



wwPDB X-ray Structure Validation Summary Report ⓘ

May 31, 2021 – 10:49 PM JST

PDB ID : 7D49
Title : X-ray crystal Structure of E.coli Dihydrofolate Reductase complexed with folate and NADP⁺ at pH4.5
Authors : Wan, Q.; Dealwis, C.
Deposited on : 2020-09-23
Resolution : 1.65 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 : 2.19
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) : 2.19

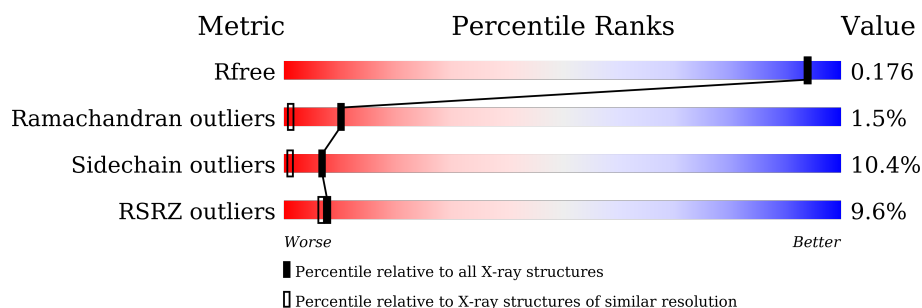
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	1827 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>9%</div> <div>92%</div> <div>8%</div> </div>
1	10-A	159	<div> <div>9%</div> <div>90%</div> <div>10%</div> </div>
1	11-A	159	<div> <div>9%</div> <div>97%</div> <div>.</div> </div>
1	12-A	159	<div> <div>9%</div> <div>91%</div> <div>9%</div> </div>
1	13-A	159	<div> <div>9%</div> <div>89%</div> <div>10%</div> </div>
1	14-A	159	<div> <div>9%</div> <div>91%</div> <div>8%</div> </div>
1	15-A	159	<div> <div>9%</div> <div>89%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	16-A	159	<div> <div>9%</div> <div>92%</div> <div>8%</div> <div>.</div> </div>
1	17-A	159	<div> <div>9%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
1	18-A	159	<div> <div>9%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	19-A	159	<div> <div>9%</div> <div>92%</div> <div>8%</div> <div></div> </div>
1	2-A	159	<div> <div>9%</div> <div>94%</div> <div>6%</div> <div></div> </div>
1	20-A	159	<div> <div>9%</div> <div>92%</div> <div>8%</div> <div></div> </div>
1	21-A	159	<div> <div>9%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>
1	22-A	159	<div> <div>9%</div> <div>94%</div> <div>6%</div> <div></div> </div>
1	23-A	159	<div> <div>9%</div> <div>91%</div> <div>9%</div> <div></div> </div>
1	24-A	159	<div> <div>9%</div> <div>91%</div> <div>9%</div> <div></div> </div>
1	25-A	159	<div> <div>9%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	26-A	159	<div> <div>9%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	27-A	159	<div> <div>9%</div> <div>87%</div> <div>13%</div> <div></div> </div>
1	28-A	159	<div> <div>9%</div> <div>91%</div> <div>9%</div> <div></div> </div>
1	29-A	159	<div> <div>9%</div> <div>91%</div> <div>9%</div> <div></div> </div>
1	3-A	159	<div> <div>9%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	30-A	159	<div> <div>9%</div> <div>94%</div> <div>5%</div> <div>.</div> </div>
1	31-A	159	<div> <div>9%</div> <div>91%</div> <div>9%</div> <div></div> </div>
1	32-A	159	<div> <div>9%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	33-A	159	<div> <div>9%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	34-A	159	<div> <div>9%</div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	35-A	159	<div> <div>9%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	36-A	159	<div> <div>9%</div> <div>86%</div> <div>14%</div> <div></div> </div>
1	37-A	159	<div> <div>9%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	38-A	159	<div> <div>9%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	39-A	159	<div> <div>9%</div> <div>84%</div> <div>16%</div> </div>
1	4-A	159	<div> <div>9%</div> <div>94%</div> <div>6%</div> </div>
1	40-A	159	<div> <div>9%</div> <div>86%</div> <div>14%</div> </div>
1	41-A	159	<div> <div>9%</div> <div>83%</div> <div>14%</div> </div>
1	42-A	159	<div> <div>9%</div> <div>85%</div> <div>14%</div> </div>
1	43-A	159	<div> <div>9%</div> <div>86%</div> <div>13%</div> </div>
1	44-A	159	<div> <div>9%</div> <div>88%</div> <div>11%</div> </div>
1	45-A	159	<div> <div>9%</div> <div>89%</div> <div>10%</div> </div>
1	46-A	159	<div> <div>9%</div> <div>88%</div> <div>11%</div> </div>
1	47-A	159	<div> <div>9%</div> <div>89%</div> <div>11%</div> </div>
1	48-A	159	<div> <div>9%</div> <div>89%</div> <div>10%</div> </div>
1	49-A	159	<div> <div>9%</div> <div>89%</div> <div>11%</div> </div>
1	5-A	159	<div> <div>9%</div> <div>93%</div> <div>7%</div> </div>
1	50-A	159	<div> <div>9%</div> <div>87%</div> <div>11%</div> </div>
1	51-A	159	<div> <div>9%</div> <div>88%</div> <div>11%</div> </div>
1	52-A	159	<div> <div>9%</div> <div>91%</div> <div>8%</div> </div>
1	53-A	159	<div> <div>9%</div> <div>89%</div> <div>10%</div> </div>
1	54-A	159	<div> <div>9%</div> <div>92%</div> <div>8%</div> </div>
1	55-A	159	<div> <div>9%</div> <div>88%</div> <div>9%</div> </div>
1	56-A	159	<div> <div>9%</div> <div>86%</div> <div>12%</div> </div>
1	57-A	159	<div> <div>9%</div> <div>89%</div> <div>10%</div> </div>
1	58-A	159	<div> <div>9%</div> <div>90%</div> <div>9%</div> </div>
1	59-A	159	<div> <div>9%</div> <div>87%</div> <div>12%</div> </div>
1	6-A	159	<div> <div>9%</div> <div>91%</div> <div>9%</div> </div>
1	60-A	159	<div> <div>9%</div> <div>86%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
1	61-A	159	<div> <div>9%</div> <div>92%</div> <div>8%</div> </div>
1	62-A	159	<div> <div>9%</div> <div>89%</div> <div>11%</div> </div>
1	63-A	159	<div> <div>9%</div> <div>88%</div> <div>12%</div> </div>
1	64-A	159	<div> <div>9%</div> <div>90%</div> <div>9%</div> </div>
1	65-A	159	<div> <div>9%</div> <div>91%</div> <div>8%</div> </div>
1	66-A	159	<div> <div>9%</div> <div>89%</div> <div>11%</div> </div>
1	67-A	159	<div> <div>9%</div> <div>91%</div> <div>9%</div> </div>
1	68-A	159	<div> <div>9%</div> <div>85%</div> <div>13%</div> </div>
1	69-A	159	<div> <div>9%</div> <div>86%</div> <div>14%</div> </div>
1	7-A	159	<div> <div>9%</div> <div>89%</div> <div>11%</div> </div>
1	70-A	159	<div> <div>9%</div> <div>86%</div> <div>14%</div> </div>
1	71-A	159	<div> <div>9%</div> <div>89%</div> <div>11%</div> </div>
1	72-A	159	<div> <div>9%</div> <div>89%</div> <div>10%</div> </div>
1	73-A	159	<div> <div>9%</div> <div>91%</div> <div>9%</div> </div>
1	74-A	159	<div> <div>9%</div> <div>92%</div> <div>8%</div> </div>
1	75-A	159	<div> <div>9%</div> <div>90%</div> <div>9%</div> </div>
1	76-A	159	<div> <div>9%</div> <div>93%</div> <div>7%</div> </div>
1	77-A	159	<div> <div>9%</div> <div>94%</div> <div>6%</div> </div>
1	78-A	159	<div> <div>9%</div> <div>89%</div> <div>11%</div> </div>
1	79-A	159	<div> <div>9%</div> <div>91%</div> <div>9%</div> </div>
1	8-A	159	<div> <div>9%</div> <div>92%</div> <div>8%</div> </div>
1	80-A	159	<div> <div>9%</div> <div>90%</div> <div>9%</div> </div>
1	9-A	159	<div> <div>9%</div> <div>86%</div> <div>14%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 113251 atoms, of which 0 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	N	O	S	0	0	0
			1268	805	216	240	7			
1	2-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	3-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	4-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	5-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	6-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	7-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	8-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	9-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	10-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	11-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	12-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	13-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	14-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	15-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	16-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	17-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	18-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	19-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	20-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	21-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	22-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	23-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	24-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	25-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	26-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	27-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	28-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	29-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	30-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	31-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	32-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	33-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	34-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	35-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	36-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	37-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	38-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	39-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	40-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	41-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	42-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	43-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	44-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	45-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	46-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	47-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	48-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	49-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	50-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	51-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	52-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	53-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	54-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	55-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	56-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	57-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	58-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	59-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	60-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	61-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	62-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	63-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	64-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	65-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	66-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	67-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	68-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	69-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	70-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	71-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	72-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	73-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	74-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	75-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	76-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	77-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	78-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			
1	79-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			

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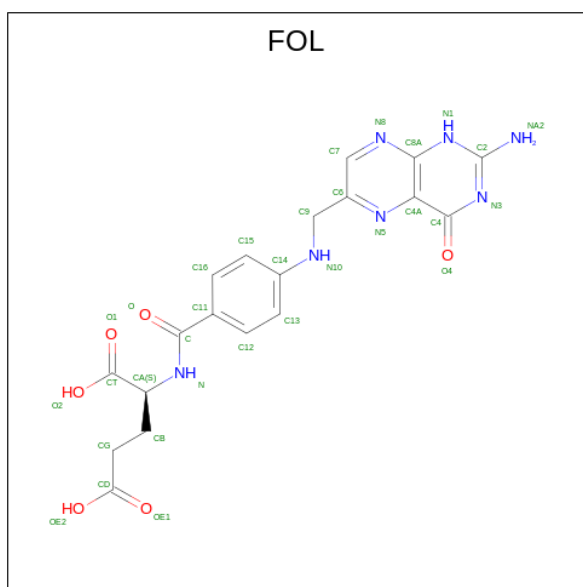
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	80-A	159	Total	C	N	O	S	0	0	0
			1268	805	216	240	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	ASP	ASN	conflict	UNP P0ABQ4

- Molecule 2 is FOLIC ACID (three-letter code: FOL) (formula: $C_{19}H_{19}N_7O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	1-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	2-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	3-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	4-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	5-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	6-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	7-A	1	Total	C	N	O	0	0
			32	19	7	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	8-A	1	Total 32	C 19	N 7	O 6	0	0
2	9-A	1	Total 32	C 19	N 7	O 6	0	0
2	10-A	1	Total 32	C 19	N 7	O 6	0	0
2	11-A	1	Total 32	C 19	N 7	O 6	0	0
2	12-A	1	Total 32	C 19	N 7	O 6	0	0
2	13-A	1	Total 32	C 19	N 7	O 6	0	0
2	14-A	1	Total 32	C 19	N 7	O 6	0	0
2	15-A	1	Total 32	C 19	N 7	O 6	0	0
2	16-A	1	Total 32	C 19	N 7	O 6	0	0
2	17-A	1	Total 32	C 19	N 7	O 6	0	0
2	18-A	1	Total 32	C 19	N 7	O 6	0	0
2	19-A	1	Total 32	C 19	N 7	O 6	0	0
2	20-A	1	Total 32	C 19	N 7	O 6	0	0
2	21-A	1	Total 32	C 19	N 7	O 6	0	0
2	22-A	1	Total 32	C 19	N 7	O 6	0	0
2	23-A	1	Total 32	C 19	N 7	O 6	0	0
2	24-A	1	Total 32	C 19	N 7	O 6	0	0
2	25-A	1	Total 32	C 19	N 7	O 6	0	0
2	26-A	1	Total 32	C 19	N 7	O 6	0	0
2	27-A	1	Total 32	C 19	N 7	O 6	0	0
2	28-A	1	Total 32	C 19	N 7	O 6	0	0

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

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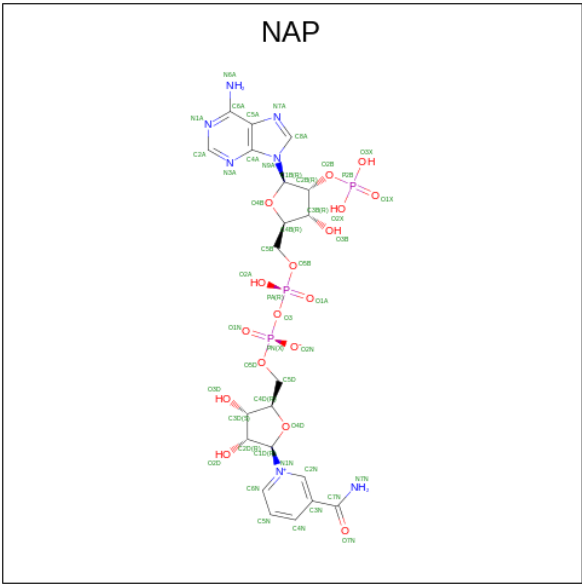
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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			32	19	7	6		
2	51-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	52-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	53-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	54-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	55-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	56-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	57-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	58-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	59-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	60-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	61-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	62-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	63-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	64-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	65-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	66-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	67-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	68-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	69-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	70-A	1	Total	C	N	O	0	0
			32	19	7	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	71-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	72-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	73-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	74-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	75-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	76-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	77-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	78-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	79-A	1	Total	C	N	O	0	0
			32	19	7	6		
2	80-A	1	Total	C	N	O	0	0
			32	19	7	6		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	1-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	2-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	3-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	4-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	5-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	6-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	7-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	8-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	9-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	10-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	11-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	12-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	13-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	14-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	15-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	16-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	17-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	18-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	19-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	20-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	21-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	22-A	1	Total 48	C 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	23-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	24-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	25-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	26-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	27-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	28-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	29-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	30-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	31-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	32-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	33-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	34-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	35-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	36-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	37-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	38-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	39-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	40-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	41-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	42-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	43-A	1	Total 48	C 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	44-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	45-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	46-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	47-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	48-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	49-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	50-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	51-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	52-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	53-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	54-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	55-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	56-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	57-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	58-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	59-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	60-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	61-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	62-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	63-A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	64-A	1	Total 48	C 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	65-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	66-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	67-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	68-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	69-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	70-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	71-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	72-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	73-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	74-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	75-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	76-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	77-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	78-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	79-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	80-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1-A	79	Total	O	0	0
			79	79		
4	2-A	68	Total	O	0	0
			68	68		
4	3-A	63	Total	O	0	0
			63	63		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	4-A	67	Total O 67 67	0	0
4	5-A	67	Total O 67 67	0	0
4	6-A	60	Total O 60 60	0	0
4	7-A	61	Total O 61 61	0	0
4	8-A	61	Total O 61 61	0	0
4	9-A	59	Total O 59 59	0	0
4	10-A	57	Total O 57 57	0	0
4	11-A	72	Total O 72 72	0	0
4	12-A	76	Total O 76 76	0	0
4	13-A	75	Total O 75 75	0	0
4	14-A	72	Total O 72 72	0	0
4	15-A	65	Total O 65 65	0	0
4	16-A	64	Total O 64 64	0	0
4	17-A	72	Total O 72 72	0	0
4	18-A	73	Total O 73 73	0	0
4	19-A	76	Total O 76 76	0	0
4	20-A	57	Total O 57 57	0	0
4	21-A	67	Total O 67 67	0	0
4	22-A	69	Total O 69 69	0	0
4	23-A	71	Total O 71 71	0	0
4	24-A	65	Total O 65 65	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	25-A	61	Total O 61 61	0	0
4	26-A	53	Total O 53 53	0	0
4	27-A	67	Total O 67 67	0	0
4	28-A	74	Total O 74 74	0	0
4	29-A	80	Total O 80 80	0	0
4	30-A	72	Total O 72 72	0	0
4	31-A	76	Total O 76 76	0	0
4	32-A	72	Total O 72 72	0	0
4	33-A	70	Total O 70 70	0	0
4	34-A	62	Total O 62 62	0	0
4	35-A	52	Total O 52 52	0	0
4	36-A	62	Total O 62 62	0	0
4	37-A	66	Total O 66 66	0	0
4	38-A	76	Total O 76 76	0	0
4	39-A	72	Total O 72 72	0	0
4	40-A	75	Total O 75 75	0	0
4	41-A	72	Total O 72 72	0	0
4	42-A	66	Total O 66 66	0	0
4	43-A	65	Total O 65 65	0	0
4	44-A	65	Total O 65 65	0	0
4	45-A	69	Total O 69 69	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	46-A	62	Total O 62 62	0	0
4	47-A	63	Total O 63 63	0	0
4	48-A	80	Total O 80 80	0	0
4	49-A	74	Total O 74 74	0	0
4	50-A	70	Total O 70 70	0	0
4	51-A	69	Total O 69 69	0	0
4	52-A	68	Total O 68 68	0	0
4	53-A	63	Total O 63 63	0	0
4	54-A	70	Total O 70 70	0	0
4	55-A	75	Total O 75 75	0	0
4	56-A	76	Total O 76 76	0	0
4	57-A	72	Total O 72 72	0	0
4	58-A	76	Total O 76 76	0	0
4	59-A	71	Total O 71 71	0	0
4	60-A	75	Total O 75 75	0	0
4	61-A	48	Total O 48 48	0	0
4	62-A	52	Total O 52 52	0	0
4	63-A	72	Total O 72 72	0	0
4	64-A	73	Total O 73 73	0	0
4	65-A	74	Total O 74 74	0	0
4	66-A	62	Total O 62 62	0	0

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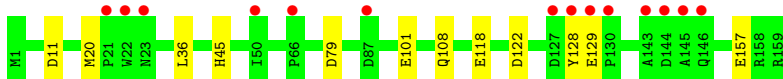
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	67-A	56	Total 56	O 56	0	0
4	68-A	56	Total 56	O 56	0	0
4	69-A	64	Total 64	O 64	0	0
4	70-A	69	Total 69	O 69	0	0
4	71-A	65	Total 65	O 65	0	0
4	72-A	71	Total 71	O 71	0	0
4	73-A	65	Total 65	O 65	0	0
4	74-A	63	Total 63	O 63	0	0
4	75-A	64	Total 64	O 64	0	0
4	76-A	61	Total 61	O 61	0	0
4	77-A	71	Total 71	O 71	0	0
4	78-A	71	Total 71	O 71	0	0
4	79-A	76	Total 76	O 76	0	0
4	80-A	71	Total 71	O 71	0	0

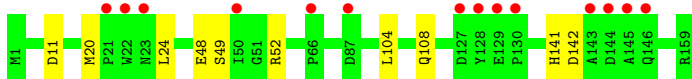
3 Residue-property plots [i](#)

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



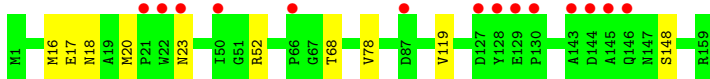
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



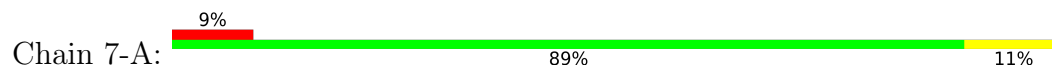
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



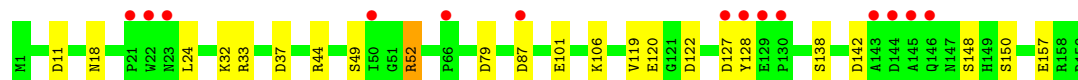
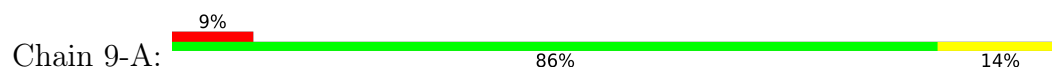
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



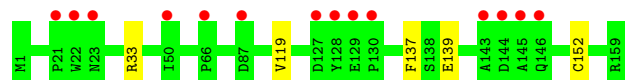
- Molecule 1: Dihydrofolate reductase



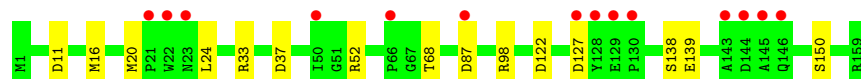
- Molecule 1: Dihydrofolate reductase



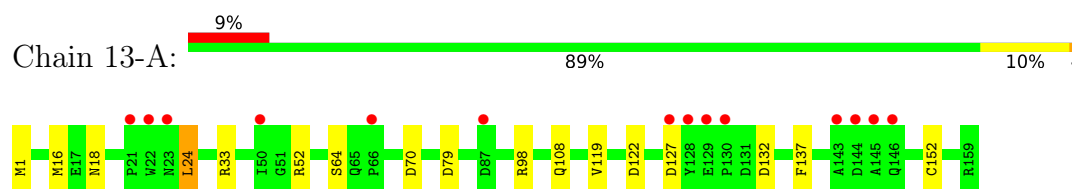
- Molecule 1: Dihydrofolate reductase



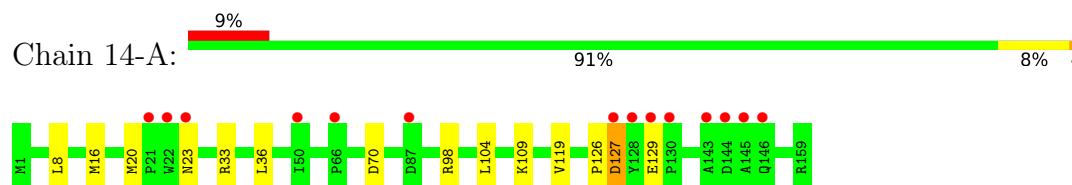
- Molecule 1: Dihydrofolate reductase



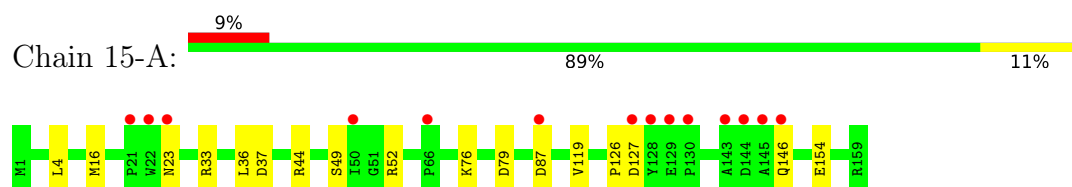
- Molecule 1: Dihydrofolate reductase



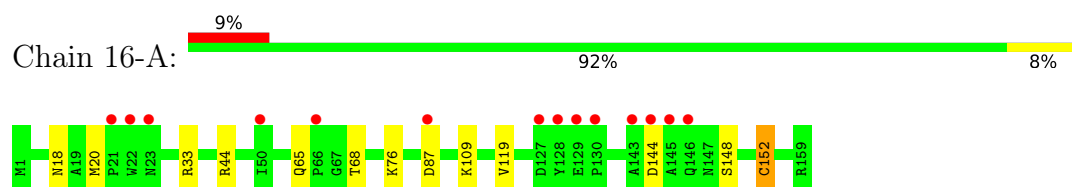
- Molecule 1: Dihydrofolate reductase



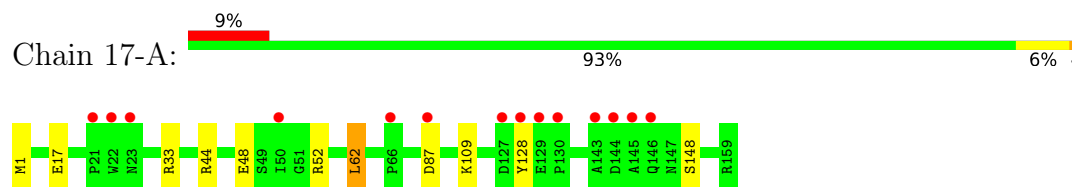
- Molecule 1: Dihydrofolate reductase



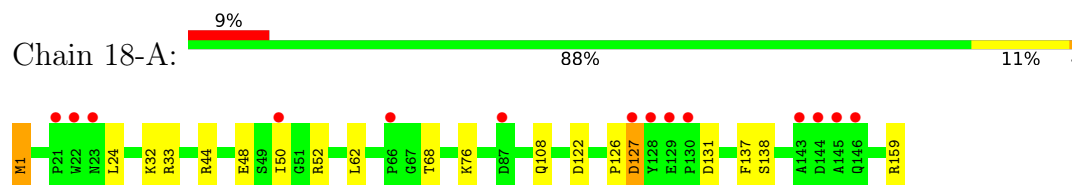
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase

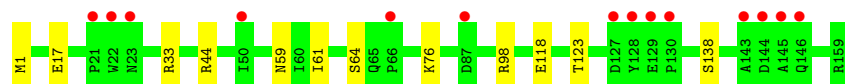


- Molecule 1: Dihydrofolate reductase

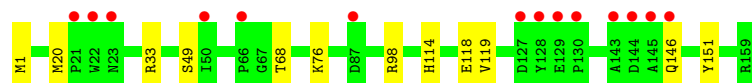


- Molecule 1: Dihydrofolate reductase





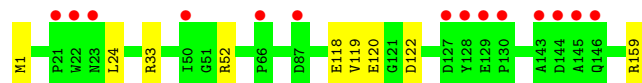
- Molecule 1: Dihydrofolate reductase



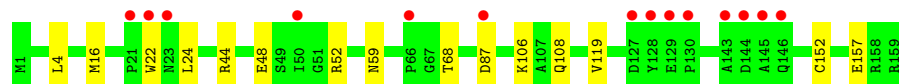
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



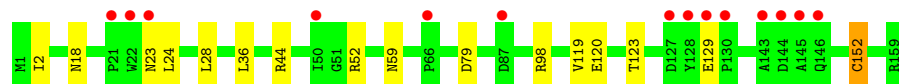
- Molecule 1: Dihydrofolate reductase



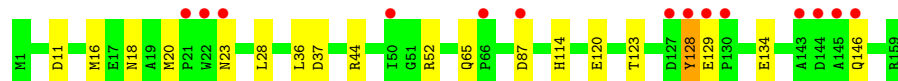
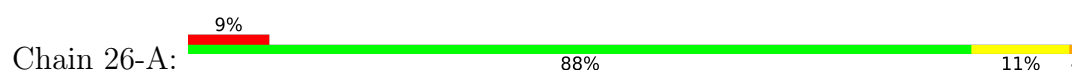
- Molecule 1: Dihydrofolate reductase



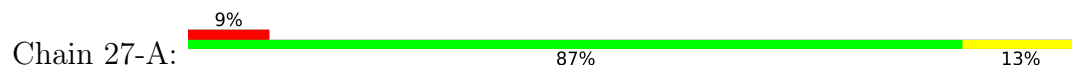
- Molecule 1: Dihydrofolate reductase



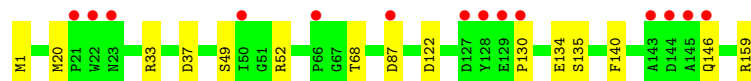
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



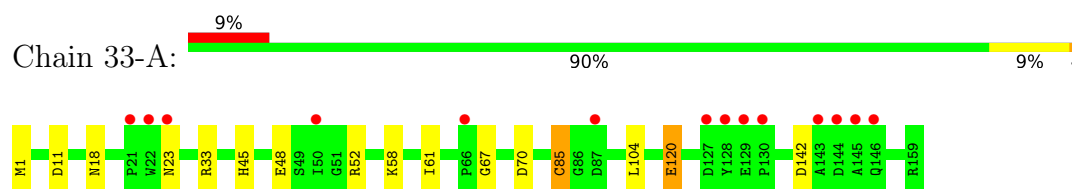
- Molecule 1: Dihydrofolate reductase



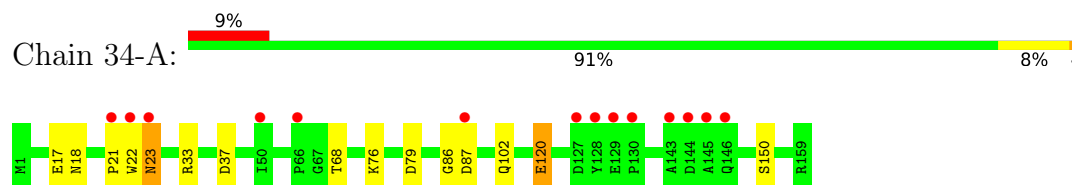
- Molecule 1: Dihydrofolate reductase



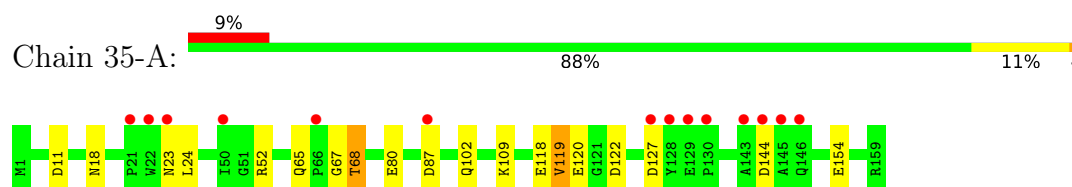
- Molecule 1: Dihydrofolate reductase



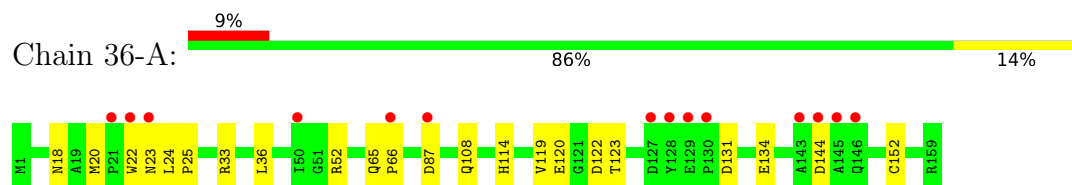
- Molecule 1: Dihydrofolate reductase



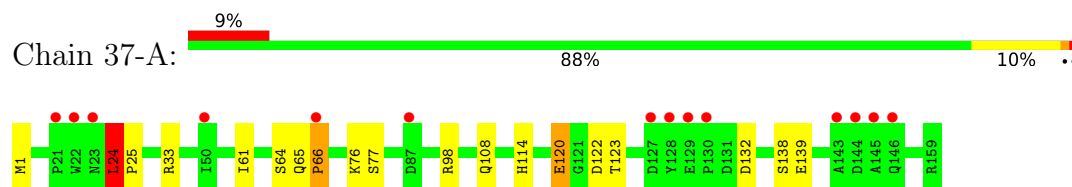
- Molecule 1: Dihydrofolate reductase



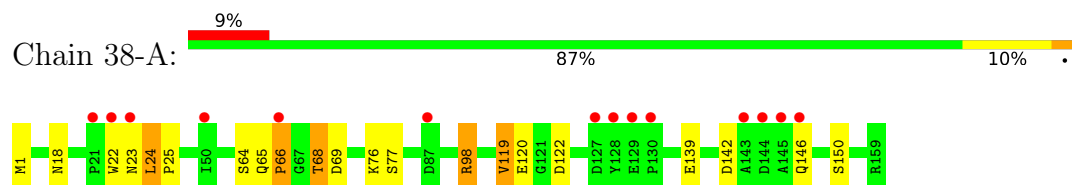
- Molecule 1: Dihydrofolate reductase



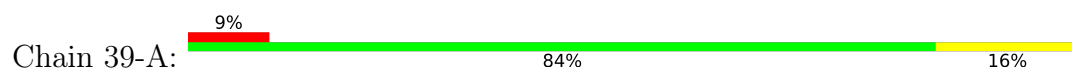
- Molecule 1: Dihydrofolate reductase

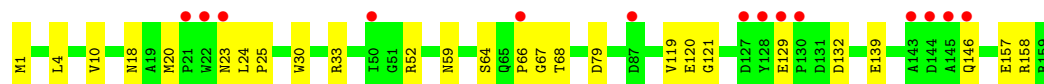


- Molecule 1: Dihydrofolate reductase

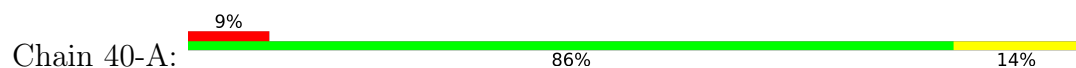


- Molecule 1: Dihydrofolate reductase

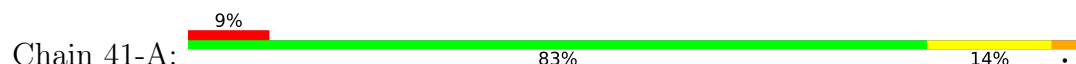




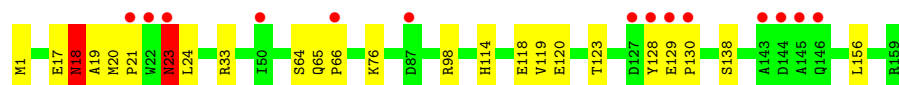
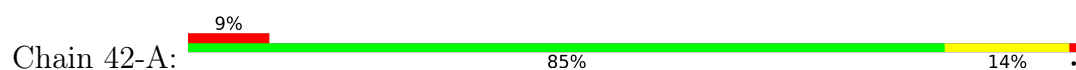
- Molecule 1: Dihydrofolate reductase



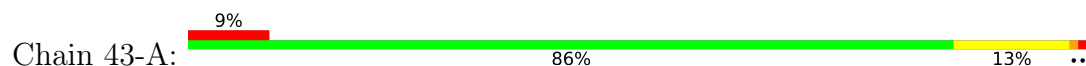
- Molecule 1: Dihydrofolate reductase



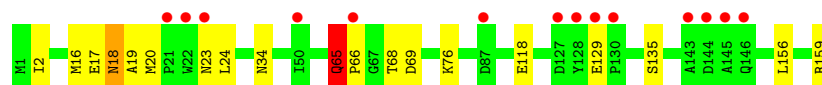
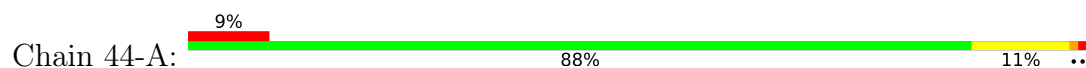
- Molecule 1: Dihydrofolate reductase



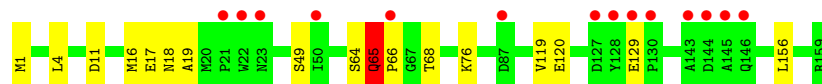
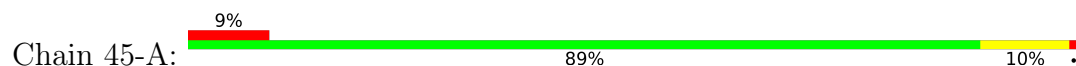
- Molecule 1: Dihydrofolate reductase



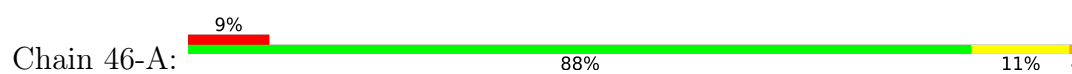
- Molecule 1: Dihydrofolate reductase



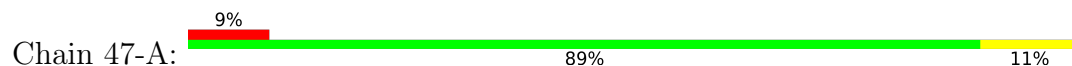
- Molecule 1: Dihydrofolate reductase



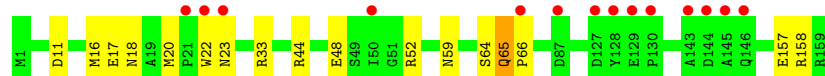
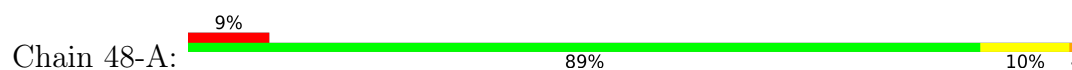
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



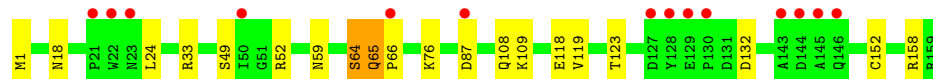
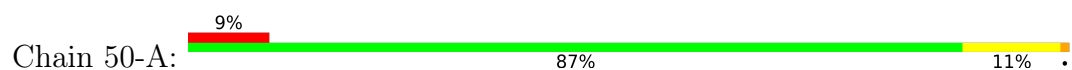
- Molecule 1: Dihydrofolate reductase



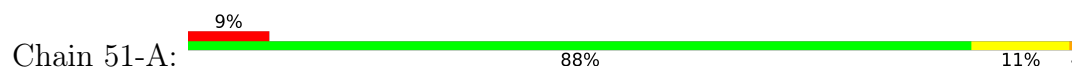
- Molecule 1: Dihydrofolate reductase



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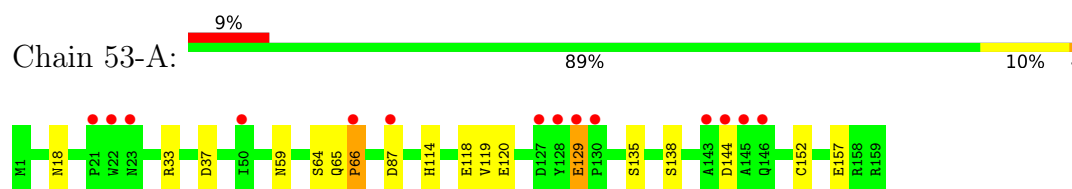
- Molecule 1: Dihydrofolate reductase



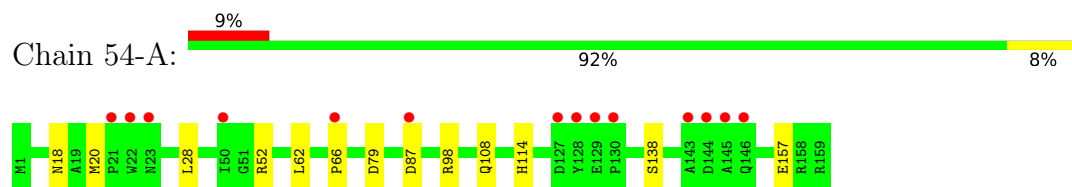
- Molecule 1: Dihydrofolate reductase



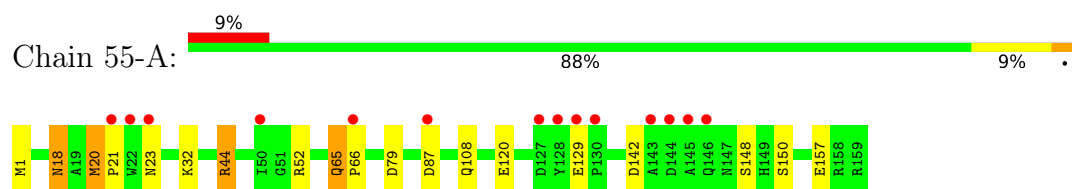
● Molecule 1: Dihydrofolate reductase



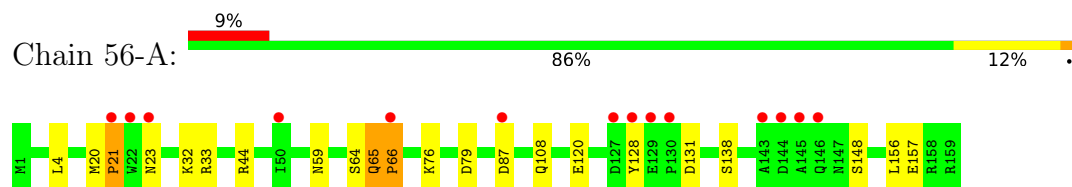
● Molecule 1: Dihydrofolate reductase



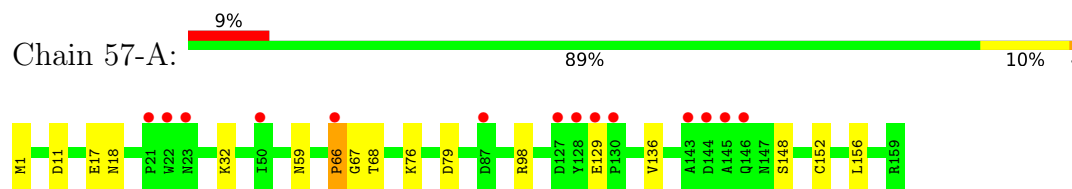
● Molecule 1: Dihydrofolate reductase



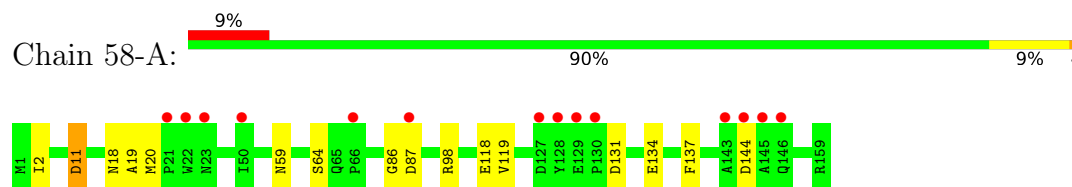
● Molecule 1: Dihydrofolate reductase



● Molecule 1: Dihydrofolate reductase



● Molecule 1: Dihydrofolate reductase

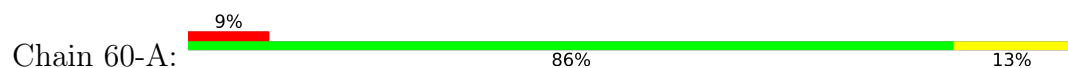


● Molecule 1: Dihydrofolate reductase

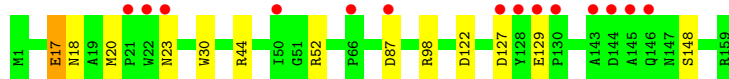




- Molecule 1: Dihydrofolate reductase



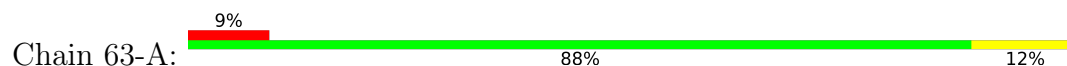
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



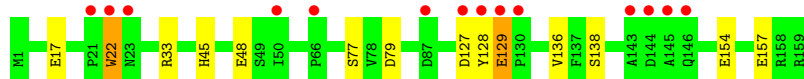
- Molecule 1: Dihydrofolate reductase



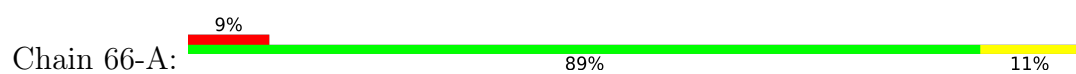
- Molecule 1: Dihydrofolate reductase



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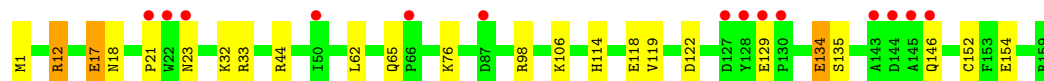
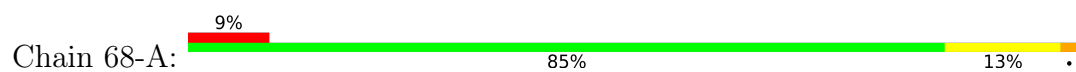
- Molecule 1: Dihydrofolate reductase



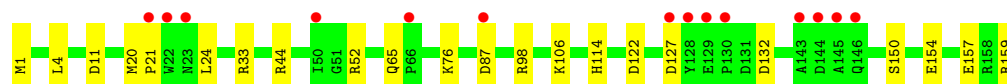
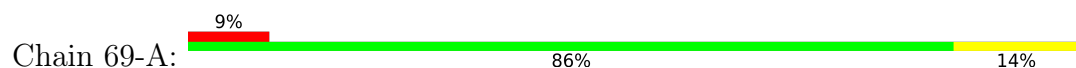
• Molecule 1: Dihydrofolate reductase



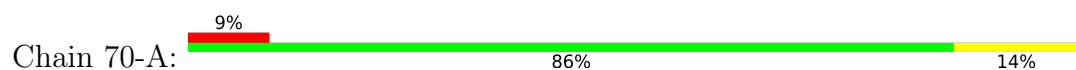
• Molecule 1: Dihydrofolate reductase



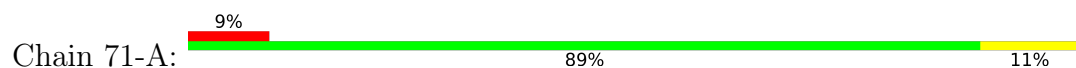
• Molecule 1: Dihydrofolate reductase



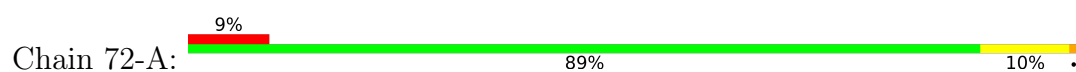
• Molecule 1: Dihydrofolate reductase



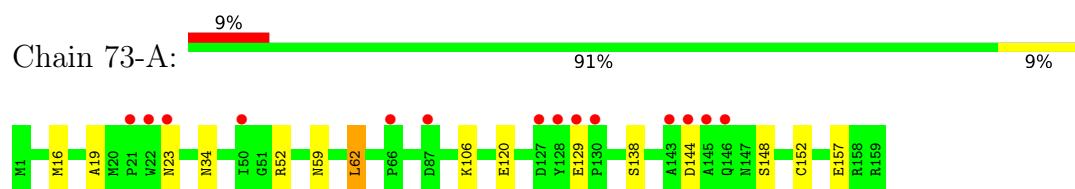
• Molecule 1: Dihydrofolate reductase



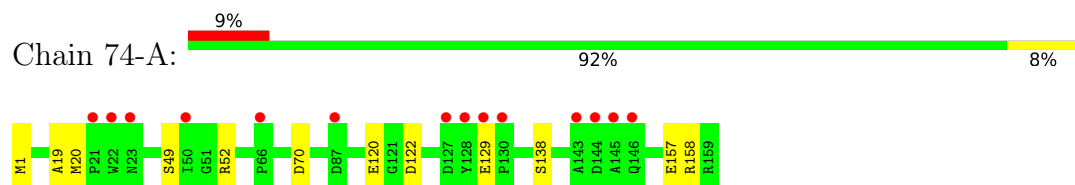
• Molecule 1: Dihydrofolate reductase



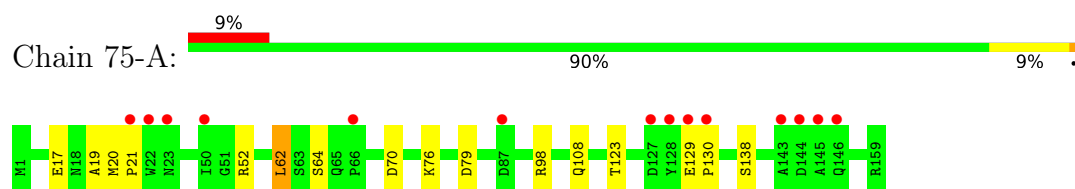
- Molecule 1: Dihydrofolate reductase



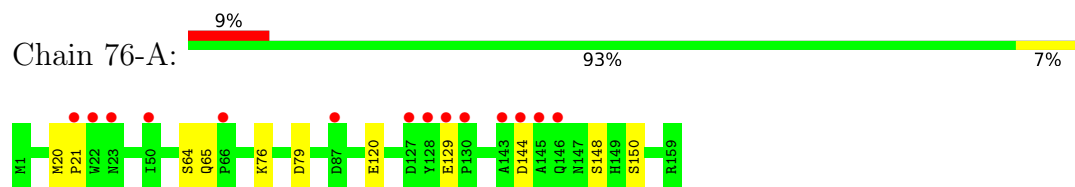
- Molecule 1: Dihydrofolate reductase



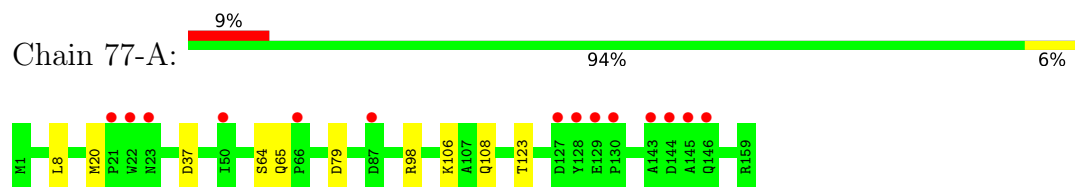
- Molecule 1: Dihydrofolate reductase



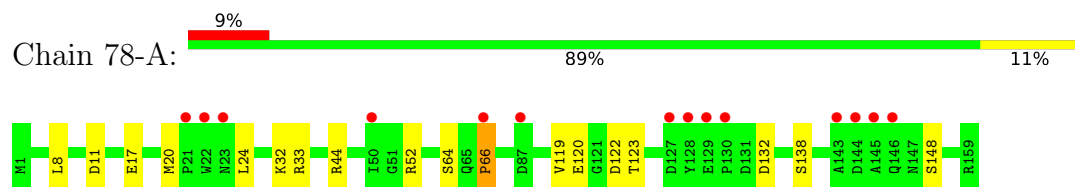
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase

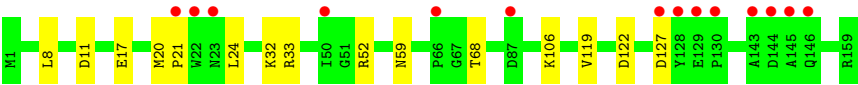


- Molecule 1: Dihydrofolate reductase

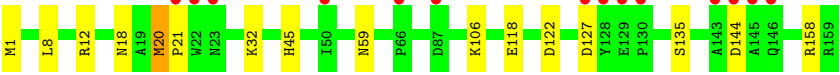


- Molecule 1: Dihydrofolate reductase





● Molecule 1: Dihydrofolate reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	34.10Å 45.59Å 99.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.31 – 1.65 27.31 – 1.65	Depositor EDS
% Data completeness (in resolution range)	91.8 (27.31-1.65) 91.3 (27.31-1.65)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 1.65Å)	Xtriage
Refinement program	PHENIX (phenix.ensemble_refinement:1.13rc2_2986)	Depositor
R, R_{free}	0.135 , 0.171 0.147 , 0.176	Depositor DCC
R_{free} test set	904 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 588.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	113251	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.25% 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: NAP, FOL

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	0.46	0/1302	0.68	0/1770
1	2-A	0.44	0/1302	0.66	0/1770
1	3-A	0.50	0/1302	0.69	3/1770 (0.2%)
1	4-A	0.46	0/1302	0.62	0/1770
1	5-A	0.43	0/1302	0.64	0/1770
1	6-A	0.41	0/1302	0.63	1/1770 (0.1%)
1	7-A	0.42	0/1302	0.66	1/1770 (0.1%)
1	8-A	0.46	1/1302 (0.1%)	0.66	1/1770 (0.1%)
1	9-A	0.45	0/1302	0.69	1/1770 (0.1%)
1	10-A	0.45	0/1302	0.66	0/1770
1	11-A	0.47	1/1302 (0.1%)	0.64	0/1770
1	12-A	0.41	0/1302	0.64	0/1770
1	13-A	0.47	1/1302 (0.1%)	0.70	2/1770 (0.1%)
1	14-A	0.45	0/1302	0.65	0/1770
1	15-A	0.40	0/1302	0.64	0/1770
1	16-A	0.43	1/1302 (0.1%)	0.64	0/1770
1	17-A	0.42	0/1302	0.64	1/1770 (0.1%)
1	18-A	0.49	1/1302 (0.1%)	0.69	2/1770 (0.1%)
1	19-A	0.43	0/1302	0.63	0/1770
1	20-A	0.40	0/1302	0.63	0/1770
1	21-A	0.44	0/1302	0.63	1/1770 (0.1%)
1	22-A	0.39	0/1302	0.61	0/1770
1	23-A	0.46	1/1302 (0.1%)	0.66	1/1770 (0.1%)
1	24-A	0.44	0/1302	0.65	1/1770 (0.1%)
1	25-A	0.48	1/1302 (0.1%)	0.64	1/1770 (0.1%)
1	26-A	0.41	0/1302	0.63	0/1770
1	27-A	0.41	0/1302	0.63	0/1770
1	28-A	0.43	0/1302	0.66	0/1770
1	29-A	0.42	0/1302	0.62	0/1770
1	30-A	0.42	0/1302	0.65	0/1770
1	31-A	0.43	0/1302	0.66	0/1770
1	32-A	0.42	0/1302	0.68	0/1770

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	33-A	0.48	1/1302 (0.1%)	0.68	1/1770 (0.1%)
1	34-A	0.44	0/1302	0.68	0/1770
1	35-A	0.44	0/1302	0.66	1/1770 (0.1%)
1	36-A	0.42	0/1302	0.64	0/1770
1	37-A	0.43	0/1302	0.69	2/1770 (0.1%)
1	38-A	0.49	1/1302 (0.1%)	0.75	2/1770 (0.1%)
1	39-A	0.44	0/1302	0.70	0/1770
1	40-A	0.46	1/1302 (0.1%)	0.71	1/1770 (0.1%)
1	41-A	0.44	0/1302	0.69	0/1770
1	42-A	0.44	0/1302	0.67	0/1770
1	43-A	0.46	0/1302	0.68	0/1770
1	44-A	0.44	0/1302	0.68	0/1770
1	45-A	0.44	0/1302	0.67	0/1770
1	46-A	0.47	0/1302	0.67	1/1770 (0.1%)
1	47-A	0.45	0/1302	0.66	0/1770
1	48-A	0.47	1/1302 (0.1%)	0.64	0/1770
1	49-A	0.45	0/1302	0.66	0/1770
1	50-A	0.44	0/1302	0.67	0/1770
1	51-A	0.42	0/1302	0.63	0/1770
1	52-A	0.42	0/1302	0.67	1/1770 (0.1%)
1	53-A	0.46	0/1302	0.67	0/1770
1	54-A	0.43	0/1302	0.64	0/1770
1	55-A	0.42	0/1302	0.68	1/1770 (0.1%)
1	56-A	0.44	0/1302	0.69	0/1770
1	57-A	0.42	0/1302	0.66	1/1770 (0.1%)
1	58-A	0.44	0/1302	0.65	0/1770
1	59-A	0.44	0/1302	0.63	0/1770
1	60-A	0.45	1/1302 (0.1%)	0.64	0/1770
1	61-A	0.44	0/1302	0.66	0/1770
1	62-A	0.39	0/1302	0.61	0/1770
1	63-A	0.50	1/1302 (0.1%)	0.70	2/1770 (0.1%)
1	64-A	0.45	0/1302	0.69	1/1770 (0.1%)
1	65-A	0.45	0/1302	0.67	0/1770
1	66-A	0.46	0/1302	0.68	1/1770 (0.1%)
1	67-A	0.44	0/1302	0.67	0/1770
1	68-A	0.54	2/1302 (0.2%)	0.73	2/1770 (0.1%)
1	69-A	0.41	0/1302	0.65	1/1770 (0.1%)
1	70-A	0.43	0/1302	0.64	0/1770
1	71-A	0.44	0/1302	0.65	1/1770 (0.1%)
1	72-A	0.43	0/1302	0.65	1/1770 (0.1%)
1	73-A	0.45	0/1302	0.72	2/1770 (0.1%)
1	74-A	0.42	0/1302	0.66	0/1770
1	75-A	0.40	0/1302	0.70	1/1770 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	76-A	0.43	0/1302	0.65	0/1770
1	77-A	0.45	0/1302	0.66	1/1770 (0.1%)
1	78-A	0.43	0/1302	0.68	0/1770
1	79-A	0.43	0/1302	0.66	0/1770
1	80-A	0.44	0/1302	0.65	0/1770
All	All	0.44	15/104160 (0.0%)	0.66	40/141600 (0.0%)

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	8-A	0	2
1	10-A	0	1
1	14-A	0	1
1	18-A	0	1
1	20-A	0	1
1	23-A	0	1
1	27-A	0	1
1	29-A	0	1
1	35-A	0	1
1	36-A	0	3
1	37-A	0	1
1	38-A	0	2
1	39-A	0	1
1	41-A	0	2
1	42-A	0	3
1	43-A	0	3
1	44-A	0	2
1	45-A	0	2
1	46-A	0	1
1	47-A	0	1
1	53-A	0	1
1	56-A	0	3
1	57-A	0	2
1	58-A	0	2
1	60-A	0	2
1	65-A	0	2
1	70-A	0	1
1	75-A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	76-A	0	1
1	80-A	0	1
All	All	0	48

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	25-A	152	CYS	CB-SG	7.93	1.95	1.82
1	11-A	152	CYS	CB-SG	-7.50	1.69	1.82
1	68-A	12	ARG	CG-CD	-7.00	1.34	1.51
1	38-A	98	ARG	CG-CD	-6.70	1.35	1.51
1	68-A	134	GLU	CG-CD	6.28	1.61	1.51

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	68-A	1	MET	CG-SD-CE	9.96	116.14	100.20
1	38-A	24	LEU	CA-CB-CG	8.55	134.96	115.30
1	3-A	16	MET	CG-SD-CE	8.12	113.20	100.20
1	71-A	28	LEU	CA-CB-CG	-7.43	98.20	115.30
1	68-A	12	ARG	CB-CG-CD	7.35	130.72	111.60

There are no chirality outliers.

5 of 48 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	128	TYR	Peptide
1	10-A	129	GLU	Peptide
1	14-A	126	PRO	Peptide
1	8-A	127	ASP	Peptide
1	8-A	128	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	1268	0	1221	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2-A	1268	0	1221	0	0
1	3-A	1268	0	1221	0	0
1	4-A	1268	0	1221	0	0
1	5-A	1268	0	1221	0	0
1	6-A	1268	0	1221	0	0
1	7-A	1268	0	1221	0	0
1	8-A	1268	0	1221	0	0
1	9-A	1268	0	1221	0	0
1	10-A	1268	0	1221	0	0
1	11-A	1268	0	1221	0	0
1	12-A	1268	0	1221	0	0
1	13-A	1268	0	1221	0	0
1	14-A	1268	0	1221	0	0
1	15-A	1268	0	1221	0	0
1	16-A	1268	0	1221	0	0
1	17-A	1268	0	1221	0	0
1	18-A	1268	0	1221	0	0
1	19-A	1268	0	1221	0	0
1	20-A	1268	0	1221	0	0
1	21-A	1268	0	1221	0	0
1	22-A	1268	0	1221	0	0
1	23-A	1268	0	1221	0	0
1	24-A	1268	0	1221	0	0
1	25-A	1268	0	1221	0	0
1	26-A	1268	0	1221	0	0
1	27-A	1268	0	1221	0	0
1	28-A	1268	0	1221	0	0
1	29-A	1268	0	1221	0	0
1	30-A	1268	0	1221	0	0
1	31-A	1268	0	1221	0	0
1	32-A	1268	0	1221	0	0
1	33-A	1268	0	1221	0	0
1	34-A	1268	0	1221	0	0
1	35-A	1268	0	1221	0	0
1	36-A	1268	0	1221	0	0
1	37-A	1268	0	1221	0	0
1	38-A	1268	0	1221	0	0
1	39-A	1268	0	1221	0	0
1	40-A	1268	0	1221	0	0
1	41-A	1268	0	1221	0	0
1	42-A	1268	0	1221	0	0
1	43-A	1268	0	1221	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	44-A	1268	0	1221	0	0
1	45-A	1268	0	1221	0	0
1	46-A	1268	0	1221	0	0
1	47-A	1268	0	1221	0	0
1	48-A	1268	0	1221	0	0
1	49-A	1268	0	1221	0	0
1	50-A	1268	0	1221	0	0
1	51-A	1268	0	1221	0	0
1	52-A	1268	0	1221	0	0
1	53-A	1268	0	1221	0	0
1	54-A	1268	0	1221	0	0
1	55-A	1268	0	1221	0	0
1	56-A	1268	0	1221	0	0
1	57-A	1268	0	1221	0	0
1	58-A	1268	0	1221	0	0
1	59-A	1268	0	1221	0	0
1	60-A	1268	0	1221	0	0
1	61-A	1268	0	1221	0	0
1	62-A	1268	0	1221	0	0
1	63-A	1268	0	1221	0	0
1	64-A	1268	0	1221	0	0
1	65-A	1268	0	1221	0	0
1	66-A	1268	0	1221	0	0
1	67-A	1268	0	1221	0	0
1	68-A	1268	0	1221	0	0
1	69-A	1268	0	1221	0	0
1	70-A	1268	0	1221	0	0
1	71-A	1268	0	1221	0	0
1	72-A	1268	0	1221	0	0
1	73-A	1268	0	1221	0	0
1	74-A	1268	0	1221	0	0
1	75-A	1268	0	1221	0	0
1	76-A	1268	0	1221	0	0
1	77-A	1268	0	1221	0	0
1	78-A	1268	0	1221	0	0
1	79-A	1268	0	1221	0	0
1	80-A	1268	0	1221	0	0
2	1-A	32	0	17	0	0
2	2-A	32	0	17	0	0
2	3-A	32	0	17	0	0
2	4-A	32	0	17	0	0
2	5-A	32	0	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	6-A	32	0	17	0	0
2	7-A	32	0	17	0	0
2	8-A	32	0	17	0	0
2	9-A	32	0	17	0	0
2	10-A	32	0	17	0	0
2	11-A	32	0	17	0	0
2	12-A	32	0	17	0	0
2	13-A	32	0	17	0	0
2	14-A	32	0	17	0	0
2	15-A	32	0	17	0	0
2	16-A	32	0	17	0	0
2	17-A	32	0	17	0	0
2	18-A	32	0	17	0	0
2	19-A	32	0	17	0	0
2	20-A	32	0	17	0	0
2	21-A	32	0	17	0	0
2	22-A	32	0	17	0	0
2	23-A	32	0	17	0	0
2	24-A	32	0	17	0	0
2	25-A	32	0	17	0	0
2	26-A	32	0	17	0	0
2	27-A	32	0	17	0	0
2	28-A	32	0	17	0	0
2	29-A	32	0	17	0	0
2	30-A	32	0	17	0	0
2	31-A	32	0	17	0	0
2	32-A	32	0	17	0	0
2	33-A	32	0	17	0	0
2	34-A	32	0	17	0	0
2	35-A	32	0	17	0	0
2	36-A	32	0	17	0	0
2	37-A	32	0	17	0	0
2	38-A	32	0	17	0	0
2	39-A	32	0	17	0	0
2	40-A	32	0	17	0	0
2	41-A	32	0	17	0	0
2	42-A	32	0	17	0	0
2	43-A	32	0	17	0	0
2	44-A	32	0	17	0	0
2	45-A	32	0	17	0	0
2	46-A	32	0	17	0	0
2	47-A	32	0	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	48-A	32	0	17	0	0
2	49-A	32	0	17	0	0
2	50-A	32	0	17	0	0
2	51-A	32	0	17	0	0
2	52-A	32	0	17	0	0
2	53-A	32	0	17	0	0
2	54-A	32	0	17	0	0
2	55-A	32	0	17	0	0
2	56-A	32	0	17	0	0
2	57-A	32	0	17	0	0
2	58-A	32	0	17	0	0
2	59-A	32	0	17	0	0
2	60-A	32	0	17	0	0
2	61-A	32	0	17	0	0
2	62-A	32	0	17	0	0
2	63-A	32	0	17	0	0
2	64-A	32	0	17	0	0
2	65-A	32	0	17	0	0
2	66-A	32	0	17	0	0
2	67-A	32	0	17	0	0
2	68-A	32	0	17	0	0
2	69-A	32	0	17	0	0
2	70-A	32	0	17	0	0
2	71-A	32	0	17	0	0
2	72-A	32	0	17	0	0
2	73-A	32	0	17	0	0
2	74-A	32	0	17	0	0
2	75-A	32	0	17	0	0
2	76-A	32	0	17	0	0
2	77-A	32	0	17	0	0
2	78-A	32	0	16	0	0
2	79-A	32	0	17	0	0
2	80-A	32	0	17	0	0
3	1-A	48	0	24	0	0
3	2-A	48	0	24	0	0
3	3-A	48	0	23	0	0
3	4-A	48	0	24	0	0
3	5-A	48	0	24	0	0
3	6-A	48	0	24	0	0
3	7-A	48	0	24	0	0
3	8-A	48	0	24	0	0
3	9-A	48	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	10-A	48	0	24	0	0
3	11-A	48	0	24	0	0
3	12-A	48	0	24	0	0
3	13-A	48	0	23	0	0
3	14-A	48	0	24	0	0
3	15-A	48	0	24	0	0
3	16-A	48	0	24	0	0
3	17-A	48	0	24	0	0
3	18-A	48	0	24	0	0
3	19-A	48	0	24	0	0
3	20-A	48	0	24	0	0
3	21-A	48	0	24	0	0
3	22-A	48	0	24	0	0
3	23-A	48	0	24	0	0
3	24-A	48	0	24	0	0
3	25-A	48	0	24	0	0
3	26-A	48	0	24	0	0
3	27-A	48	0	24	0	0
3	28-A	48	0	24	0	0
3	29-A	48	0	24	0	0
3	30-A	48	0	24	0	0
3	31-A	48	0	24	0	0
3	32-A	48	0	24	0	0
3	33-A	48	0	24	0	0
3	34-A	48	0	24	0	0
3	35-A	48	0	24	0	0
3	36-A	48	0	24	0	0
3	37-A	48	0	24	0	0
3	38-A	48	0	24	0	0
3	39-A	48	0	24	0	0
3	40-A	48	0	24	0	0
3	41-A	48	0	24	0	0
3	42-A	48	0	24	0	0
3	43-A	48	0	24	0	0
3	44-A	48	0	24	0	0
3	45-A	48	0	24	0	0
3	46-A	48	0	24	0	0
3	47-A	48	0	24	0	0
3	48-A	48	0	24	0	0
3	49-A	48	0	24	0	0
3	50-A	48	0	24	0	0
3	51-A	48	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	52-A	48	0	23	0	0
3	53-A	48	0	24	0	0
3	54-A	48	0	24	0	0
3	55-A	48	0	24	0	0
3	56-A	48	0	24	0	0
3	57-A	48	0	24	0	0
3	58-A	48	0	24	0	0
3	59-A	48	0	24	0	0
3	60-A	48	0	24	0	0
3	61-A	48	0	23	0	0
3	62-A	48	0	24	0	0
3	63-A	48	0	24	0	0
3	64-A	48	0	24	0	0
3	65-A	48	0	24	0	0
3	66-A	48	0	23	0	0
3	67-A	48	0	23	0	0
3	68-A	48	0	24	0	0
3	69-A	48	0	24	0	0
3	70-A	48	0	23	0	0
3	71-A	48	0	24	0	0
3	72-A	48	0	24	0	0
3	73-A	48	0	24	0	0
3	74-A	48	0	23	0	0
3	75-A	48	0	24	0	0
3	76-A	48	0	24	0	0
3	77-A	48	0	24	0	0
3	78-A	48	0	24	0	0
3	79-A	48	0	24	0	0
3	80-A	48	0	23	0	0
4	1-A	79	0	0	0	0
4	2-A	68	0	0	0	0
4	3-A	63	0	0	0	0
4	4-A	67	0	0	0	0
4	5-A	67	0	0	0	0
4	6-A	60	0	0	0	0
4	7-A	61	0	0	0	0
4	8-A	61	0	0	0	0
4	9-A	59	0	0	0	0
4	10-A	57	0	0	0	0
4	11-A	72	0	0	0	0
4	12-A	76	0	0	0	0
4	13-A	75	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	14-A	72	0	0	0	0
4	15-A	65	0	0	0	0
4	16-A	64	0	0	0	0
4	17-A	72	0	0	0	0
4	18-A	73	0	0	0	0
4	19-A	76	0	0	0	0
4	20-A	57	0	0	0	0
4	21-A	67	0	0	0	0
4	22-A	69	0	0	0	0
4	23-A	71	0	0	0	0
4	24-A	65	0	0	0	0
4	25-A	61	0	0	0	0
4	26-A	53	0	0	0	0
4	27-A	67	0	0	0	0
4	28-A	74	0	0	0	0
4	29-A	80	0	0	0	0
4	30-A	72	0	0	0	0
4	31-A	76	0	0	0	0
4	32-A	72	0	0	0	0
4	33-A	70	0	0	0	0
4	34-A	62	0	0	0	0
4	35-A	52	0	0	0	0
4	36-A	62	0	0	0	0
4	37-A	66	0	0	0	0
4	38-A	76	0	0	0	0
4	39-A	72	0	0	0	0
4	40-A	75	0	0	0	0
4	41-A	72	0	0	0	0
4	42-A	66	0	0	0	0
4	43-A	65	0	0	0	0
4	44-A	65	0	0	0	0
4	45-A	69	0	0	0	0
4	46-A	62	0	0	0	0
4	47-A	63	0	0	0	0
4	48-A	80	0	0	0	0
4	49-A	74	0	0	0	0
4	50-A	70	0	0	0	0
4	51-A	69	0	0	0	0
4	52-A	68	0	0	0	0
4	53-A	63	0	0	0	0
4	54-A	70	0	0	0	0
4	55-A	75	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	56-A	76	0	0	0	0
4	57-A	72	0	0	0	0
4	58-A	76	0	0	0	0
4	59-A	71	0	0	0	0
4	60-A	75	0	0	0	0
4	61-A	48	0	0	0	0
4	62-A	52	0	0	0	0
4	63-A	72	0	0	0	0
4	64-A	73	0	0	0	0
4	65-A	74	0	0	0	0
4	66-A	62	0	0	0	0
4	67-A	56	0	0	0	0
4	68-A	56	0	0	0	0
4	69-A	64	0	0	0	0
4	70-A	69	0	0	0	0
4	71-A	65	0	0	0	0
4	72-A	71	0	0	0	0
4	73-A	65	0	0	0	0
4	74-A	63	0	0	0	0
4	75-A	64	0	0	0	0
4	76-A	61	0	0	0	0
4	77-A	71	0	0	0	0
4	78-A	71	0	0	0	0
4	79-A	76	0	0	0	0
4	80-A	71	0	0	0	0
All	All	113251	0	100950	0	0

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

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	2-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	3-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	8
1	4-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	5-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	6-A	157/159 (99%)	152 (97%)	4 (2%)	1 (1%)	25	8
1	7-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	12	1
1	8-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	8
1	9-A	157/159 (99%)	149 (95%)	5 (3%)	3 (2%)	8	0
1	10-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	11-A	157/159 (99%)	154 (98%)	2 (1%)	1 (1%)	25	8
1	12-A	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
1	13-A	157/159 (99%)	147 (94%)	9 (6%)	1 (1%)	25	8
1	14-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	1
1	15-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	16-A	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
1	17-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	18-A	157/159 (99%)	146 (93%)	9 (6%)	2 (1%)	12	1
1	19-A	157/159 (99%)	152 (97%)	5 (3%)	0	100	100
1	20-A	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
1	21-A	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
1	22-A	157/159 (99%)	148 (94%)	9 (6%)	0	100	100
1	23-A	157/159 (99%)	149 (95%)	8 (5%)	0	100	100
1	24-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	8
1	25-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	12	1
1	26-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	1
1	27-A	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
1	28-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	8
1	29-A	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	30-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	12	1
1	31-A	157/159 (99%)	149 (95%)	4 (2%)	4 (2%)	5	0
1	32-A	157/159 (99%)	146 (93%)	8 (5%)	3 (2%)	8	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	33-A	157/159 (99%)	145 (92%)	10 (6%)	2 (1%)	12	1
1	34-A	157/159 (99%)	142 (90%)	9 (6%)	6 (4%)	3	0
1	35-A	157/159 (99%)	146 (93%)	6 (4%)	5 (3%)	4	0
1	36-A	157/159 (99%)	145 (92%)	11 (7%)	1 (1%)	25	8
1	37-A	157/159 (99%)	146 (93%)	6 (4%)	5 (3%)	4	0
1	38-A	157/159 (99%)	139 (88%)	11 (7%)	7 (4%)	2	0
1	39-A	157/159 (99%)	146 (93%)	6 (4%)	5 (3%)	4	0
1	40-A	157/159 (99%)	140 (89%)	11 (7%)	6 (4%)	3	0
1	41-A	157/159 (99%)	142 (90%)	4 (2%)	11 (7%)	1	0
1	42-A	157/159 (99%)	142 (90%)	8 (5%)	7 (4%)	2	0
1	43-A	157/159 (99%)	140 (89%)	9 (6%)	8 (5%)	2	0
1	44-A	157/159 (99%)	148 (94%)	3 (2%)	6 (4%)	3	0
1	45-A	157/159 (99%)	148 (94%)	5 (3%)	4 (2%)	5	0
1	46-A	157/159 (99%)	149 (95%)	4 (2%)	4 (2%)	5	0
1	47-A	157/159 (99%)	146 (93%)	4 (2%)	7 (4%)	2	0
1	48-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	8	0
1	49-A	157/159 (99%)	145 (92%)	9 (6%)	3 (2%)	8	0
1	50-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	8	0
1	51-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	8	0
1	52-A	157/159 (99%)	154 (98%)	1 (1%)	2 (1%)	12	1
1	53-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	5	0
1	54-A	157/159 (99%)	147 (94%)	8 (5%)	2 (1%)	12	1
1	55-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	4	0
1	56-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	5	0
1	57-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	8	0
1	58-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	4	0
1	59-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	5	0
1	60-A	157/159 (99%)	145 (92%)	7 (4%)	5 (3%)	4	0
1	61-A	157/159 (99%)	145 (92%)	9 (6%)	3 (2%)	8	0
1	62-A	157/159 (99%)	153 (98%)	2 (1%)	2 (1%)	12	1
1	63-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	12	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	64-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	25	8
1	65-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	1
1	66-A	157/159 (99%)	147 (94%)	8 (5%)	2 (1%)	12	1
1	67-A	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	68-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	1
1	69-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	25	8
1	70-A	157/159 (99%)	150 (96%)	7 (4%)	0	100	100
1	71-A	157/159 (99%)	153 (98%)	4 (2%)	0	100	100
1	72-A	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
1	73-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	8
1	74-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	8
1	75-A	157/159 (99%)	151 (96%)	4 (2%)	2 (1%)	12	1
1	76-A	157/159 (99%)	145 (92%)	11 (7%)	1 (1%)	25	8
1	77-A	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
1	78-A	157/159 (99%)	150 (96%)	6 (4%)	1 (1%)	25	8
1	79-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	25	8
1	80-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	12	1
All	All	12560/12720 (99%)	11875 (94%)	502 (4%)	183 (2%)	10	1

5 of 183 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	9-A	18	ASN
1	9-A	128	TYR
1	18-A	127	ASP
1	26-A	129	GLU
1	32-A	21	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	136/136 (100%)	125 (92%)	11 (8%)	11	2
1	2-A	136/136 (100%)	126 (93%)	10 (7%)	13	2
1	3-A	136/136 (100%)	124 (91%)	12 (9%)	10	1
1	4-A	136/136 (100%)	126 (93%)	10 (7%)	13	2
1	5-A	136/136 (100%)	125 (92%)	11 (8%)	11	2
1	6-A	136/136 (100%)	123 (90%)	13 (10%)	8	1
1	7-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	8-A	136/136 (100%)	126 (93%)	10 (7%)	13	2
1	9-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	10-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	11-A	136/136 (100%)	133 (98%)	3 (2%)	52	27
1	12-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	13-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	14-A	136/136 (100%)	124 (91%)	12 (9%)	10	1
1	15-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	16-A	136/136 (100%)	123 (90%)	13 (10%)	8	1
1	17-A	136/136 (100%)	125 (92%)	11 (8%)	11	2
1	18-A	136/136 (100%)	120 (88%)	16 (12%)	5	1
1	19-A	136/136 (100%)	124 (91%)	12 (9%)	10	1
1	20-A	136/136 (100%)	125 (92%)	11 (8%)	11	2
1	21-A	136/136 (100%)	124 (91%)	12 (9%)	10	1
1	22-A	136/136 (100%)	127 (93%)	9 (7%)	16	3
1	23-A	136/136 (100%)	124 (91%)	12 (9%)	10	1
1	24-A	136/136 (100%)	124 (91%)	12 (9%)	10	1
1	25-A	136/136 (100%)	122 (90%)	14 (10%)	7	1
1	26-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	27-A	136/136 (100%)	117 (86%)	19 (14%)	3	0
1	28-A	136/136 (100%)	122 (90%)	14 (10%)	7	1
1	29-A	136/136 (100%)	123 (90%)	13 (10%)	8	1
1	30-A	136/136 (100%)	128 (94%)	8 (6%)	19	3
1	31-A	136/136 (100%)	125 (92%)	11 (8%)	11	2
1	32-A	136/136 (100%)	119 (88%)	17 (12%)	4	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	33-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	34-A	136/136 (100%)	125 (92%)	11 (8%)	11	2
1	35-A	136/136 (100%)	122 (90%)	14 (10%)	7	1
1	36-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	37-A	136/136 (100%)	120 (88%)	16 (12%)	5	1
1	38-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	39-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	40-A	136/136 (100%)	120 (88%)	16 (12%)	5	1
1	41-A	136/136 (100%)	117 (86%)	19 (14%)	3	0
1	42-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	43-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	44-A	136/136 (100%)	122 (90%)	14 (10%)	7	1
1	45-A	136/136 (100%)	123 (90%)	13 (10%)	8	1
1	46-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	47-A	136/136 (100%)	125 (92%)	11 (8%)	11	2
1	48-A	136/136 (100%)	122 (90%)	14 (10%)	7	1
1	49-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	50-A	136/136 (100%)	117 (86%)	19 (14%)	3	0
1	51-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	52-A	136/136 (100%)	124 (91%)	12 (9%)	10	1
1	53-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	54-A	136/136 (100%)	125 (92%)	11 (8%)	11	2
1	55-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	56-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	57-A	136/136 (100%)	124 (91%)	12 (9%)	10	1
1	58-A	136/136 (100%)	126 (93%)	10 (7%)	13	2
1	59-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	60-A	136/136 (100%)	120 (88%)	16 (12%)	5	1
1	61-A	136/136 (100%)	125 (92%)	11 (8%)	11	2
1	62-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	63-A	136/136 (100%)	122 (90%)	14 (10%)	7	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	64-A	136/136 (100%)	120 (88%)	16 (12%)	5	1
1	65-A	136/136 (100%)	124 (91%)	12 (9%)	10	1
1	66-A	136/136 (100%)	120 (88%)	16 (12%)	5	1
1	67-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	68-A	136/136 (100%)	114 (84%)	22 (16%)	2	0
1	69-A	136/136 (100%)	116 (85%)	20 (15%)	3	0
1	70-A	136/136 (100%)	113 (83%)	23 (17%)	2	0
1	71-A	136/136 (100%)	120 (88%)	16 (12%)	5	1
1	72-A	136/136 (100%)	119 (88%)	17 (12%)	4	0
1	73-A	136/136 (100%)	123 (90%)	13 (10%)	8	1
1	74-A	136/136 (100%)	125 (92%)	11 (8%)	11	2
1	75-A	136/136 (100%)	123 (90%)	13 (10%)	8	1
1	76-A	136/136 (100%)	127 (93%)	9 (7%)	16	3
1	77-A	136/136 (100%)	127 (93%)	9 (7%)	16	3
1	78-A	136/136 (100%)	118 (87%)	18 (13%)	4	0
1	79-A	136/136 (100%)	122 (90%)	14 (10%)	7	1
1	80-A	136/136 (100%)	122 (90%)	14 (10%)	7	1
All	All	10880/10880 (100%)	9748 (90%)	1132 (10%)	7	1

5 of 1132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	67-A	98	ARG
1	68-A	152	CYS
1	67-A	52	ARG
1	73-A	138	SER
1	31-A	79	ASP

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

160 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAP	65-A	202	-	45,52,52	4.05	11 (24%)	56,80,80	1.66	6 (10%)
3	NAP	41-A	202	-	45,52,52	4.11	11 (24%)	56,80,80	1.55	6 (10%)
3	NAP	47-A	202	-	45,52,52	4.07	11 (24%)	56,80,80	1.61	5 (8%)
3	NAP	29-A	202	-	45,52,52	4.10	11 (24%)	56,80,80	1.56	6 (10%)
2	FOL	69-A	201	-	28,34,34	1.49	5 (17%)	36,47,47	2.92	18 (50%)
2	FOL	12-A	201	-	28,34,34	1.21	2 (7%)	36,47,47	2.15	9 (25%)
2	FOL	73-A	201	-	28,34,34	1.51	5 (17%)	36,47,47	3.56	19 (52%)
2	FOL	28-A	201	-	28,34,34	1.22	2 (7%)	36,47,47	2.02	7 (19%)
2	FOL	67-A	201	-	28,34,34	1.32	4 (14%)	36,47,47	2.88	16 (44%)
3	NAP	2-A	202	-	45,52,52	4.09	11 (24%)	56,80,80	1.62	6 (10%)
2	FOL	56-A	201	-	28,34,34	1.25	2 (7%)	36,47,47	2.38	12 (33%)
2	FOL	11-A	201	-	28,34,34	1.25	2 (7%)	36,47,47	2.15	8 (22%)
2	FOL	6-A	201	-	28,34,34	1.22	2 (7%)	36,47,47	2.16	9 (25%)
3	NAP	28-A	202	-	45,52,52	4.09	11 (24%)	56,80,80	1.68	5 (8%)
2	FOL	79-A	201	-	28,34,34	1.33	3 (10%)	36,47,47	2.30	9 (25%)
3	NAP	46-A	202	-	45,52,52	4.11	11 (24%)	56,80,80	1.55	5 (8%)
2	FOL	9-A	201	-	28,34,34	1.25	2 (7%)	36,47,47	2.28	10 (27%)
2	FOL	63-A	201	-	28,34,34	1.37	2 (7%)	36,47,47	2.88	14 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	68-A	202	-	45,52,52	4.08	11 (24%)	56,80,80	1.55	6 (10%)
3	NAP	78-A	202	-	45,52,52	4.12	11 (24%)	56,80,80	1.58	5 (8%)
3	NAP	73-A	202	-	45,52,52	4.10	11 (24%)	56,80,80	1.57	6 (10%)
3	NAP	61-A	202	-	45,52,52	4.09	11 (24%)	56,80,80	1.54	7 (12%)
3	NAP	71-A	202	-	45,52,52	4.07	11 (24%)	56,80,80	1.66	6 (10%)
2	FOL	71-A	201	-	28,34,34	1.19	3 (10%)	36,47,47	2.83	16 (44%)
2	FOL	77-A	201	-	28,34,34	1.32	3 (10%)	36,47,47	2.54	9 (25%)
2	FOL	46-A	201	-	28,34,34	1.12	2 (7%)	36,47,47	2.34	11 (30%)
3	NAP	11-A	202	-	45,52,52	4.06	11 (24%)	56,80,80	1.57	6 (10%)
3	NAP	10-A	202	-	45,52,52	4.05	11 (24%)	56,80,80	1.66	6 (10%)
3	NAP	52-A	202	-	45,52,52	4.10	11 (24%)	56,80,80	1.59	6 (10%)
3	NAP	5-A	202	-	45,52,52	4.09	11 (24%)	56,80,80	1.58	6 (10%)
3	NAP	66-A	202	-	45,52,52	4.05	11 (24%)	56,80,80	1.66	7 (12%)
3	NAP	24-A	202	-	45,52,52	4.10	11 (24%)	56,80,80	1.53	7 (12%)
2	FOL	58-A	201	-	28,34,34	1.23	2 (7%)	36,47,47	2.48	13 (36%)
2	FOL	36-A	201	-	28,34,34	1.19	2 (7%)	36,47,47	2.07	7 (19%)
3	NAP	70-A	202	-	45,52,52	4.09	11 (24%)	56,80,80	1.60	6 (10%)
2	FOL	57-A	201	-	28,34,34	1.24	2 (7%)	36,47,47	2.51	13 (36%)
3	NAP	35-A	202	-	45,52,52	4.15	11 (24%)	56,80,80	1.58	6 (10%)
2	FOL	13-A	201	-	28,34,34	1.25	2 (7%)	36,47,47	2.10	7 (19%)
3	NAP	43-A	202	-	45,52,52	4.06	11 (24%)	56,80,80	1.60	6 (10%)
2	FOL	14-A	201	-	28,34,34	1.25	2 (7%)	36,47,47	2.35	10 (27%)
2	FOL	44-A	201	-	28,34,34	1.16	2 (7%)	36,47,47	2.14	7 (19%)
3	NAP	26-A	202	-	45,52,52	4.09	11 (24%)	56,80,80	1.51	6 (10%)
3	NAP	44-A	202	-	45,52,52	4.07	11 (24%)	56,80,80	1.64	7 (12%)
2	FOL	65-A	201	-	28,34,34	1.38	2 (7%)	36,47,47	2.53	13 (36%)
3	NAP	19-A	202	-	45,52,52	4.09	11 (24%)	56,80,80	1.63	6 (10%)
2	FOL	16-A	201	-	28,34,34	1.18	2 (7%)	36,47,47	2.15	9 (25%)
3	NAP	7-A	202	-	45,52,52	4.14	11 (24%)	56,80,80	1.65	6 (10%)
2	FOL	5-A	201	-	28,34,34	1.27	2 (7%)	36,47,47	2.23	8 (22%)
3	NAP	39-A	202	-	45,52,52	4.16	11 (24%)	56,80,80	1.58	6 (10%)
2	FOL	40-A	201	-	28,34,34	1.26	2 (7%)	36,47,47	2.64	14 (38%)
3	NAP	49-A	202	-	45,52,52	4.09	11 (24%)	56,80,80	1.64	7 (12%)
2	FOL	41-A	201	-	28,34,34	1.20	2 (7%)	36,47,47	2.24	9 (25%)
2	FOL	50-A	201	-	28,34,34	1.22	2 (7%)	36,47,47	2.12	8 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FOL	7-A	201	-	28,34,34	1.20	2 (7%)	36,47,47	2.17	9 (25%)
3	NAP	53-A	202	-	45,52,52	4.07	11 (24%)	56,80,80	1.62	6 (10%)
2	FOL	37-A	201	-	28,34,34	1.19	3 (10%)	36,47,47	2.21	10 (27%)
3	NAP	20-A	202	-	45,52,52	4.10	11 (24%)	56,80,80	1.52	5 (8%)
2	FOL	18-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.24	8 (22%)
3	NAP	4-A	202	-	45,52,52	4.08	11 (24%)	56,80,80	1.60	7 (12%)
2	FOL	32-A	201	-	28,34,34	1.16	2 (7%)	36,47,47	2.11	8 (22%)
3	NAP	16-A	202	-	45,52,52	4.09	11 (24%)	56,80,80	1.59	5 (8%)
2	FOL	30-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.20	9 (25%)
2	FOL	25-A	201	-	28,34,34	1.18	2 (7%)	36,47,47	2.51	11 (30%)
3	NAP	55-A	202	-	45,52,52	4.08	11 (24%)	56,80,80	1.69	5 (8%)
2	FOL	21-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.10	6 (16%)
3	NAP	13-A	202	-	45,52,52	4.10	11 (24%)	56,80,80	1.59	4 (7%)
3	NAP	37-A	202	-	45,52,52	4.14	11 (24%)	56,80,80	1.63	5 (8%)
2	FOL	20-A	201	-	28,34,34	1.16	2 (7%)	36,47,47	2.24	11 (30%)
2	FOL	8-A	201	-	28,34,34	1.16	2 (7%)	36,47,47	2.27	12 (33%)
2	FOL	4-A	201	-	28,34,34	1.20	2 (7%)	36,47,47	2.25	10 (27%)
2	FOL	51-A	201	-	28,34,34	1.19	2 (7%)	36,47,47	2.16	8 (22%)
2	FOL	42-A	201	-	28,34,34	1.20	2 (7%)	36,47,47	2.19	8 (22%)
3	NAP	22-A	202	-	45,52,52	4.10	11 (24%)	56,80,80	1.60	7 (12%)
2	FOL	22-A	201	-	28,34,34	1.20	2 (7%)	36,47,47	2.26	9 (25%)
2	FOL	55-A	201	-	28,34,34	1.21	2 (7%)	36,47,47	2.45	12 (33%)
3	NAP	25-A	202	-	45,52,52	4.10	11 (24%)	56,80,80	1.59	7 (12%)
2	FOL	26-A	201	-	28,34,34	1.24	3 (10%)	36,47,47	2.26	11 (30%)
3	NAP	57-A	202	-	45,52,52	4.07	11 (24%)	56,80,80	1.62	6 (10%)
2	FOL	66-A	201	-	28,34,34	1.44	3 (10%)	36,47,47	2.48	11 (30%)
3	NAP	77-A	202	-	45,52,52	4.11	11 (24%)	56,80,80	1.50	5 (8%)
2	FOL	10-A	201	-	28,34,34	1.21	2 (7%)	36,47,47	2.30	12 (33%)
2	FOL	33-A	201	-	28,34,34	1.23	3 (10%)	36,47,47	2.24	10 (27%)
2	FOL	54-A	201	-	28,34,34	1.16	2 (7%)	36,47,47	2.39	13 (36%)
3	NAP	14-A	202	-	45,52,52	4.14	11 (24%)	56,80,80	1.50	5 (8%)
3	NAP	51-A	202	-	45,52,52	4.07	11 (24%)	56,80,80	1.51	5 (8%)
3	NAP	32-A	202	-	45,52,52	4.12	11 (24%)	56,80,80	1.49	4 (7%)
2	FOL	27-A	201	-	28,34,34	1.21	2 (7%)	36,47,47	2.10	8 (22%)
2	FOL	2-A	201	-	28,34,34	1.21	2 (7%)	36,47,47	2.17	9 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	54-A	202	-	45,52,52	4.18	11 (24%)	56,80,80	1.61	6 (10%)
3	NAP	1-A	202	-	45,52,52	4.11	11 (24%)	56,80,80	1.61	6 (10%)
3	NAP	38-A	202	-	45,52,52	4.11	11 (24%)	56,80,80	1.57	5 (8%)
3	NAP	80-A	202	-	45,52,52	3.99	11 (24%)	56,80,80	1.75	7 (12%)
2	FOL	34-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.17	8 (22%)
3	NAP	79-A	202	-	45,52,52	4.08	11 (24%)	56,80,80	1.52	4 (7%)
3	NAP	33-A	202	-	45,52,52	4.08	11 (24%)	56,80,80	1.51	6 (10%)
3	NAP	58-A	202	-	45,52,52	4.06	11 (24%)	56,80,80	1.56	5 (8%)
3	NAP	72-A	202	-	45,52,52	4.12	11 (24%)	56,80,80	1.58	5 (8%)
3	NAP	36-A	202	-	45,52,52	4.11	11 (24%)	56,80,80	1.59	6 (10%)
3	NAP	12-A	202	-	45,52,52	4.07	11 (24%)	56,80,80	1.60	6 (10%)
3	NAP	3-A	202	-	45,52,52	4.11	11 (24%)	56,80,80	1.55	6 (10%)
2	FOL	70-A	201	-	28,34,34	1.46	5 (17%)	36,47,47	2.62	14 (38%)
2	FOL	47-A	201	-	28,34,34	1.18	2 (7%)	36,47,47	2.30	9 (25%)
2	FOL	64-A	201	-	28,34,34	1.39	3 (10%)	36,47,47	2.93	16 (44%)
2	FOL	31-A	201	-	28,34,34	1.30	2 (7%)	36,47,47	2.22	7 (19%)
3	NAP	9-A	202	-	45,52,52	4.09	11 (24%)	56,80,80	1.60	5 (8%)
3	NAP	17-A	202	-	45,52,52	4.07	11 (24%)	56,80,80	1.56	5 (8%)
3	NAP	64-A	202	-	45,52,52	4.08	11 (24%)	56,80,80	1.60	6 (10%)
2	FOL	19-A	201	-	28,34,34	1.18	2 (7%)	36,47,47	2.29	10 (27%)
2	FOL	23-A	201	-	28,34,34	1.09	2 (7%)	36,47,47	2.27	6 (16%)
3	NAP	8-A	202	-	45,52,52	4.08	12 (26%)	56,80,80	1.51	4 (7%)
3	NAP	31-A	202	-	45,52,52	4.11	11 (24%)	56,80,80	1.48	4 (7%)
2	FOL	38-A	201	-	28,34,34	1.23	3 (10%)	36,47,47	2.22	10 (27%)
3	NAP	40-A	202	-	45,52,52	4.12	11 (24%)	56,80,80	1.64	6 (10%)
2	FOL	35-A	201	-	28,34,34	1.19	2 (7%)	36,47,47	2.17	10 (27%)
2	FOL	80-A	201	-	28,34,34	1.27	2 (7%)	36,47,47	2.38	10 (27%)
3	NAP	6-A	202	-	45,52,52	4.12	11 (24%)	56,80,80	1.55	6 (10%)
2	FOL	49-A	201	-	28,34,34	1.15	2 (7%)	36,47,47	2.33	10 (27%)
3	NAP	62-A	202	-	45,52,52	4.09	11 (24%)	56,80,80	1.58	6 (10%)
2	FOL	43-A	201	-	28,34,34	1.21	2 (7%)	36,47,47	2.19	8 (22%)
2	FOL	17-A	201	-	28,34,34	1.20	3 (10%)	36,47,47	2.21	9 (25%)
2	FOL	52-A	201	-	28,34,34	1.19	2 (7%)	36,47,47	2.42	11 (30%)
2	FOL	39-A	201	-	28,34,34	1.27	3 (10%)	36,47,47	2.36	11 (30%)
3	NAP	21-A	202	-	45,52,52	4.09	11 (24%)	56,80,80	1.53	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	48-A	202	-	45,52,52	4.04	11 (24%)	56,80,80	1.65	6 (10%)
3	NAP	27-A	202	-	45,52,52	4.10	11 (24%)	56,80,80	1.47	6 (10%)
3	NAP	42-A	202	-	45,52,52	4.08	11 (24%)	56,80,80	1.66	7 (12%)
2	FOL	45-A	201	-	28,34,34	1.20	2 (7%)	36,47,47	2.26	9 (25%)
3	NAP	56-A	202	-	45,52,52	4.06	11 (24%)	56,80,80	1.55	5 (8%)
3	NAP	75-A	202	-	45,52,52	4.12	11 (24%)	56,80,80	1.63	6 (10%)
2	FOL	61-A	201	-	28,34,34	1.21	2 (7%)	36,47,47	2.38	11 (30%)
3	NAP	69-A	202	-	45,52,52	4.07	11 (24%)	56,80,80	1.61	6 (10%)
3	NAP	34-A	202	-	45,52,52	4.11	11 (24%)	56,80,80	1.66	6 (10%)
2	FOL	53-A	201	-	28,34,34	1.15	2 (7%)	36,47,47	2.30	10 (27%)
2	FOL	59-A	201	-	28,34,34	1.26	2 (7%)	36,47,47	2.19	11 (30%)
2	FOL	68-A	201	-	28,34,34	1.15	2 (7%)	36,47,47	2.47	14 (38%)
2	FOL	15-A	201	-	28,34,34	1.24	2 (7%)	36,47,47	2.23	9 (25%)
3	NAP	30-A	202	-	45,52,52	4.10	11 (24%)	56,80,80	1.56	5 (8%)
3	NAP	76-A	202	-	45,52,52	4.14	11 (24%)	56,80,80	1.54	6 (10%)
2	FOL	24-A	201	-	28,34,34	1.16	2 (7%)	36,47,47	2.17	8 (22%)
2	FOL	78-A	201	-	28,34,34	1.63	4 (14%)	36,47,47	2.36	9 (25%)
3	NAP	59-A	202	-	45,52,52	4.10	11 (24%)	56,80,80	1.51	5 (8%)
3	NAP	23-A	202	-	45,52,52	4.09	11 (24%)	56,80,80	1.63	5 (8%)
2	FOL	3-A	201	-	28,34,34	1.22	2 (7%)	36,47,47	2.24	8 (22%)
2	FOL	48-A	201	-	28,34,34	1.15	2 (7%)	36,47,47	2.41	14 (38%)
2	FOL	62-A	201	-	28,34,34	1.17	2 (7%)	36,47,47	2.18	9 (25%)
3	NAP	45-A	202	-	45,52,52	4.09	11 (24%)	56,80,80	1.59	7 (12%)
2	FOL	74-A	201	-	28,34,34	1.32	2 (7%)	36,47,47	2.60	11 (30%)
3	NAP	50-A	202	-	45,52,52	4.06	11 (24%)	56,80,80	1.62	7 (12%)
3	NAP	18-A	202	-	45,52,52	4.00	11 (24%)	56,80,80	1.59	5 (8%)
2	FOL	75-A	201	-	28,34,34	1.26	2 (7%)	36,47,47	2.22	8 (22%)
3	NAP	60-A	202	-	45,52,52	4.08	11 (24%)	56,80,80	1.63	4 (7%)
3	NAP	67-A	202	-	45,52,52	4.01	11 (24%)	56,80,80	1.59	6 (10%)
2	FOL	60-A	201	-	28,34,34	1.33	3 (10%)	36,47,47	2.38	11 (30%)
3	NAP	63-A	202	-	45,52,52	4.06	11 (24%)	56,80,80	1.60	6 (10%)
2	FOL	1-A	201	-	28,34,34	1.24	2 (7%)	36,47,47	2.22	9 (25%)
2	FOL	29-A	201	-	28,34,34	1.21	3 (10%)	36,47,47	2.31	11 (30%)
3	NAP	74-A	202	-	45,52,52	4.09	12 (26%)	56,80,80	1.73	6 (10%)
2	FOL	76-A	201	-	28,34,34	1.36	3 (10%)	36,47,47	2.40	13 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	15-A	202	-	45,52,52	4.11	11 (24%)	56,80,80	1.59	5 (8%)
2	FOL	72-A	201	-	28,34,34	1.57	5 (17%)	36,47,47	3.80	19 (52%)

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
3	NAP	65-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	41-A	202	-	-	2/31/67/67	0/5/5/5
3	NAP	47-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	69-A	201	-	-	8/16/22/22	0/3/3/3
2	FOL	12-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	73-A	201	-	-	6/16/22/22	0/3/3/3
2	FOL	28-A	201	-	-	0/16/22/22	0/3/3/3
2	FOL	67-A	201	-	-	8/16/22/22	0/3/3/3
3	NAP	2-A	202	-	-	2/31/67/67	0/5/5/5
2	FOL	56-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	11-A	201	-	-	4/16/22/22	0/3/3/3
2	FOL	6-A	201	-	-	0/16/22/22	0/3/3/3
3	NAP	28-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	79-A	201	-	-	4/16/22/22	0/3/3/3
3	NAP	46-A	202	-	-	5/31/67/67	0/5/5/5
2	FOL	9-A	201	-	-	6/16/22/22	0/3/3/3
2	FOL	63-A	201	-	-	3/16/22/22	0/3/3/3
3	NAP	68-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	78-A	202	-	-	2/31/67/67	0/5/5/5
3	NAP	73-A	202	-	-	5/31/67/67	0/5/5/5
3	NAP	61-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	71-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	71-A	201	-	-	11/16/22/22	0/3/3/3
2	FOL	77-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	46-A	201	-	-	3/16/22/22	0/3/3/3
3	NAP	11-A	202	-	-	1/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	10-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	52-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	5-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	66-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	24-A	202	-	-	2/31/67/67	0/5/5/5
2	FOL	58-A	201	-	-	6/16/22/22	0/3/3/3
2	FOL	36-A	201	-	-	1/16/22/22	0/3/3/3
3	NAP	70-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	57-A	201	-	-	6/16/22/22	0/3/3/3
3	NAP	35-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	13-A	201	-	-	0/16/22/22	0/3/3/3
3	NAP	43-A	202	-	-	2/31/67/67	0/5/5/5
2	FOL	14-A	201	-	-	0/16/22/22	0/3/3/3
2	FOL	44-A	201	-	-	0/16/22/22	0/3/3/3
3	NAP	26-A	202	-	-	5/31/67/67	0/5/5/5
3	NAP	44-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	65-A	201	-	-	1/16/22/22	0/3/3/3
3	NAP	19-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	16-A	201	-	-	1/16/22/22	0/3/3/3
3	NAP	7-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	5-A	201	-	-	3/16/22/22	0/3/3/3
3	NAP	39-A	202	-	-	2/31/67/67	0/5/5/5
2	FOL	40-A	201	-	-	3/16/22/22	0/3/3/3
3	NAP	49-A	202	-	-	2/31/67/67	0/5/5/5
2	FOL	41-A	201	-	-	1/16/22/22	0/3/3/3
2	FOL	50-A	201	-	-	1/16/22/22	0/3/3/3
2	FOL	7-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	53-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	37-A	201	-	-	1/16/22/22	0/3/3/3
3	NAP	20-A	202	-	-	5/31/67/67	0/5/5/5
2	FOL	18-A	201	-	-	3/16/22/22	0/3/3/3
3	NAP	4-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	32-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	16-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	30-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	25-A	201	-	-	5/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	55-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	21-A	201	-	-	1/16/22/22	0/3/3/3
3	NAP	13-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	37-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	20-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	8-A	201	-	-	4/16/22/22	0/3/3/3
2	FOL	4-A	201	-	-	0/16/22/22	0/3/3/3
2	FOL	51-A	201	-	-	0/16/22/22	0/3/3/3
2	FOL	42-A	201	-	-	3/16/22/22	0/3/3/3
3	NAP	22-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	22-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	55-A	201	-	-	6/16/22/22	0/3/3/3
3	NAP	25-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	26-A	201	-	-	4/16/22/22	0/3/3/3
3	NAP	57-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	66-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	77-A	202	-	-	1/31/67/67	0/5/5/5
2	FOL	10-A	201	-	-	4/16/22/22	0/3/3/3
2	FOL	33-A	201	-	-	4/16/22/22	0/3/3/3
2	FOL	54-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	14-A	202	-	-	2/31/67/67	0/5/5/5
3	NAP	51-A	202	-	-	2/31/67/67	0/5/5/5
3	NAP	32-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	27-A	201	-	-	0/16/22/22	0/3/3/3
2	FOL	2-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	54-A	202	-	-	10/31/67/67	0/5/5/5
3	NAP	1-A	202	-	-	2/31/67/67	0/5/5/5
3	NAP	38-A	202	-	-	1/31/67/67	0/5/5/5
3	NAP	80-A	202	-	-	6/31/67/67	0/5/5/5
2	FOL	34-A	201	-	-	0/16/22/22	0/3/3/3
3	NAP	79-A	202	-	-	2/31/67/67	0/5/5/5
3	NAP	33-A	202	-	-	2/31/67/67	0/5/5/5
3	NAP	58-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	72-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	36-A	202	-	-	3/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	12-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	3-A	202	-	-	2/31/67/67	0/5/5/5
2	FOL	70-A	201	-	-	6/16/22/22	0/3/3/3
2	FOL	47-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	64-A	201	-	-	10/16/22/22	0/3/3/3
2	FOL	31-A	201	-	-	4/16/22/22	0/3/3/3
3	NAP	9-A	202	-	-	1/31/67/67	0/5/5/5
3	NAP	17-A	202	-	-	1/31/67/67	0/5/5/5
3	NAP	64-A	202	-	-	2/31/67/67	0/5/5/5
2	FOL	19-A	201	-	-	1/16/22/22	0/3/3/3
2	FOL	23-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	8-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	31-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	38-A	201	-	-	6/16/22/22	0/3/3/3
3	NAP	40-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	35-A	201	-	-	5/16/22/22	0/3/3/3
2	FOL	80-A	201	-	-	9/16/22/22	0/3/3/3
3	NAP	6-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	49-A	201	-	-	3/16/22/22	0/3/3/3
3	NAP	62-A	202	-	-	2/31/67/67	0/5/5/5
2	FOL	43-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	17-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	52-A	201	-	-	2/16/22/22	0/3/3/3
2	FOL	39-A	201	-	-	4/16/22/22	0/3/3/3
3	NAP	21-A	202	-	-	2/31/67/67	0/5/5/5
3	NAP	48-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	27-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	42-A	202	-	-	1/31/67/67	0/5/5/5
2	FOL	45-A	201	-	-	1/16/22/22	0/3/3/3
3	NAP	56-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	75-A	202	-	-	5/31/67/67	0/5/5/5
2	FOL	61-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	69-A	202	-	-	2/31/67/67	0/5/5/5
3	NAP	34-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	53-A	201	-	-	3/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	59-A	201	-	-	3/16/22/22	0/3/3/3
2	FOL	68-A	201	-	-	7/16/22/22	0/3/3/3
2	FOL	15-A	201	-	-	4/16/22/22	0/3/3/3
3	NAP	30-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	76-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	24-A	201	-	-	4/16/22/22	0/3/3/3
2	FOL	78-A	201	-	-	4/16/22/22	0/3/3/3
3	NAP	59-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	23-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	3-A	201	-	-	4/16/22/22	0/3/3/3
2	FOL	48-A	201	-	-	4/16/22/22	0/3/3/3
2	FOL	62-A	201	-	-	6/16/22/22	0/3/3/3
3	NAP	45-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	74-A	201	-	-	7/16/22/22	0/3/3/3
3	NAP	50-A	202	-	-	3/31/67/67	0/5/5/5
3	NAP	18-A	202	-	-	4/31/67/67	0/5/5/5
2	FOL	75-A	201	-	-	5/16/22/22	0/3/3/3
3	NAP	60-A	202	-	-	4/31/67/67	0/5/5/5
3	NAP	67-A	202	-	-	2/31/67/67	0/5/5/5
2	FOL	60-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	63-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	1-A	201	-	-	0/16/22/22	0/3/3/3
2	FOL	29-A	201	-	-	2/16/22/22	0/3/3/3
3	NAP	74-A	202	-	-	3/31/67/67	0/5/5/5
2	FOL	76-A	201	-	-	6/16/22/22	0/3/3/3
3	NAP	15-A	202	-	-	6/31/67/67	0/5/5/5
2	FOL	72-A	201	-	-	9/16/22/22	0/3/3/3

The worst 5 of 1072 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	55-A	202	NAP	C2D-C1D	-15.25	1.30	1.53
3	54-A	202	NAP	C2D-C1D	-15.22	1.30	1.53
3	14-A	202	NAP	C2D-C1D	-15.09	1.30	1.53
3	79-A	202	NAP	C2D-C1D	-15.09	1.30	1.53
3	19-A	202	NAP	C2D-C1D	-15.03	1.31	1.53

The worst 5 of 1290 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	72-A	201	FOL	CA-N-C	13.66	139.95	122.34
2	73-A	201	FOL	N8-C8A-N1	10.18	127.44	115.82
2	67-A	201	FOL	N8-C8A-N1	9.63	126.81	115.82
2	64-A	201	FOL	N8-C8A-N1	9.06	126.16	115.82
2	63-A	201	FOL	CA-N-C	8.69	133.55	122.34

There are no chirality outliers.

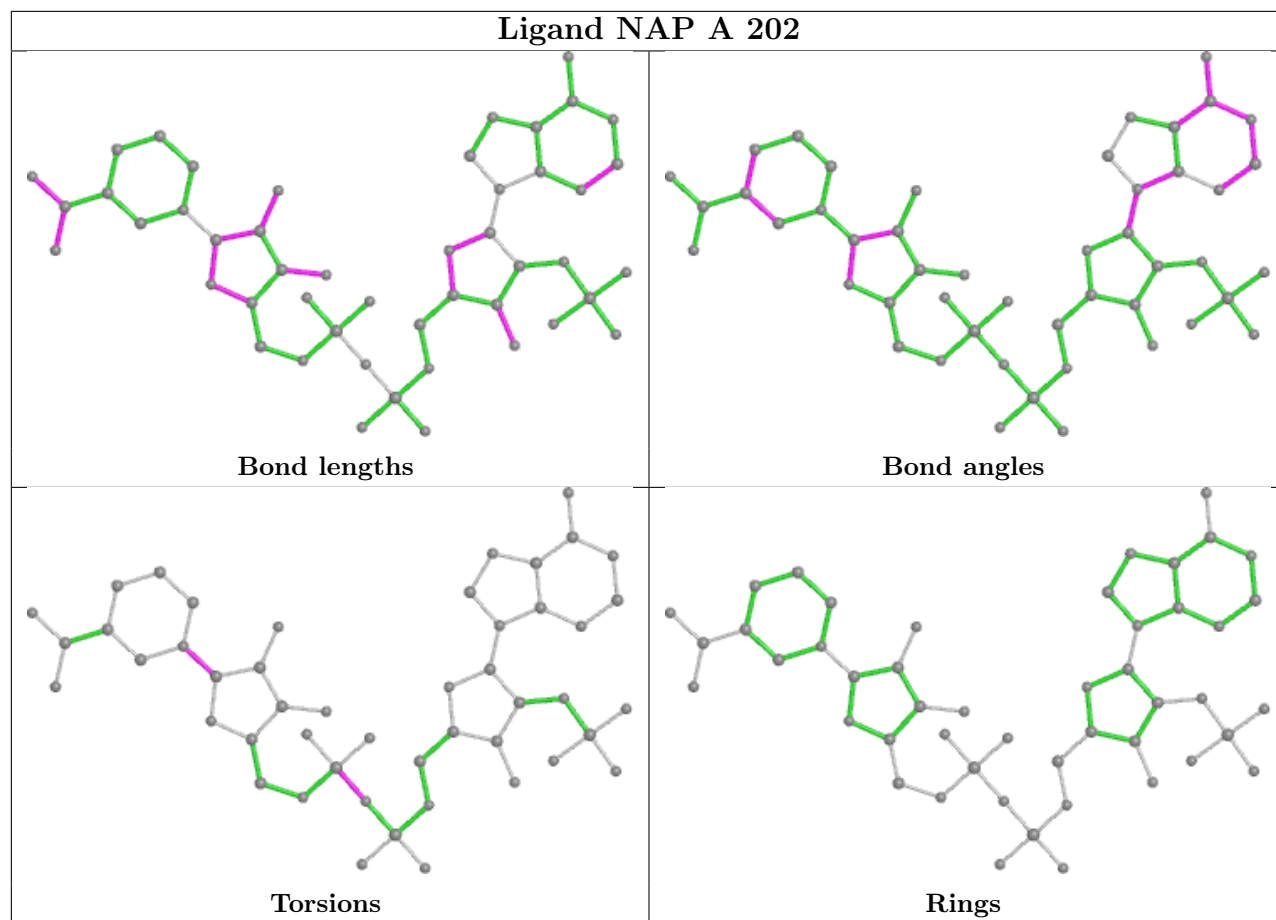
5 of 532 torsion outliers are listed below:

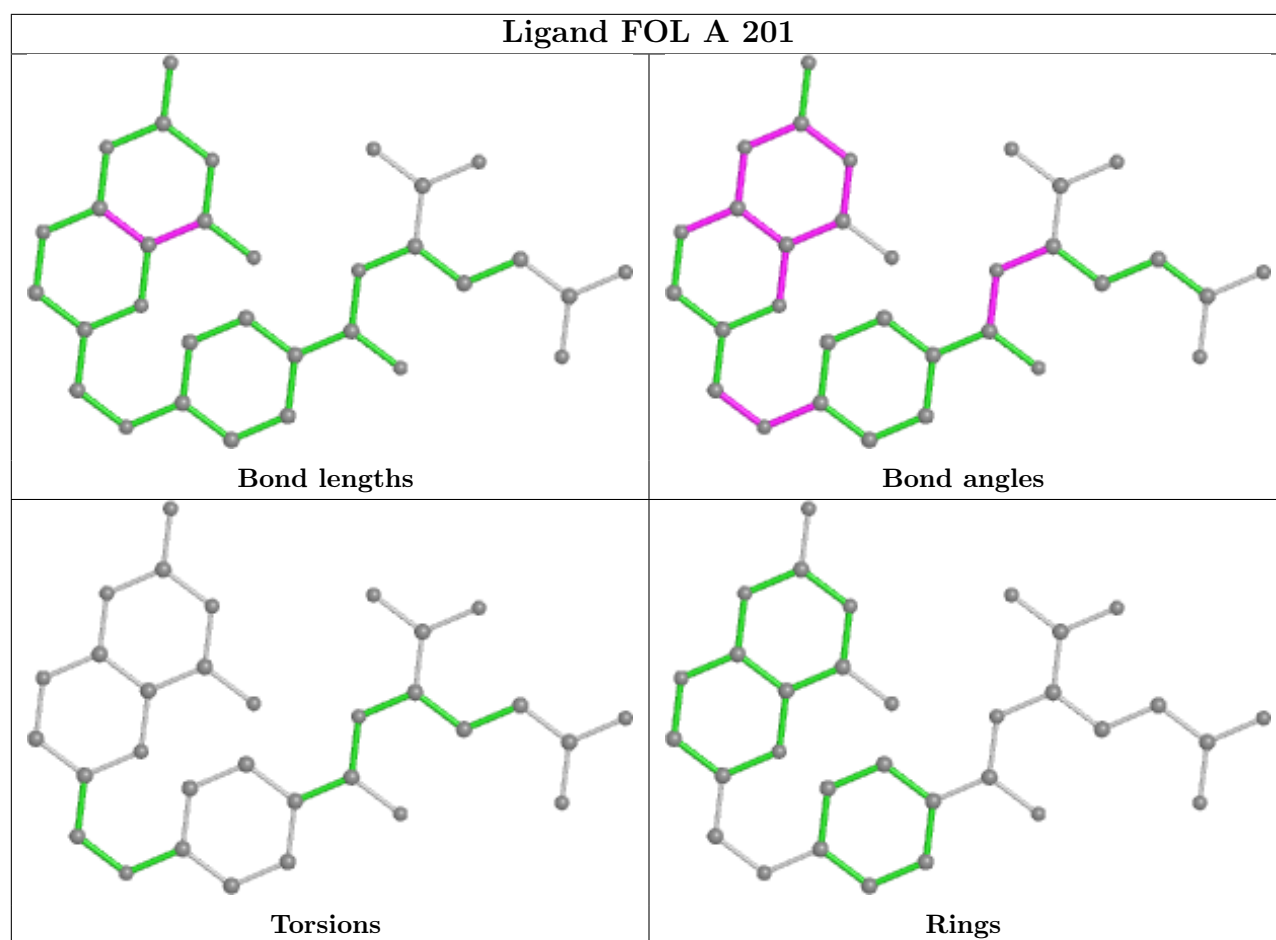
Mol	Chain	Res	Type	Atoms
2	2-A	201	FOL	N-CA-CB-CG
2	2-A	201	FOL	CT-CA-CB-CG
2	5-A	201	FOL	CT-CA-CB-CG
2	7-A	201	FOL	CB-CA-N-C
2	7-A	201	FOL	CT-CA-N-C

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(Å²)	Q<0.9
1	1-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	2-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	3-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	4-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	5-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	6-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	7-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	8-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	9-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	10-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	11-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	12-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	13-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	14-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	15-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	16-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	17-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	18-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	19-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	20-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	21-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	22-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	23-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	24-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	25-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	26-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	27-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	28-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	29-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	30-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	31-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	32-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	33-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	34-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	35-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	36-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	37-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	38-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	39-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	40-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	41-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	42-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	43-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	44-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	45-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	46-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	47-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	48-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	49-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	50-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	51-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	52-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	53-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	54-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	55-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	56-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	57-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	58-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	59-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	60-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	61-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	62-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	63-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	64-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	65-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	66-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	67-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	68-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	69-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	70-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	71-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	72-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	73-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	74-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	75-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	76-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	77-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	78-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	79-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
1	80-A	159/159 (100%)	0.62	14 (8%)	10	9	8, 13, 18, 22	159 (100%)
All	All	12720/12720 (100%)	0.62	1120 (8%)	8	9	8, 13, 18, 22	12720 (100%)

The worst 5 of 1120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	127	ASP	4.7
1	2-A	127	ASP	4.7
1	3-A	127	ASP	4.7

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Mol	Chain	Res	Type	RSRZ
1	4-A	127	ASP	4.7
1	5-A	127	ASP	4.7

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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
3	NAP	1-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	2-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	3-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	4-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	5-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	6-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	7-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	8-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	9-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	10-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	11-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	12-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	13-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	14-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	15-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	16-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	17-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	18-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	19-A	202	48/48	0.95	0.12	9,12,16,18	48
3	NAP	20-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	21-A	202	48/48	0.95	0.12	9,12,16,17	48

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAP	22-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	23-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	24-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	25-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	26-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	27-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	28-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	29-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	30-A	202	48/48	0.95	0.12	9,12,16,18	48
3	NAP	31-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	32-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	33-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	34-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	35-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	36-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	37-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	38-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	39-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	40-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	41-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	42-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	43-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	44-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	45-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	46-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	47-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	48-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	49-A	202	48/48	0.95	0.12	9,12,17,17	48
3	NAP	50-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	51-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	52-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	53-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	54-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	55-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	56-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	57-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	58-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	59-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	60-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	61-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	62-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	63-A	202	48/48	0.95	0.12	9,12,16,17	48

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAP	64-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	65-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	66-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	67-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	68-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	69-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	70-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	71-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	72-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	73-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	74-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	75-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	76-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	77-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	78-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	79-A	202	48/48	0.95	0.12	9,12,16,17	48
3	NAP	80-A	202	48/48	0.95	0.12	9,12,16,17	48
2	FOL	1-A	201	32/32	0.97	0.09	9,11,17,19	32
2	FOL	2-A	201	32/32	0.97	0.09	9,11,17,19	32
2	FOL	3-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	4-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	5-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	6-A	201	32/32	0.97	0.09	9,11,17,19	32
2	FOL	7-A	201	32/32	0.97	0.09	9,11,17,18	32
2	FOL	8-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	9-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	10-A	201	32/32	0.97	0.09	9,11,17,18	32
2	FOL	11-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	12-A	201	32/32	0.97	0.09	9,11,17,18	32
2	FOL	13-A	201	32/32	0.97	0.09	9,11,17,18	32
2	FOL	14-A	201	32/32	0.97	0.09	9,11,17,19	32
2	FOL	15-A	201	32/32	0.97	0.09	9,11,17,19	32
2	FOL	16-A	201	32/32	0.97	0.09	9,11,16,18	32
2	FOL	17-A	201	32/32	0.97	0.09	9,11,17,18	32
2	FOL	18-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	19-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	20-A	201	32/32	0.97	0.09	9,11,17,18	32
2	FOL	21-A	201	32/32	0.97	0.09	9,11,16,18	32
2	FOL	22-A	201	32/32	0.97	0.09	9,11,17,19	32
2	FOL	23-A	201	32/32	0.97	0.09	9,11,17,19	32
2	FOL	24-A	201	32/32	0.97	0.09	9,11,16,18	32
2	FOL	25-A	201	32/32	0.97	0.09	9,11,16,16	32

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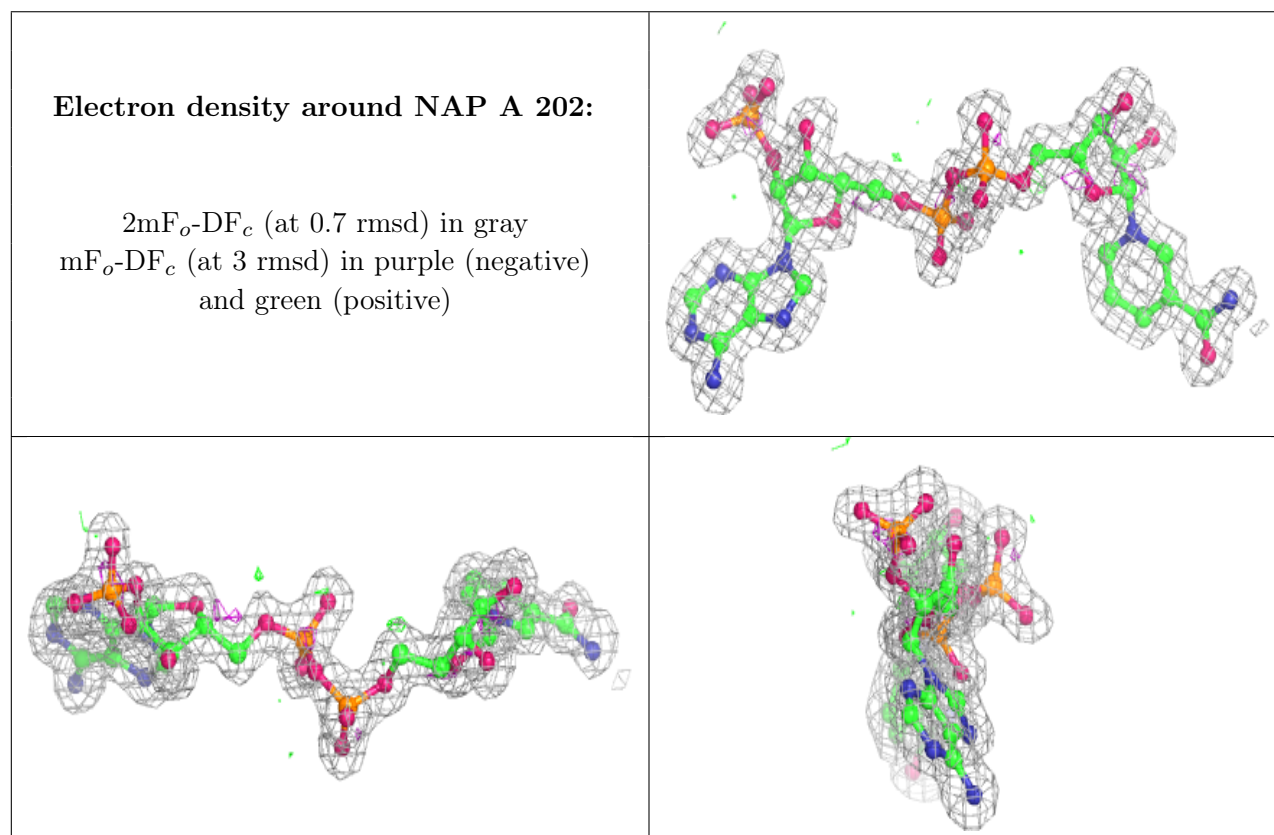
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FOL	26-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	27-A	201	32/32	0.97	0.09	9,11,17,18	32
2	FOL	28-A	201	32/32	0.97	0.09	9,11,17,18	32
2	FOL	29-A	201	32/32	0.97	0.09	9,11,17,17	32
2	FOL	30-A	201	32/32	0.97	0.09	9,11,17,18	32
2	FOL	31-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	32-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	33-A	201	32/32	0.97	0.09	9,11,16,16	32
2	FOL	34-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	35-A	201	32/32	0.97	0.09	9,11,17,18	32
2	FOL	36-A	201	32/32	0.97	0.09	9,11,17,19	32
2	FOL	37-A	201	32/32	0.97	0.09	9,11,17,19	32
2	FOL	38-A	201	32/32	0.97	0.09	9,11,18,19	32
2	FOL	39-A	201	32/32	0.97	0.09	9,11,18,19	32
2	FOL	40-A	201	32/32	0.97	0.09	9,11,19,20	32
2	FOL	41-A	201	32/32	0.97	0.09	9,11,17,18	32
2	FOL	42-A	201	32/32	0.97	0.09	9,11,17,19	32
2	FOL	43-A	201	32/32	0.97	0.09	9,11,17,17	32
2	FOL	44-A	201	32/32	0.97	0.09	9,11,17,18	32
2	FOL	45-A	201	32/32	0.97	0.09	9,11,17,18	32
2	FOL	46-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	47-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	48-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	49-A	201	32/32	0.97	0.09	9,11,15,16	32
2	FOL	50-A	201	32/32	0.97	0.09	9,11,17,18	32
2	FOL	51-A	201	32/32	0.97	0.09	9,11,17,17	32
2	FOL	52-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	53-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	54-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	55-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	56-A	201	32/32	0.97	0.09	9,11,16,16	32
2	FOL	57-A	201	32/32	0.97	0.09	9,11,16,18	32
2	FOL	58-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	59-A	201	32/32	0.97	0.09	9,11,15,16	32
2	FOL	60-A	201	32/32	0.97	0.09	9,11,15,16	32
2	FOL	61-A	201	32/32	0.97	0.09	9,11,14,15	32
2	FOL	62-A	201	32/32	0.97	0.09	9,11,14,15	32
2	FOL	63-A	201	32/32	0.97	0.09	9,11,14,15	32
2	FOL	64-A	201	32/32	0.97	0.09	9,12,16,17	32
2	FOL	65-A	201	32/32	0.97	0.09	9,11,16,16	32
2	FOL	66-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	67-A	201	32/32	0.97	0.09	9,12,16,17	32

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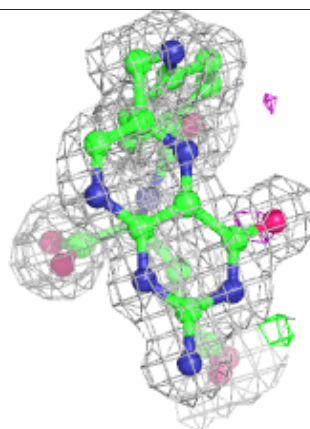
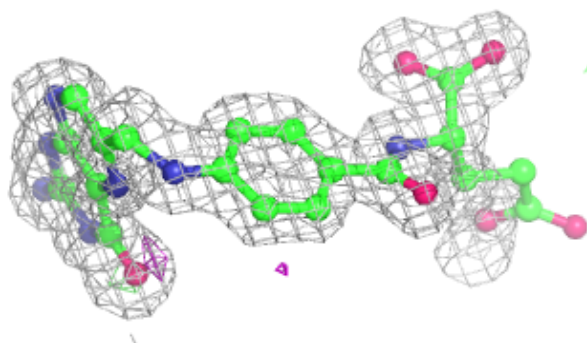
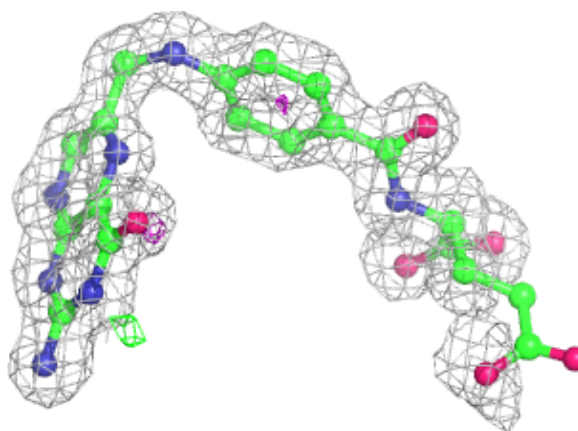
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FOL	68-A	201	32/32	0.97	0.09	9,11,16,16	32
2	FOL	69-A	201	32/32	0.97	0.09	9,11,15,16	32
2	FOL	70-A	201	32/32	0.97	0.09	9,11,15,16	32
2	FOL	71-A	201	32/32	0.97	0.09	9,11,16,18	32
2	FOL	72-A	201	32/32	0.97	0.09	9,11,17,18	32
2	FOL	73-A	201	32/32	0.97	0.09	9,12,18,19	32
2	FOL	74-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	75-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	76-A	201	32/32	0.97	0.09	9,11,15,16	32
2	FOL	77-A	201	32/32	0.97	0.09	9,11,15,16	32
2	FOL	78-A	201	32/32	0.97	0.09	9,11,15,17	32
2	FOL	79-A	201	32/32	0.97	0.09	9,11,16,17	32
2	FOL	80-A	201	32/32	0.97	0.09	9,11,16,17	32

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)



6.5 Other polymers ⓘ

There are no such residues in this entry.