2/2/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	22-A	152	1	-	2/2/6/8	-
1	CSD	9-A	152	1	-	2/2/6/8	-
1	CSD	100-A	152	1	-	2/2/6/8	-
1	CSD	43-A	152	1	-	2/2/6/8	-
1	CSD	94-A	152	1	-	2/2/6/8	-
1	CSD	62-A	152	1	-	2/2/6/8	-
1	CSD	102-A	152	1	-	2/2/6/8	-
1	CSD	59-A	152	1	-	2/2/6/8	-
1	CSD	81-A	152	1	-	2/2/6/8	-
1	CSD	90-A	152	1	-	2/2/6/8	-
1	CSD	84-A	152	1	-	2/2/6/8	-
1	CSD	12-A	152	1	-	2/2/6/8	-
1	CSD	17-A	152	1	-	2/2/6/8	-
1	CSD	112-A	152	1	-	2/2/6/8	-
1	CSD	21-A	152	1	-	2/2/6/8	-
1	CSD	74-A	152	1	-	2/2/6/8	-
1	CSD	61-A	152	1	-	2/2/6/8	-
1	CSD	96-A	152	1	-	2/2/6/8	-
1	CSD	36-A	152	1	-	2/2/6/8	-
1	CSD	113-A	152	1	-	2/2/6/8	-
1	CSD	39-A	152	1	-	2/2/6/8	-
1	CSD	99-A	152	1	-	2/2/6/8	-
1	CSD	118-A	152	1	-	2/2/6/8	-
1	CSD	95-A	152	1	-	2/2/6/8	-
1	CSD	54-A	152	1	-	2/2/6/8	-
1	CSD	122-A	152	1	-	2/2/6/8	-
1	CSD	83-A	152	1	-	2/2/6/8	-
1	CSD	23-A	152	1	-	2/2/6/8	-
1	CSD	79-A	152	1	-	2/2/6/8	-

There are no bond length outliers.

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	52-A	152	CSD	OD1-SG-CB	4.88	114.83	105.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	48-A	152	CSD	OD1-SG-CB	4.88	114.83	105.54
1	70-A	152	CSD	OD1-SG-CB	4.88	114.83	105.54
1	58-A	152	CSD	OD1-SG-CB	4.88	114.83	105.54
1	63-A	152	CSD	OD1-SG-CB	4.88	114.83	105.54

There are no chirality outliers.

5 of 250 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	52-A	152	CSD	N-CA-CB-SG
1	52-A	152	CSD	CA-CB-SG-OD1
1	48-A	152	CSD	N-CA-CB-SG
1	48-A	152	CSD	CA-CB-SG-OD1
1	70-A	152	CSD	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 500 ligands modelled in this entry, 250 are monoatomic - leaving 250 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	31-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	34-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	124-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	54-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	26-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	14-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	36-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	124-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	20-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	7-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	99-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	72-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	51-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	97-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	79-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	82-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	80-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	66-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	11-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	3-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	67-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	40-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	74-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	55-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	25-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	78-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	45-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	99-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	16-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	83-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	76-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	125-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	85-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	87-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	44-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	64-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	24-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	3-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	68-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	52-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	111-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	18-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	94-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	60-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	110-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	28-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	84-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	91-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	100-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	15-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	5-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	67-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	70-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	35-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	35-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	31-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	80-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	22-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	41-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	103-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	23-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	78-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	57-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	52-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	73-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	22-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	88-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	32-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	119-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	39-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	2-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	50-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	7-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	1-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	13-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	79-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	97-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	55-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	98-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	10-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	43-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	85-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	62-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	112-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	116-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	40-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	93-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	96-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	17-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	77-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	6-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	69-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	98-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	12-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	111-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	89-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	75-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	106-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	95-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	25-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	34-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	29-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	64-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	59-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	32-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	115-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	8-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	42-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	46-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	102-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	93-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	114-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	81-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	71-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	58-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	108-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	74-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	21-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	53-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	63-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	117-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	56-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	66-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	39-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	49-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	61-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	90-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	48-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	6-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	62-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	18-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	65-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	58-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	102-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	47-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	81-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	120-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	51-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	104-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	33-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	76-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	20-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	101-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	29-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	30-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	70-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	88-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	63-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	117-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	109-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	19-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	44-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	100-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	105-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	71-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	120-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	86-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	16-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	38-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	38-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	41-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	69-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	17-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	122-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	47-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	95-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	106-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	43-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	8-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	92-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	13-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	84-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	61-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	59-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	50-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	45-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	24-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	122-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	123-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	89-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	42-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	5-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	30-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	113-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	115-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	49-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	4-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	118-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	27-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	114-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	110-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	105-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	94-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	103-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	11-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	86-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	10-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	91-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	119-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	73-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	87-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	77-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	125-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	37-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	37-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	104-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	19-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	68-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	121-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	92-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	113-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	56-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	4-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	123-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	33-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	118-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	48-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	26-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	12-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	121-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	72-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	9-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	83-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	23-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	108-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	2-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	21-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	82-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	90-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	15-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	107-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	101-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	116-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	28-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	36-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	112-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	14-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	75-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	109-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	53-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
3	NAP	9-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	46-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	57-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	54-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	60-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	1-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	65-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)
2	FOL	27-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)
3	NAP	96-A	202	-	45,52,52	2.96	9 (20%)	56,80,80	1.33	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	107-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.29	10 (27%)

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	31-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	34-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	124-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	54-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	26-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	14-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	36-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	124-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	20-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	7-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	99-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	72-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	51-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	97-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	79-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	82-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	80-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	66-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	11-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	3-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	67-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	40-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	74-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	55-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	25-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	78-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	45-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	99-A	202	-	-	3/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	16-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	83-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	76-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	125-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	85-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	87-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	44-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	64-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	24-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	3-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	68-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	52-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	111-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	18-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	94-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	60-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	110-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	28-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	84-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	91-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	100-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	15-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	5-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	67-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	70-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	35-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	35-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	31-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	80-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	22-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	41-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	103-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	23-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	78-A	202	-	-	3/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	57-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	52-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	73-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	22-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	88-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	32-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	119-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	39-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	2-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	50-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	7-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	1-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	13-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	79-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	97-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	55-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	98-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	10-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	43-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	85-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	62-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	112-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	116-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	40-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	93-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	96-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	17-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	77-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	6-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	69-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	98-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	12-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	111-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	89-A	202	-	-	3/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	75-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	106-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	95-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	25-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	34-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	29-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	64-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	59-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	32-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	115-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	8-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	42-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	46-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	102-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	93-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	114-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	81-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	71-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	58-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	108-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	74-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	21-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	53-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	63-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	117-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	56-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	66-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	39-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	49-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	61-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	90-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	48-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	6-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	62-A	202	-	-	3/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	18-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	65-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	58-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	102-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	47-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	81-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	120-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	51-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	104-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	33-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	76-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	20-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	101-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	29-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	30-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	70-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	88-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	63-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	117-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	109-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	19-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	44-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	100-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	105-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	71-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	120-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	86-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	16-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	38-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	38-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	41-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	69-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	17-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	122-A	202	-	-	3/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	47-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	95-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	106-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	43-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	8-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	92-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	13-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	84-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	61-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	59-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	50-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	45-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	24-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	122-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	123-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	89-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	42-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	5-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	30-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	113-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	115-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	49-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	4-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	118-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	27-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	114-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	110-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	105-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	94-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	103-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	11-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	86-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	10-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	91-A	202	-	-	3/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	119-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	73-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	87-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	77-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	125-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	37-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	37-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	104-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	19-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	68-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	121-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	92-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	113-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	56-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	4-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	123-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	33-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	118-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	48-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	26-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	12-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	121-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	72-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	9-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	83-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	23-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	108-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	2-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	21-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	82-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	90-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	15-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	107-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	101-A	201	-	-	5/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	116-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	28-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	36-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	112-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	14-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	75-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	109-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	53-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	9-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	46-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	57-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	54-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	60-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	1-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	65-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	27-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	96-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	107-A	201	-	-	5/16/22/22	0/3/3/3

The worst 5 of 1375 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	80-A	202	NAP	C2D-C1D	-11.57	1.36	1.53
3	66-A	202	NAP	C2D-C1D	-11.57	1.36	1.53
3	24-A	202	NAP	C2D-C1D	-11.57	1.36	1.53
3	94-A	202	NAP	C2D-C1D	-11.57	1.36	1.53
3	35-A	202	NAP	C2D-C1D	-11.57	1.36	1.53

The worst 5 of 2250 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	31-A	201	FOL	N8-C8A-N1	6.92	123.72	115.82
2	99-A	201	FOL	N8-C8A-N1	6.92	123.72	115.82
2	51-A	201	FOL	N8-C8A-N1	6.92	123.72	115.82
2	82-A	201	FOL	N8-C8A-N1	6.92	123.72	115.82
2	21-A	201	FOL	N8-C8A-N1	6.92	123.72	115.82

There are no chirality outliers.

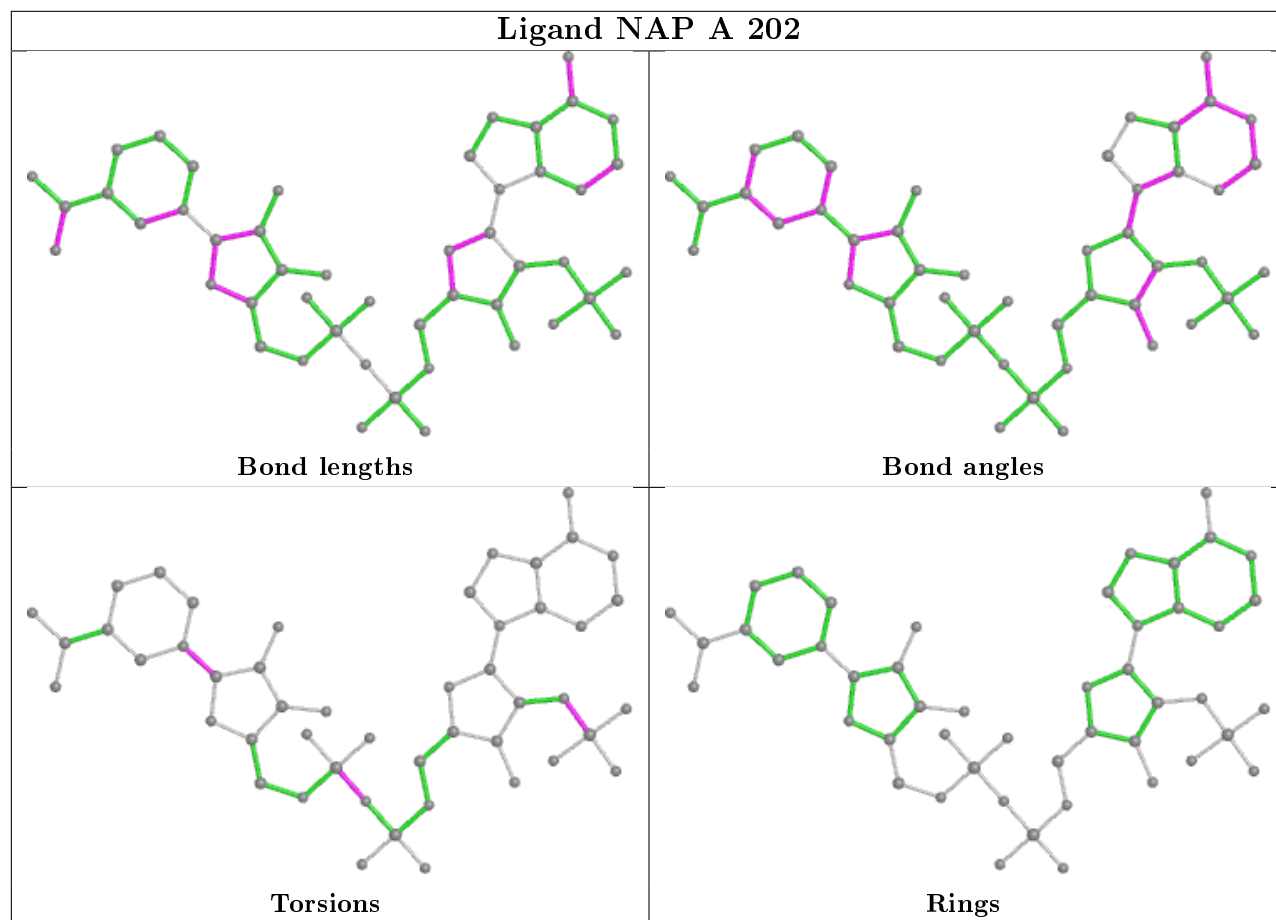
5 of 1000 torsion outliers are listed below:

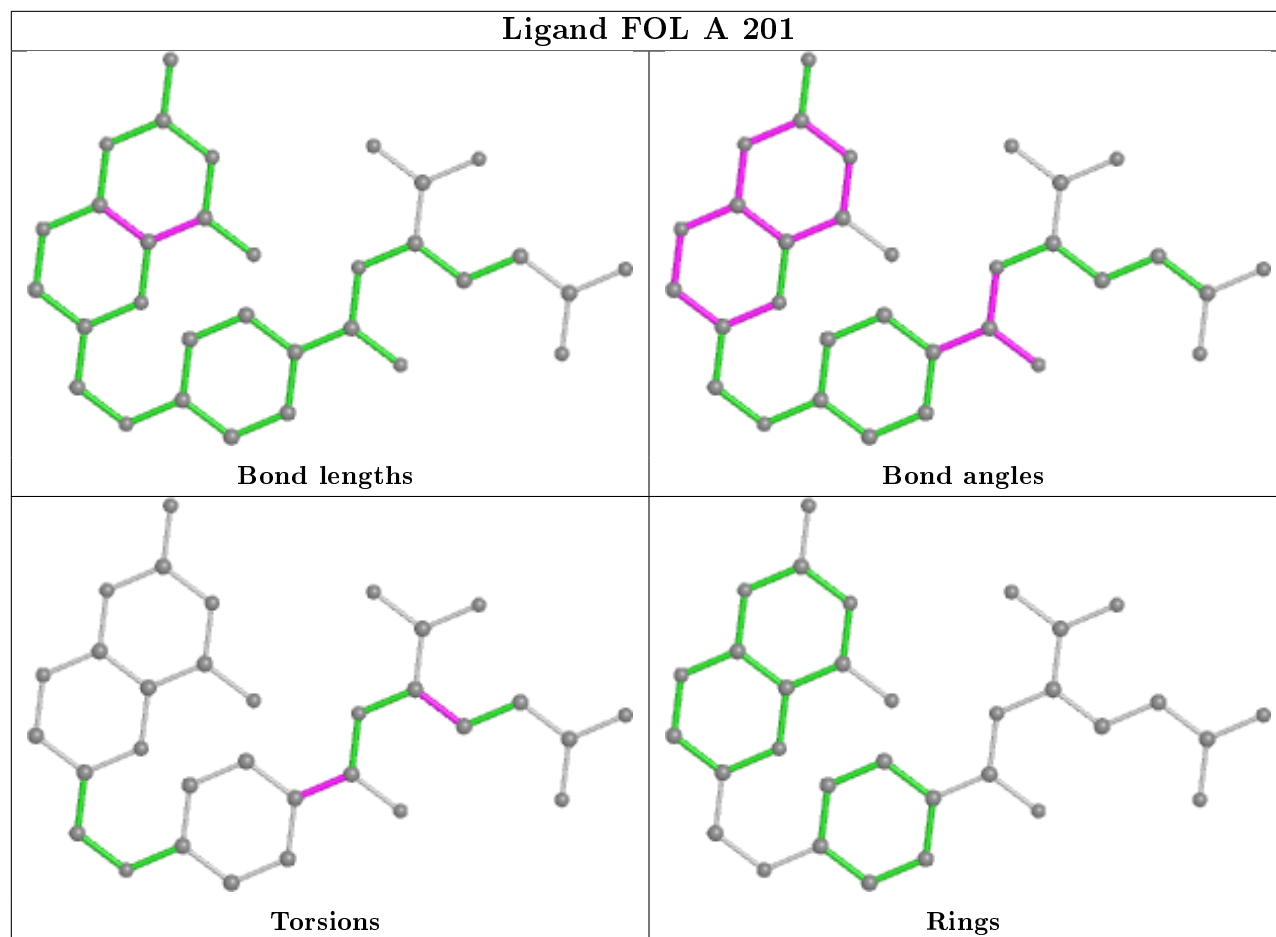
Mol	Chain	Res	Type	Atoms
3	80-A	202	NAP	O4D-C1D-N1N-C6N
3	66-A	202	NAP	O4D-C1D-N1N-C6N
3	24-A	202	NAP	O4D-C1D-N1N-C6N
3	94-A	202	NAP	O4D-C1D-N1N-C6N
3	35-A	202	NAP	O4D-C1D-N1N-C6N

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	1-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	2-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	3-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	4-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	5-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	6-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	7-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	8-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	9-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	10-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	11-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	12-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	13-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	14-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	15-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	16-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	17-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	18-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	19-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	20-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	21-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	22-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	23-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	24-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	25-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	26-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	27-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	28-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	29-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	30-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	31-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	32-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	33-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	34-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	35-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	36-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	37-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	38-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	39-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	40-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	41-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	42-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	43-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	44-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	45-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	46-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	47-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	48-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	49-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	50-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	51-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	52-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	53-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	54-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	55-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	56-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	57-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	58-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	59-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	60-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	61-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	62-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	63-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	64-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	65-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	66-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	67-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	68-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	69-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	70-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	71-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	72-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	73-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	74-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	75-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	76-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	77-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	78-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	79-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	80-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	81-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	82-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	83-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	84-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	85-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	86-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	87-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	88-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	89-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	90-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	91-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	92-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	93-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	94-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	95-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	96-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	97-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	98-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	99-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	100-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	101-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	102-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	103-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	104-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	105-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	106-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	107-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	108-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	109-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	110-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	111-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	112-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	113-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	114-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	115-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	116-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)
1	117-A	158/159 (99%)	0.58	10 (6%)	20	19	9, 12, 15, 17	158 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	118-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	119-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	120-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	121-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	122-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	123-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	124-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
1	125-A	158/159 (99%)	0.58	10 (6%)	20 19	9, 12, 15, 17	158 (100%)
All	All	19750/19875 (99%)	0.58	1250 (6%)	18 19	9, 12, 15, 17	19750 (100%)

The worst 5 of 1250 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	22	TRP	13.0
1	2-A	22	TRP	13.0
1	3-A	22	TRP	13.0
1	4-A	22	TRP	13.0
1	5-A	22	TRP	13.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	CSD	52-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	48-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	70-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	58-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	63-A	152	8/9	0.98	0.11	10,11,11,12	11
1	CSD	121-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	85-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	37-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	8-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	19-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	65-A	152	8/9	0.98	0.11	10,11,12,12	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CSD	5-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	107-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	30-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	88-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	40-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	2-A	152	8/9	0.98	0.11	10,11,11,12	11
1	CSD	103-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	16-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	38-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	41-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	114-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	105-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	50-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	28-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	125-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	106-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	75-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	6-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	35-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	20-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	92-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	49-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	97-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	64-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	31-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	89-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	76-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	24-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	51-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	33-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	110-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	60-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	56-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	15-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	4-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	124-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	10-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	109-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	11-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	42-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	72-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	120-A	152	8/9	0.98	0.11	10,11,12,12	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CSD	45-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	18-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	68-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	53-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	117-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	101-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	104-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	111-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	57-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	14-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	98-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	93-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	29-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	71-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	26-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	55-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	115-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	86-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	47-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	91-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	73-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	44-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	1-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	119-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	3-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	67-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	123-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	116-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	80-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	78-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	87-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	66-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	13-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	46-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	77-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	32-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	108-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	82-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	7-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	69-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	27-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	25-A	152	8/9	0.98	0.11	10,11,12,12	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	CSD	34-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	22-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	9-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	100-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	43-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	94-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	62-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	102-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	59-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	81-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	90-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	84-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	12-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	17-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	112-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	21-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	74-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	61-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	96-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	36-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	113-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	39-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	99-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	118-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	95-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	54-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	122-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	83-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	23-A	152	8/9	0.98	0.11	10,11,12,12	11
1	CSD	79-A	152	8/9	0.98	0.11	10,11,12,12	11

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FOL	31-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	99-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	51-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	82-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	21-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	55-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	76-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	18-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	60-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	80-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	23-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	57-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	62-A	201	32/32	0.97	0.10	9,10,13,14	49
2	FOL	111-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	39-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	61-A	201	32/32	0.97	0.10	9,10,13,13	49
2	FOL	48-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	120-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	104-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	30-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	117-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	41-A	201	32/32	0.97	0.10	9,10,11,11	49
2	FOL	54-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	45-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	116-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	113-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	103-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	77-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	123-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	26-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	46-A	201	32/32	0.97	0.10	9,10,11,11	49
2	FOL	36-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	20-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	72-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	79-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	67-A	201	32/32	0.97	0.10	9,10,13,13	49
2	FOL	87-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	64-A	201	32/32	0.97	0.10	9,10,13,14	49
2	FOL	110-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	91-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	5-A	201	32/32	0.97	0.10	9,10,11,11	49
2	FOL	81-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	50-A	201	32/32	0.97	0.10	9,10,12,12	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FOL	112-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	93-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	98-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	6-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	95-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	25-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	29-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	13-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	19-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	100-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	16-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	38-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	69-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	43-A	201	32/32	0.97	0.10	9,9,11,11	49
2	FOL	92-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	84-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	85-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	119-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	10-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	125-A	201	32/32	0.97	0.10	9,9,12,13	49
2	FOL	121-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	9-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	14-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	75-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	107-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	124-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	40-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	7-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	74-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	78-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	35-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	73-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	2-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	97-A	201	32/32	0.97	0.10	9,10,11,13	49
2	FOL	12-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	59-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	32-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	115-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	102-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	58-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	53-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	63-A	201	32/32	0.97	0.10	9,10,13,14	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FOL	49-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	42-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	88-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	17-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	106-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	24-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	122-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	89-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	4-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	114-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	94-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	56-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	33-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	101-A	201	32/32	0.97	0.10	9,9,11,12	49
2	FOL	65-A	201	32/32	0.97	0.10	9,10,13,14	49
2	FOL	27-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	34-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	11-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	118-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	44-A	201	32/32	0.97	0.10	9,10,11,11	49
2	FOL	3-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	28-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	70-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	52-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	22-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	83-A	201	32/32	0.97	0.10	9,10,11,12	49
2	FOL	96-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	8-A	201	32/32	0.97	0.10	9,9,12,12	49
2	FOL	108-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	66-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	90-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	47-A	201	32/32	0.97	0.10	9,10,11,11	49
2	FOL	109-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	105-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	71-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	86-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	37-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	68-A	201	32/32	0.97	0.10	9,10,12,13	49
2	FOL	15-A	201	32/32	0.97	0.10	9,10,12,12	49
2	FOL	1-A	201	32/32	0.97	0.10	9,10,11,12	49
3	NAP	88-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	75-A	204	1/1	0.99	0.30	11,11,11,11	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAP	81-A	202	48/48	0.99	0.09	9,10,12,12	73
3	NAP	43-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	71-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	10-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	74-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	17-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	3-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	56-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	94-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	80-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	61-A	204	1/1	0.99	0.30	12,12,12,12	1
3	NAP	62-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	41-A	204	1/1	0.99	0.30	10,10,10,10	1
4	MN	96-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	58-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	107-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	110-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	6-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	25-A	204	1/1	0.99	0.30	10,10,10,10	1
4	MN	35-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	4-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	76-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	101-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	29-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	7-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	35-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	119-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	113-A	204	1/1	0.99	0.30	12,12,12,12	1
4	MN	12-A	204	1/1	0.99	0.30	9,9,9,9	1
4	MN	120-A	204	1/1	0.99	0.30	12,12,12,12	1
4	MN	62-A	204	1/1	0.99	0.30	13,13,13,13	1
4	MN	15-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	23-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	70-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	103-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	61-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	59-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	31-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	63-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	30-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	46-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	1-A	202	48/48	0.99	0.09	9,10,12,12	73

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAP	11-A	202	48/48	0.99	0.09	9,10,12,12	73
3	NAP	44-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	120-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	89-A	204	1/1	0.99	0.30	12,12,12,12	1
3	NAP	118-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	37-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	104-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	51-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	50-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	124-A	204	1/1	0.99	0.30	12,12,12,12	1
3	NAP	7-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	45-A	204	1/1	0.99	0.30	10,10,10,10	1
4	MN	117-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	69-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	5-A	204	1/1	0.99	0.30	9,9,9,9	1
4	MN	2-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	66-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	109-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	71-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	48-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	100-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	65-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	80-A	204	1/1	0.99	0.30	12,12,12,12	1
4	MN	6-A	204	1/1	0.99	0.30	9,9,9,9	1
4	MN	68-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	54-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	105-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	122-A	204	1/1	0.99	0.30	13,13,13,13	1
4	MN	63-A	204	1/1	0.99	0.30	12,12,12,12	1
3	NAP	39-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	97-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	99-A	204	1/1	0.99	0.30	12,12,12,12	1
4	MN	59-A	204	1/1	0.99	0.30	12,12,12,12	1
4	MN	79-A	204	1/1	0.99	0.30	12,12,12,12	1
4	MN	36-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	99-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	83-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	125-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	70-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	68-A	202	48/48	0.99	0.09	9,10,12,12	73
3	NAP	52-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	111-A	202	48/48	0.99	0.09	9,10,12,13	73

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAP	84-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	100-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	48-A	204	1/1	0.99	0.30	10,10,10,10	1
4	MN	16-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	115-A	202	48/48	0.99	0.09	9,10,12,12	73
3	NAP	31-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	103-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	55-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	32-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	86-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	106-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	108-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	34-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	91-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	98-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	89-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	74-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	39-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	41-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	87-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	34-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	8-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	37-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	104-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	84-A	204	1/1	0.99	0.30	12,12,12,12	1
4	MN	38-A	204	1/1	0.99	0.30	12,12,12,12	1
3	NAP	114-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	121-A	202	48/48	0.99	0.09	9,10,12,12	73
3	NAP	110-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	44-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	24-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	90-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	66-A	204	1/1	0.99	0.30	13,13,13,13	1
4	MN	94-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	82-A	204	1/1	0.99	0.30	12,12,12,12	1
3	NAP	51-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	85-A	204	1/1	0.99	0.30	12,12,12,12	1
4	MN	30-A	204	1/1	0.99	0.30	9,9,9,9	1
3	NAP	72-A	202	48/48	0.99	0.09	9,10,12,12	73
3	NAP	38-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	82-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	47-A	202	48/48	0.99	0.09	9,10,12,13	73

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAP	36-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	60-A	204	1/1	0.99	0.30	12,12,12,12	1
3	NAP	112-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	53-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	123-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	72-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	116-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	29-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	105-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	28-A	204	1/1	0.99	0.30	10,10,10,10	1
4	MN	64-A	204	1/1	0.99	0.30	13,13,13,13	1
4	MN	107-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	81-A	204	1/1	0.99	0.30	12,12,12,12	1
3	NAP	96-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	90-A	204	1/1	0.99	0.30	12,12,12,12	1
4	MN	20-A	204	1/1	0.99	0.30	10,10,10,10	1
4	MN	77-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	12-A	202	48/48	0.99	0.09	9,10,12,12	73
3	NAP	108-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	21-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	95-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	77-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	115-A	204	1/1	0.99	0.30	12,12,12,12	1
4	MN	57-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	14-A	204	1/1	0.99	0.30	10,10,10,10	1
4	MN	116-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	57-A	202	48/48	0.99	0.09	9,10,12,12	73
3	NAP	23-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	55-A	204	1/1	0.99	0.30	12,12,12,12	1
3	NAP	69-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	111-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	56-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	14-A	202	48/48	0.99	0.09	9,10,12,12	73
3	NAP	124-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	67-A	204	1/1	0.99	0.30	13,13,13,13	1
4	MN	119-A	204	1/1	0.99	0.30	13,13,13,13	1
3	NAP	25-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	33-A	204	1/1	0.99	0.30	10,10,10,10	1
4	MN	13-A	204	1/1	0.99	0.30	10,10,10,10	1
4	MN	83-A	204	1/1	0.99	0.30	12,12,12,12	1
3	NAP	40-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	91-A	204	1/1	0.99	0.30	12,12,12,12	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MN	123-A	204	1/1	0.99	0.30	12,12,12,12	1
3	NAP	26-A	202	48/48	0.99	0.09	9,10,12,12	73
3	NAP	45-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	27-A	204	1/1	0.99	0.30	10,10,10,10	1
4	MN	9-A	204	1/1	0.99	0.30	9,9,9,9	1
3	NAP	16-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	18-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	22-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	78-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	78-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	85-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	121-A	204	1/1	0.99	0.30	12,12,12,12	1
3	NAP	117-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	118-A	204	1/1	0.99	0.30	12,12,12,12	1
3	NAP	13-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	79-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	112-A	204	1/1	0.99	0.30	12,12,12,12	1
4	MN	40-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	75-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	106-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	86-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	8-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	52-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	46-A	202	48/48	0.99	0.09	9,10,12,12	73
3	NAP	93-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	101-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	102-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	32-A	204	1/1	0.99	0.30	10,10,10,10	1
4	MN	11-A	204	1/1	0.99	0.30	10,10,10,10	1
4	MN	92-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	15-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	18-A	202	48/48	0.99	0.09	9,10,12,12	73
3	NAP	58-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	102-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	24-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	64-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	98-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	97-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	47-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	33-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	20-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	21-A	204	1/1	0.99	0.30	10,10,10,10	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MN	3-A	204	1/1	0.99	0.30	9,9,9,9	1
3	NAP	67-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	26-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	10-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	125-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	122-A	202	48/48	0.99	0.09	9,10,12,12	73
3	NAP	95-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	42-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	50-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	54-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	5-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	93-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	49-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	27-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	53-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	43-A	204	1/1	0.99	0.30	9,9,9,9	1
4	MN	76-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	73-A	202	48/48	0.99	0.09	9,10,12,12	73
3	NAP	87-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	1-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	19-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	42-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	17-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	92-A	202	48/48	0.99	0.09	9,10,12,13	73
3	NAP	113-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	109-A	204	1/1	0.99	0.30	11,11,11,11	1
4	MN	19-A	204	1/1	0.99	0.30	10,10,10,10	1
4	MN	73-A	204	1/1	0.99	0.30	11,11,11,11	1
3	NAP	2-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	88-A	204	1/1	0.99	0.30	12,12,12,12	1
4	MN	49-A	204	1/1	0.99	0.30	10,10,10,10	1
4	MN	65-A	204	1/1	0.99	0.30	13,13,13,13	1
3	NAP	28-A	202	48/48	0.99	0.09	9,10,12,13	73
4	MN	4-A	204	1/1	0.99	0.30	9,9,9,9	1
4	MN	22-A	204	1/1	0.99	0.30	10,10,10,10	1
3	NAP	9-A	202	48/48	0.99	0.09	9,10,12,12	73
3	NAP	60-A	202	48/48	0.99	0.09	9,10,12,12	73
4	MN	114-A	204	1/1	0.99	0.30	12,12,12,12	1
4	MN	89-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	5-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	50-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	93-A	203	1/1	1.00	0.20	13,13,13,13	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MN	121-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	55-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	51-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	98-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	87-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	83-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	88-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	3-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	58-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	86-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	82-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	44-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	92-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	13-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	29-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	117-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	104-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	111-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	108-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	61-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	106-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	91-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	32-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	20-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	30-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	60-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	114-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	107-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	53-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	80-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	77-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	37-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	34-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	21-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	84-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	47-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	105-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	18-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	118-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	90-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	4-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	94-A	203	1/1	1.00	0.20	13,13,13,13	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MN	76-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	102-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	69-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	115-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	8-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	124-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	100-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	25-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	31-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	36-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	17-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	63-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	65-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	110-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	42-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	54-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	120-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	7-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	35-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	109-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	40-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	43-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	39-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	125-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	99-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	49-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	12-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	67-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	73-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	122-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	85-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	24-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	15-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	81-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	33-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	103-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	22-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	28-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	66-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	45-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	14-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	116-A	203	1/1	1.00	0.20	14,14,14,14	1

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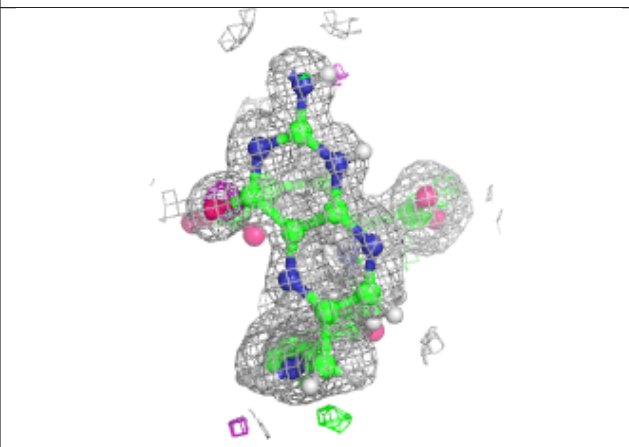
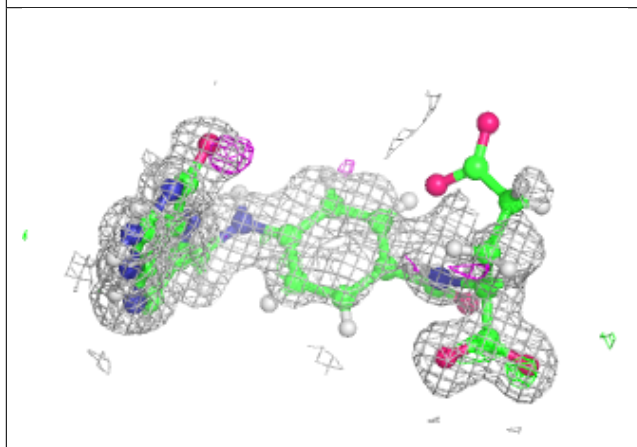
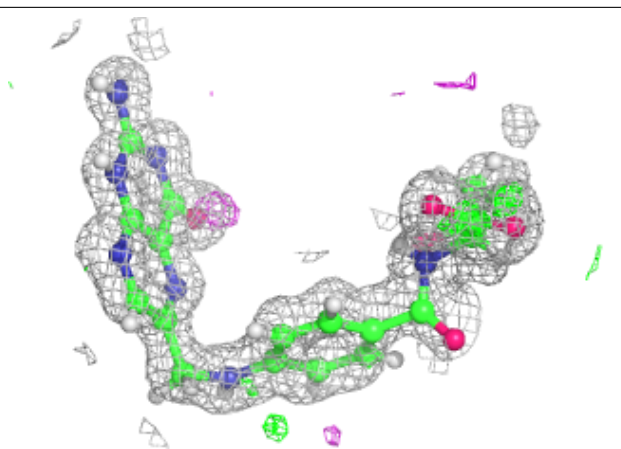
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MN	113-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	59-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	52-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	10-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	57-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	71-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	123-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	78-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	119-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	56-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	19-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	6-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	16-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	2-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	64-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	96-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	70-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	72-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	62-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	79-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	48-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	97-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	1-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	11-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	74-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	112-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	68-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	27-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	26-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	23-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	9-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	95-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	41-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	101-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	38-A	203	1/1	1.00	0.20	14,14,14,14	1
4	MN	75-A	203	1/1	1.00	0.20	13,13,13,13	1
4	MN	46-A	203	1/1	1.00	0.20	13,13,13,13	1

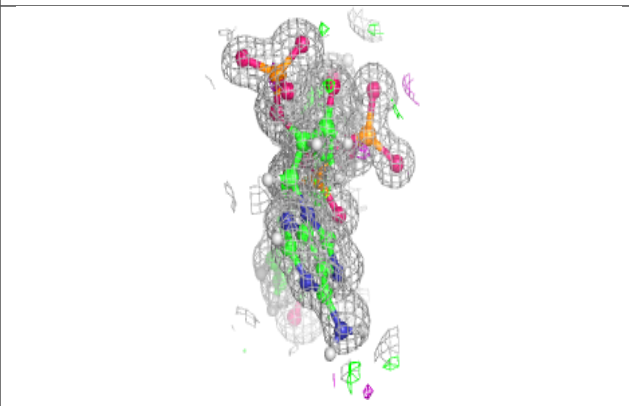
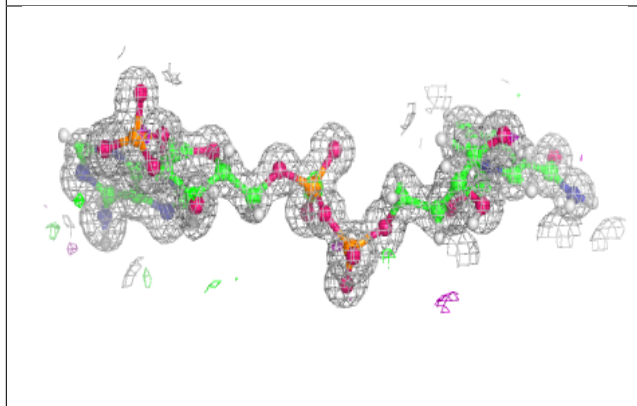
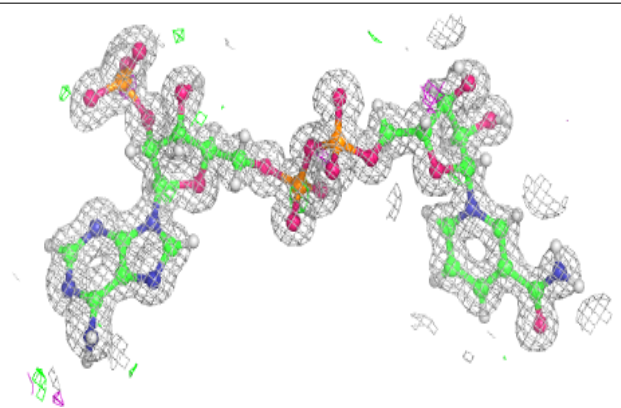
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FOL A 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NAP A 202:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.