



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 12:13 AM UTC

PDB ID : 7D4X / pdb\_00007d4x  
Title : X-ray crystal Structure of E.coli Dihydrofolate Reductase complexed with folate and NADP+ at pH7.0  
Authors : Wan, Q.; Dealwis, C.  
Deposited on : 2020-09-24  
Resolution : 1.60 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

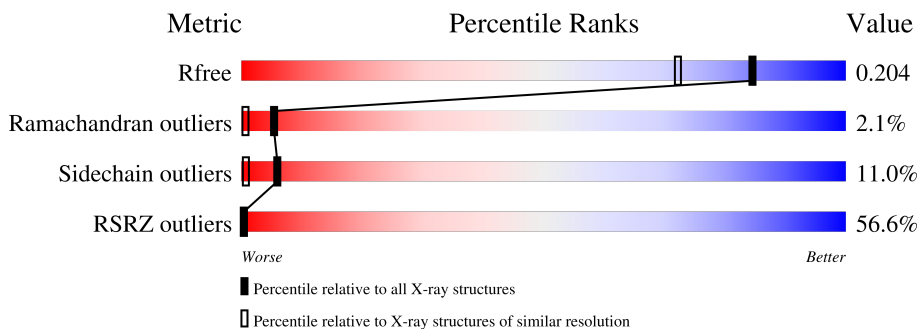
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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.














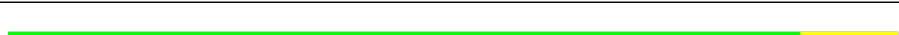

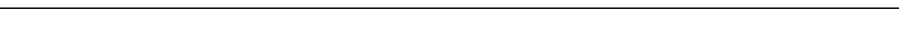
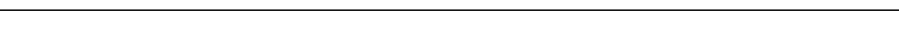
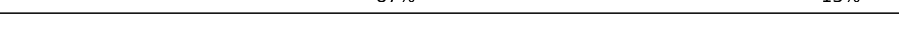

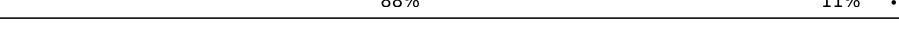







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4673 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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  $\geq 3$ , 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	
1	10-A	159	
1	11-A	159	
1	12-A	159	
1	13-A	159	
1	14-A	159	
1	15-A	159	

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Mol	Chain	Length	Quality of chain
1	16-A	159	 88% 11% .
1	17-A	159	 88% 11% .
1	18-A	159	 88% 11% .
1	19-A	159	 88% 11% .
1	2-A	159	 89% 9% .
1	20-A	159	 89% 11%
1	21-A	159	 89% 11%
1	22-A	159	 88% 11% .
1	23-A	159	 89% 11%
1	24-A	159	 88% 12%
1	25-A	159	 89% 9% .
1	26-A	159	 89% 11%
1	27-A	159	 88% 11% .
1	28-A	159	 89% 10% .
1	29-A	159	 87% 13% .
1	3-A	159	 89% 11%
1	30-A	159	 88% 11% .
1	31-A	159	 88% 12%
1	32-A	159	 89% 11%
1	33-A	159	 89% 11%
1	34-A	159	 90% 10%
1	35-A	159	 90% 10%
1	36-A	159	 89% 9% .
1	37-A	159	 90% 10%
1	38-A	159	 89% 11%

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Mol	Chain	Length	Quality of chain	
1	39-A	159	89%	11%
1	4-A	159	89%	11%
1	40-A	159	87%	13%
1	41-A	159	87%	13%
1	42-A	159	87%	13%
1	43-A	159	87%	13%
1	44-A	159	87%	13%
1	45-A	159	87%	12%
1	46-A	159	89%	11%
1	47-A	159	89%	10%
1	48-A	159	87%	13%
1	49-A	159	87%	11%
1	5-A	159	89%	11%
1	50-A	159	86%	12%
1	51-A	159	86%	13%
1	52-A	159	86%	14%
1	53-A	159	86%	13%
1	54-A	159	87%	11%
1	6-A	159	88%	11%
1	7-A	159	90%	9%
1	8-A	159	89%	10%
1	9-A	159	89%	11%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 76092 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
			Total	C	N	O	S			
1	1-A	159	1268	805	216	240	7	0	0	0
1	2-A	159	1268	805	216	240	7	0	0	0
1	3-A	159	1268	805	216	240	7	0	0	0
1	4-A	159	1268	805	216	240	7	0	0	0
1	5-A	159	1268	805	216	240	7	0	0	0
1	6-A	159	1268	805	216	240	7	0	0	0
1	7-A	159	1268	805	216	240	7	0	0	0
1	8-A	159	1268	805	216	240	7	0	0	0
1	9-A	159	1268	805	216	240	7	0	0	0
1	10-A	159	1268	805	216	240	7	0	0	0
1	11-A	159	1268	805	216	240	7	0	0	0
1	12-A	159	1268	805	216	240	7	0	0	0
1	13-A	159	1268	805	216	240	7	0	0	0
1	14-A	159	1268	805	216	240	7	0	0	0
1	15-A	159	1268	805	216	240	7	0	0	0
1	16-A	159	1268	805	216	240	7	0	0	0

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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
			Total	C	N	O	S			
1	38-A	159	1268	805	216	240	7	0	0	0
1	39-A	159	1268	805	216	240	7	0	0	0
1	40-A	159	1268	805	216	240	7	0	0	0
1	41-A	159	1268	805	216	240	7	0	0	0
1	42-A	159	1268	805	216	240	7	0	0	0
1	43-A	159	1268	805	216	240	7	0	0	0
1	44-A	159	1268	805	216	240	7	0	0	0
1	45-A	159	1268	805	216	240	7	0	0	0
1	46-A	159	1268	805	216	240	7	0	0	0
1	47-A	159	1268	805	216	240	7	0	0	0
1	48-A	159	1268	805	216	240	7	0	0	0
1	49-A	159	1268	805	216	240	7	0	0	0
1	50-A	159	1268	805	216	240	7	0	0	0
1	51-A	159	1268	805	216	240	7	0	0	0
1	52-A	159	1268	805	216	240	7	0	0	0
1	53-A	159	1268	805	216	240	7	0	0	0
1	54-A	159	1268	805	216	240	7	0	0	0

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 (CCD ID: FOL) (formula: C<sub>19</sub>H<sub>19</sub>N<sub>7</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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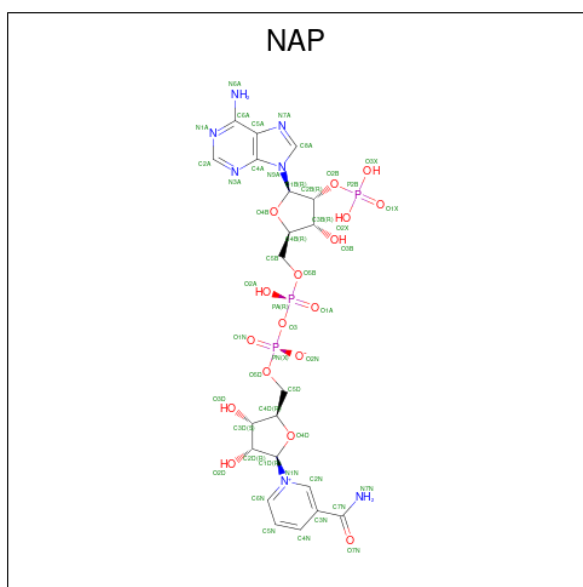
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	15-A	1	Total 32	C 19	N 7	O 6	0	0
2	16-A	1	Total 32	C 19	N 7	O 6	0	0
2	17-A	1	Total 32	C 19	N 7	O 6	0	0
2	18-A	1	Total 32	C 19	N 7	O 6	0	0
2	19-A	1	Total 32	C 19	N 7	O 6	0	0
2	20-A	1	Total 32	C 19	N 7	O 6	0	0
2	21-A	1	Total 32	C 19	N 7	O 6	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
2	29-A	1	Total 32	C 19	N 7	O 6	0	0
2	30-A	1	Total 32	C 19	N 7	O 6	0	0
2	31-A	1	Total 32	C 19	N 7	O 6	0	0
2	32-A	1	Total 32	C 19	N 7	O 6	0	0
2	33-A	1	Total 32	C 19	N 7	O 6	0	0
2	34-A	1	Total 32	C 19	N 7	O 6	0	0
2	35-A	1	Total 32	C 19	N 7	O 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		
2	50-A	1	Total	C	N	O	0	0
			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		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	15-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	16-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	17-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	18-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	19-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	20-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	21-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	22-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	23-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	24-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	25-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	26-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	27-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	28-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	29-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	30-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	31-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	32-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	33-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	34-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	35-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	36-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	37-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	38-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	39-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	40-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	41-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	42-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	43-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	44-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	45-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	46-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	47-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	48-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	49-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	50-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	51-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	52-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	53-A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	54-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	68	Total O 68 68	0	0
4	2-A	65	Total O 65 65	0	0
4	3-A	62	Total O 62 62	0	0
4	4-A	63	Total O 63 63	0	0
4	5-A	59	Total O 59 59	0	0
4	6-A	56	Total O 56 56	0	0
4	7-A	62	Total O 62 62	0	0
4	8-A	67	Total O 67 67	0	0
4	9-A	70	Total O 70 70	0	0
4	10-A	59	Total O 59 59	0	0
4	11-A	58	Total O 58 58	0	0
4	12-A	61	Total O 61 61	0	0
4	13-A	65	Total O 65 65	0	0
4	14-A	67	Total O 67 67	0	0
4	15-A	69	Total O 69 69	0	0
4	16-A	63	Total O 63 63	0	0
4	17-A	59	Total O 59 59	0	0
4	18-A	57	Total O 57 57	0	0
4	19-A	54	Total O 54 54	0	0
4	20-A	61	Total O 61 61	0	0
4	21-A	61	Total O 61 61	0	0
4	22-A	54	Total O 54 54	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	23-A	60	Total O 60 60	0	0
4	24-A	61	Total O 61 61	0	0
4	25-A	51	Total O 51 51	0	0
4	26-A	59	Total O 59 59	0	0
4	27-A	73	Total O 73 73	0	0
4	28-A	54	Total O 54 54	0	0
4	29-A	53	Total O 53 53	0	0
4	30-A	51	Total O 51 51	0	0
4	31-A	64	Total O 64 64	0	0
4	32-A	62	Total O 62 62	0	0
4	33-A	65	Total O 65 65	0	0
4	34-A	54	Total O 54 54	0	0
4	35-A	69	Total O 69 69	0	0
4	36-A	56	Total O 56 56	0	0
4	37-A	55	Total O 55 55	0	0
4	38-A	66	Total O 66 66	0	0
4	39-A	58	Total O 58 58	0	0
4	40-A	64	Total O 64 64	0	0
4	41-A	58	Total O 58 58	0	0
4	42-A	61	Total O 61 61	0	0
4	43-A	57	Total O 57 57	0	0

*Continued on next page...*

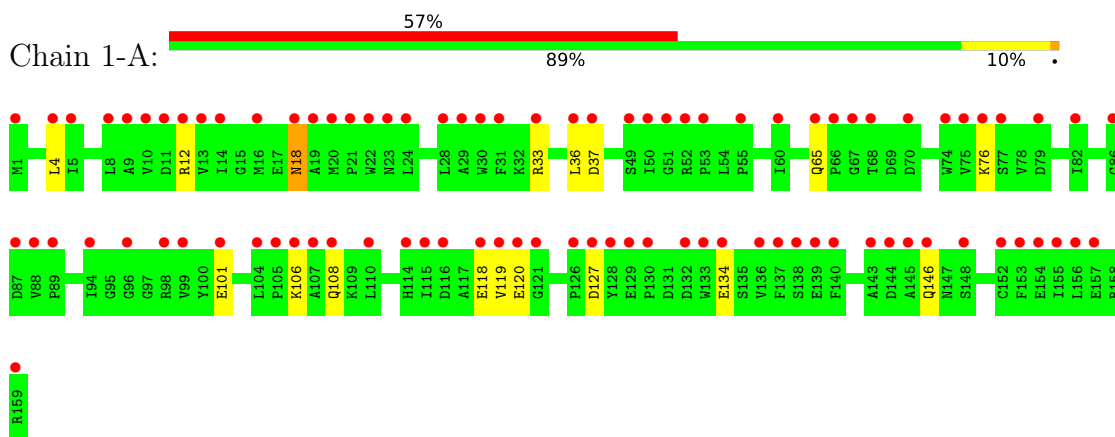
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	44-A	73	Total 73	O 73	0	0
4	45-A	77	Total 77	O 77	0	0
4	46-A	63	Total 63	O 63	0	0
4	47-A	64	Total 64	O 64	0	0
4	48-A	63	Total 63	O 63	0	0
4	49-A	61	Total 61	O 61	0	0
4	50-A	57	Total 57	O 57	0	0
4	51-A	63	Total 63	O 63	0	0
4	52-A	50	Total 50	O 50	0	0
4	53-A	53	Total 53	O 53	0	0
4	54-A	65	Total 65	O 65	0	0

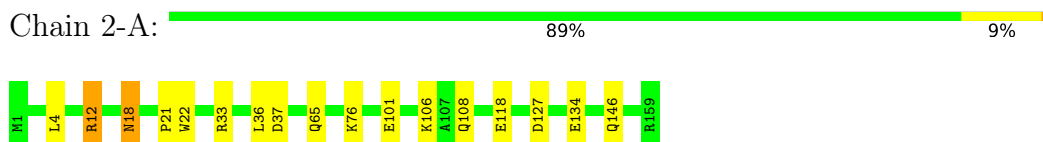
### 3 Residue-property plots [i](#)

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.

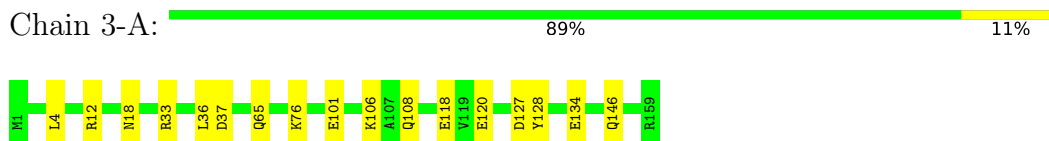
- Molecule 1: Dihydrofolate reductase



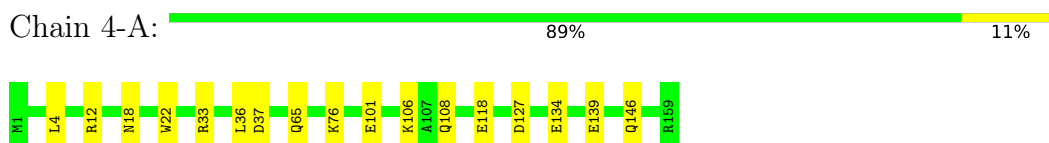
- Molecule 1: Dihydrofolate reductase



- 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

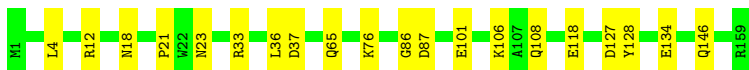


- Molecule 1: Dihydrofolate reductase

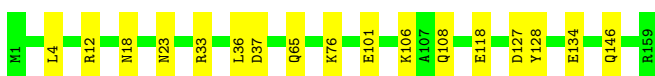




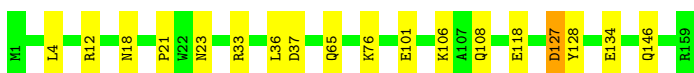
- Molecule 1: Dihydrofolate reductase



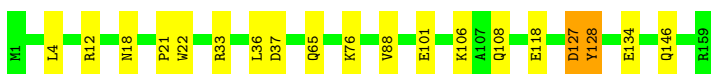
- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase





- Molecule 1: Dihydrofolate reductase

Chain 20-A:   89% 11%



- Molecule 1: Dihydrofolate reductase

Chain 21-A:   89% 11%



- Molecule 1: Dihydrofolate reductase

Chain 22-A:    88% 11%



- Molecule 1: Dihydrofolate reductase

Chain 23-A:   89% 11%



- Molecule 1: Dihydrofolate reductase

Chain 24-A:   88% 12%



- Molecule 1: Dihydrofolate reductase

Chain 25-A:    89% 9%



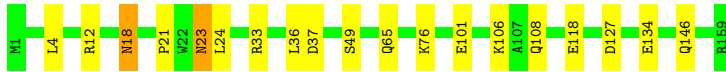
- Molecule 1: Dihydrofolate reductase

Chain 26-A:   89% 11%



- Molecule 1: Dihydrofolate reductase

Chain 27-A: 88% 11%



- Molecule 1: Dihydrofolate reductase

Chain 28-A: 89% 10%



- Molecule 1: Dihydrofolate reductase

Chain 29-A: 87% 13%



- Molecule 1: Dihydrofolate reductase

Chain 30-A: 88% 11%



- Molecule 1: Dihydrofolate reductase

Chain 31-A: 88% 12%



- Molecule 1: Dihydrofolate reductase

Chain 32-A: 89% 11%



- Molecule 1: Dihydrofolate reductase

Chain 33-A: 89% 11%



- Molecule 1: Dihydrofolate reductase

Chain 34-A: 90% 10%



- Molecule 1: Dihydrofolate reductase

Chain 35-A: 90% 10%



- Molecule 1: Dihydrofolate reductase

Chain 36-A: 89% 9%



- Molecule 1: Dihydrofolate reductase

Chain 37-A: 90% 10%



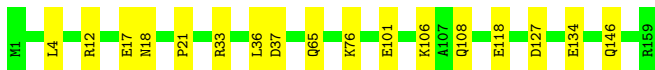
- Molecule 1: Dihydrofolate reductase

Chain 38-A: 89% 11%



- Molecule 1: Dihydrofolate reductase

Chain 39-A: 89% 11%



- Molecule 1: Dihydrofolate reductase

Chain 40-A: 87% 13%



- Molecule 1: Dihydrofolate reductase

Chain 41-A:   87% 13%



- Molecule 1: Dihydrofolate reductase

Chain 42-A:   87% 13%



- Molecule 1: Dihydrofolate reductase

Chain 43-A:   87% 13%



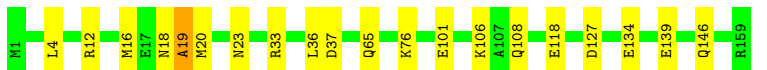
- Molecule 1: Dihydrofolate reductase

Chain 44-A:   87% 13%



- Molecule 1: Dihydrofolate reductase

Chain 45-A:    87% 12% 1%



- Molecule 1: Dihydrofolate reductase

Chain 46-A:   89% 11%



- Molecule 1: Dihydrofolate reductase

Chain 47-A:    89% 10% 1%



- Molecule 1: Dihydrofolate reductase



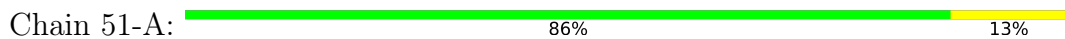
- Molecule 1: Dihydrofolate reductase



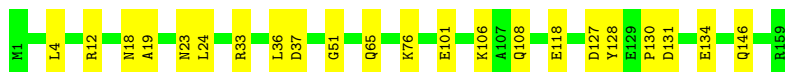
- Molecule 1: Dihydrofolate reductase



- 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, $\alpha$ , $\beta$ , $\gamma$	34.29Å 45.62Å 98.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.41 – 1.60 27.41 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (27.41-1.60) 97.0 (27.41-1.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.53 (at 1.60Å)	Xtrriage
Refinement program	PHENIX (phenix.ensemble_refinement:1.13rc2_2986)	Depositor
R, $R_{free}$	0.155 , 0.189 0.167 , 0.204	Depositor DCC
$R_{free}$ test set	1068 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtrriage
Anisotropy	0.344	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.01 , 20.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	76092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.06	0/1302	0.12	0/1770
1	2-A	0.06	0/1302	0.12	0/1770
1	3-A	0.06	0/1302	0.12	0/1770
1	4-A	0.06	0/1302	0.12	0/1770
1	5-A	0.06	0/1302	0.12	0/1770
1	6-A	0.06	0/1302	0.12	0/1770
1	7-A	0.06	0/1302	0.12	0/1770
1	8-A	0.06	0/1302	0.12	0/1770
1	9-A	0.06	0/1302	0.12	0/1770
1	10-A	0.06	0/1302	0.12	0/1770
1	11-A	0.06	0/1302	0.12	0/1770
1	12-A	0.06	0/1302	0.12	0/1770
1	13-A	0.06	0/1302	0.12	0/1770
1	14-A	0.06	0/1302	0.12	0/1770
1	15-A	0.06	0/1302	0.12	0/1770
1	16-A	0.06	0/1302	0.12	0/1770
1	17-A	0.06	0/1302	0.12	0/1770
1	18-A	0.06	0/1302	0.12	0/1770
1	19-A	0.06	0/1302	0.12	0/1770
1	20-A	0.06	0/1302	0.12	0/1770
1	21-A	0.06	0/1302	0.12	0/1770
1	22-A	0.06	0/1302	0.12	0/1770
1	23-A	0.06	0/1302	0.12	0/1770
1	24-A	0.06	0/1302	0.12	0/1770
1	25-A	0.06	0/1302	0.12	0/1770
1	26-A	0.06	0/1302	0.12	0/1770
1	27-A	0.06	0/1302	0.12	0/1770
1	28-A	0.06	0/1302	0.12	0/1770
1	29-A	0.06	0/1302	0.12	0/1770
1	30-A	0.06	0/1302	0.12	0/1770
1	31-A	0.06	0/1302	0.12	0/1770
1	32-A	0.06	0/1302	0.12	0/1770

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	33-A	0.06	0/1302	0.12	0/1770
1	34-A	0.06	0/1302	0.12	0/1770
1	35-A	0.06	0/1302	0.12	0/1770
1	36-A	0.06	0/1302	0.12	0/1770
1	37-A	0.06	0/1302	0.12	0/1770
1	38-A	0.06	0/1302	0.12	0/1770
1	39-A	0.06	0/1302	0.12	0/1770
1	40-A	0.06	0/1302	0.12	0/1770
1	41-A	0.06	0/1302	0.12	0/1770
1	42-A	0.06	0/1302	0.12	0/1770
1	43-A	0.06	0/1302	0.12	0/1770
1	44-A	0.06	0/1302	0.12	0/1770
1	45-A	0.06	0/1302	0.12	0/1770
1	46-A	0.06	0/1302	0.12	0/1770
1	47-A	0.06	0/1302	0.12	0/1770
1	48-A	0.06	0/1302	0.12	0/1770
1	49-A	0.06	0/1302	0.12	0/1770
1	50-A	0.06	0/1302	0.12	0/1770
1	51-A	0.06	0/1302	0.12	0/1770
1	52-A	0.06	0/1302	0.12	0/1770
1	53-A	0.06	0/1302	0.12	0/1770
1	54-A	0.06	0/1302	0.12	0/1770
All	All	0.06	0/70308	0.12	0/95580

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	6-A	0	1
1	8-A	0	1
1	10-A	0	3
1	11-A	0	1
1	13-A	0	1
1	15-A	0	1
1	16-A	0	1
1	17-A	0	1
1	19-A	0	1
1	20-A	0	2
1	22-A	0	1
1	23-A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	24-A	0	1
1	25-A	0	1
1	27-A	0	2
1	28-A	0	2
1	30-A	0	1
1	31-A	0	1
1	32-A	0	1
1	36-A	0	1
1	40-A	0	1
1	41-A	0	1
1	42-A	0	1
1	43-A	0	1
1	44-A	0	1
1	45-A	0	3
1	47-A	0	1
1	48-A	0	3
1	49-A	0	1
1	50-A	0	3
1	51-A	0	2
1	52-A	0	2
1	53-A	0	4
1	54-A	0	5
All	All	0	54

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 54 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	10-A	127	ASP	Peptide
1	10-A	152	CYS	Peptide
1	10-A	20	MET	Peptide
1	6-A	88	VAL	Peptide
1	8-A	130	PRO	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	42-A	1268	0	1221	0	0
1	43-A	1268	0	1221	0	0
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
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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
3	1-A	48	0	25	0	0
3	2-A	48	0	25	0	0
3	3-A	48	0	25	0	0
3	4-A	48	0	25	0	0
3	5-A	48	0	25	0	0
3	6-A	48	0	25	0	0
3	7-A	48	0	25	0	0
3	8-A	48	0	23	0	0
3	9-A	48	0	24	0	0
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	24	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	18-A	48	0	24	0	0
3	19-A	48	0	23	0	0
3	20-A	48	0	24	0	0
3	21-A	48	0	24	0	0
3	22-A	48	0	25	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	25	0	0
3	29-A	48	0	25	0	0
3	30-A	48	0	25	0	0
3	31-A	48	0	24	0	0
3	32-A	48	0	24	0	0
3	33-A	48	0	25	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	25	0	0
3	47-A	48	0	25	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
3	52-A	48	0	24	0	0
3	53-A	48	0	24	0	0
3	54-A	48	0	24	0	0
4	1-A	68	0	0	0	0
4	2-A	65	0	0	0	0
4	3-A	62	0	0	0	0
4	4-A	63	0	0	0	0
4	5-A	59	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	6-A	56	0	0	0	0
4	7-A	62	0	0	0	0
4	8-A	67	0	0	0	0
4	9-A	70	0	0	0	0
4	10-A	59	0	0	0	0
4	11-A	58	0	0	0	0
4	12-A	61	0	0	0	0
4	13-A	65	0	0	0	0
4	14-A	67	0	0	0	0
4	15-A	69	0	0	0	0
4	16-A	63	0	0	0	0
4	17-A	59	0	0	0	0
4	18-A	57	0	0	0	0
4	19-A	54	0	0	0	0
4	20-A	61	0	0	0	0
4	21-A	61	0	0	0	0
4	22-A	54	0	0	0	0
4	23-A	60	0	0	0	0
4	24-A	61	0	0	0	0
4	25-A	51	0	0	0	0
4	26-A	59	0	0	0	0
4	27-A	73	0	0	0	0
4	28-A	54	0	0	0	0
4	29-A	53	0	0	0	0
4	30-A	51	0	0	0	0
4	31-A	64	0	0	0	0
4	32-A	62	0	0	0	0
4	33-A	65	0	0	0	0
4	34-A	54	0	0	0	0
4	35-A	69	0	0	0	0
4	36-A	56	0	0	0	0
4	37-A	55	0	0	0	0
4	38-A	66	0	0	0	0
4	39-A	58	0	0	0	0
4	40-A	64	0	0	0	0
4	41-A	58	0	0	0	0
4	42-A	61	0	0	0	0
4	43-A	57	0	0	0	0
4	44-A	73	0	0	0	0
4	45-A	77	0	0	0	0
4	46-A	63	0	0	0	0
4	47-A	64	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	48-A	63	0	0	0	0
4	49-A	61	0	0	0	0
4	50-A	57	0	0	0	0
4	51-A	63	0	0	0	0
4	52-A	50	0	0	0	0
4	53-A	53	0	0	0	0
4	54-A	65	0	0	0	0
All	All	76092	0	68160	0	0

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

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1-A	157/159 (99%)	142 (90%)	12 (8%)	3 (2%)	6	1
1	2-A	157/159 (99%)	142 (90%)	11 (7%)	4 (2%)	4	0
1	3-A	157/159 (99%)	148 (94%)	7 (4%)	2 (1%)	9	2
1	4-A	157/159 (99%)	141 (90%)	14 (9%)	2 (1%)	9	2
1	5-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	9	2
1	6-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	4	0
1	7-A	157/159 (99%)	147 (94%)	8 (5%)	2 (1%)	9	2
1	8-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	9	2
1	9-A	157/159 (99%)	147 (94%)	8 (5%)	2 (1%)	9	2
1	10-A	157/159 (99%)	143 (91%)	12 (8%)	2 (1%)	9	2
1	11-A	157/159 (99%)	142 (90%)	11 (7%)	4 (2%)	4	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	12-A	157/159 (99%)	143 (91%)	6 (4%)	8 (5%)	1	0
1	13-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	4	0
1	14-A	157/159 (99%)	150 (96%)	5 (3%)	2 (1%)	9	2
1	15-A	157/159 (99%)	146 (93%)	8 (5%)	3 (2%)	6	1
1	16-A	157/159 (99%)	147 (94%)	5 (3%)	5 (3%)	3	0
1	17-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	4	0
1	18-A	157/159 (99%)	148 (94%)	4 (2%)	5 (3%)	3	0
1	19-A	157/159 (99%)	144 (92%)	9 (6%)	4 (2%)	4	0
1	20-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	21	7
1	21-A	157/159 (99%)	144 (92%)	11 (7%)	2 (1%)	9	2
1	22-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	4	0
1	23-A	157/159 (99%)	147 (94%)	9 (6%)	1 (1%)	21	7
1	24-A	157/159 (99%)	143 (91%)	11 (7%)	3 (2%)	6	1
1	25-A	157/159 (99%)	149 (95%)	5 (3%)	3 (2%)	6	1
1	26-A	157/159 (99%)	145 (92%)	10 (6%)	2 (1%)	9	2
1	27-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	4	0
1	28-A	157/159 (99%)	147 (94%)	7 (4%)	3 (2%)	6	1
1	29-A	157/159 (99%)	145 (92%)	5 (3%)	7 (4%)	2	0
1	30-A	157/159 (99%)	145 (92%)	8 (5%)	4 (2%)	4	0
1	31-A	157/159 (99%)	148 (94%)	6 (4%)	3 (2%)	6	1
1	32-A	157/159 (99%)	146 (93%)	9 (6%)	2 (1%)	9	2
1	33-A	157/159 (99%)	153 (98%)	2 (1%)	2 (1%)	9	2
1	34-A	157/159 (99%)	151 (96%)	5 (3%)	1 (1%)	21	7
1	35-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	21	7
1	36-A	157/159 (99%)	145 (92%)	9 (6%)	3 (2%)	6	1
1	37-A	157/159 (99%)	149 (95%)	7 (4%)	1 (1%)	21	7
1	38-A	157/159 (99%)	144 (92%)	10 (6%)	3 (2%)	6	1
1	39-A	157/159 (99%)	143 (91%)	12 (8%)	2 (1%)	9	2
1	40-A	157/159 (99%)	147 (94%)	6 (4%)	4 (2%)	4	0
1	41-A	157/159 (99%)	146 (93%)	6 (4%)	5 (3%)	3	0
1	42-A	157/159 (99%)	149 (95%)	4 (2%)	4 (2%)	4	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	43-A	157/159 (99%)	148 (94%)	5 (3%)	4 (2%)	4	0
1	44-A	157/159 (99%)	139 (88%)	14 (9%)	4 (2%)	4	0
1	45-A	157/159 (99%)	144 (92%)	10 (6%)	3 (2%)	6	1
1	46-A	157/159 (99%)	149 (95%)	6 (4%)	2 (1%)	9	2
1	47-A	157/159 (99%)	145 (92%)	10 (6%)	2 (1%)	9	2
1	48-A	157/159 (99%)	143 (91%)	11 (7%)	3 (2%)	6	1
1	49-A	157/159 (99%)	145 (92%)	6 (4%)	6 (4%)	2	0
1	50-A	157/159 (99%)	144 (92%)	6 (4%)	7 (4%)	2	0
1	51-A	157/159 (99%)	142 (90%)	8 (5%)	7 (4%)	2	0
1	52-A	157/159 (99%)	144 (92%)	8 (5%)	5 (3%)	3	0
1	53-A	157/159 (99%)	144 (92%)	7 (4%)	6 (4%)	2	0
1	54-A	157/159 (99%)	135 (86%)	18 (12%)	4 (2%)	4	0
All	All	8478/8586 (99%)	7863 (93%)	433 (5%)	182 (2%)	5	1

5 of 182 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-A	21	PRO
1	4-A	139	GLU
1	6-A	127	ASP
1	8-A	127	ASP
1	9-A	126	PRO

### 5.3.2 Protein sidechains [i](#)

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%)	121 (89%)	15 (11%)	6	1
1	2-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	3-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	4-A	136/136 (100%)	121 (89%)	15 (11%)	6	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	6-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	7-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	8-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	9-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	10-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	11-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
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%)	121 (89%)	15 (11%)	6	1
1	15-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	16-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	17-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	18-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	19-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	20-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	21-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	22-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	23-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	24-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	25-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	26-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	27-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	28-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	29-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	30-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	31-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	32-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	33-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	34-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	35-A	136/136 (100%)	121 (89%)	15 (11%)	6	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	36-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	37-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	38-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	39-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	40-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	41-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	42-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	43-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	44-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	45-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	46-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	47-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	48-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	49-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	50-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	51-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	52-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	53-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
1	54-A	136/136 (100%)	121 (89%)	15 (11%)	6	1
All	All	7344/7344 (100%)	6534 (89%)	810 (11%)	6	1

5 of 810 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	31-A	134	GLU
1	39-A	33	ARG
1	54-A	36	LEU
1	32-A	118	GLU
1	31-A	127	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 223 such sidechains are listed below:

Mol	Chain	Res	Type
1	28-A	141	HIS

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Mol	Chain	Res	Type
1	54-A	65	GLN
1	34-A	146	GLN
1	54-A	23	ASN
1	48-A	141	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

108 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	31-A	202	-	50,52,52	3.22	12 (24%)	71,80,80	1.54	15 (21%)
2	FOL	4-A	201	-	34,34,34	1.03	1 (2%)	43,47,47	1.94	12 (27%)
2	FOL	36-A	201	-	34,34,34	1.09	1 (2%)	43,47,47	1.43	6 (13%)
3	NAP	13-A	202	-	50,52,52	3.28	13 (26%)	71,80,80	1.54	14 (19%)
3	NAP	23-A	202	-	50,52,52	3.23	12 (24%)	71,80,80	1.53	12 (16%)
3	NAP	7-A	202	-	50,52,52	3.23	13 (26%)	71,80,80	1.60	15 (21%)
3	NAP	26-A	202	-	50,52,52	3.28	13 (26%)	71,80,80	1.59	13 (18%)
3	NAP	21-A	202	-	50,52,52	3.25	13 (26%)	71,80,80	1.63	14 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FOL	49-A	201	-	34,34,34	0.98	2 (5%)	43,47,47	1.47	4 (9%)
2	FOL	35-A	201	-	34,34,34	1.01	2 (5%)	43,47,47	1.26	2 (4%)
3	NAP	35-A	202	-	50,52,52	3.27	13 (26%)	71,80,80	1.57	16 (22%)
3	NAP	54-A	202	-	50,52,52	3.26	11 (22%)	71,80,80	1.57	12 (16%)
3	NAP	33-A	202	-	50,52,52	3.20	12 (24%)	71,80,80	1.54	11 (15%)
2	FOL	15-A	201	-	34,34,34	1.10	2 (5%)	43,47,47	1.43	4 (9%)
3	NAP	15-A	202	-	50,52,52	3.36	14 (28%)	71,80,80	1.96	15 (21%)
2	FOL	8-A	201	-	34,34,34	1.05	2 (5%)	43,47,47	1.89	9 (20%)
3	NAP	5-A	202	-	50,52,52	3.24	13 (26%)	71,80,80	1.53	12 (16%)
3	NAP	8-A	202	-	50,52,52	3.23	13 (26%)	71,80,80	1.59	15 (21%)
3	NAP	32-A	202	-	50,52,52	3.26	15 (30%)	71,80,80	1.52	16 (22%)
2	FOL	2-A	201	-	34,34,34	1.08	4 (11%)	43,47,47	1.35	5 (11%)
2	FOL	10-A	201	-	34,34,34	1.05	2 (5%)	43,47,47	1.41	4 (9%)
3	NAP	2-A	202	-	50,52,52	3.28	14 (28%)	71,80,80	1.61	15 (21%)
2	FOL	25-A	201	-	34,34,34	0.96	2 (5%)	43,47,47	1.32	4 (9%)
3	NAP	25-A	202	-	50,52,52	3.25	13 (26%)	71,80,80	1.56	12 (16%)
3	NAP	30-A	202	-	50,52,52	3.24	12 (24%)	71,80,80	1.55	16 (22%)
3	NAP	10-A	202	-	50,52,52	3.25	13 (26%)	71,80,80	1.63	15 (21%)
2	FOL	14-A	201	-	34,34,34	1.07	2 (5%)	43,47,47	1.24	2 (4%)
3	NAP	40-A	202	-	50,52,52	3.27	11 (22%)	71,80,80	1.57	13 (18%)
2	FOL	29-A	201	-	34,34,34	1.03	1 (2%)	43,47,47	1.33	4 (9%)
3	NAP	45-A	202	-	50,52,52	3.26	13 (26%)	71,80,80	1.65	15 (21%)
2	FOL	6-A	201	-	34,34,34	1.03	3 (8%)	43,47,47	1.90	11 (25%)
2	FOL	38-A	201	-	34,34,34	1.11	2 (5%)	43,47,47	1.49	5 (11%)
2	FOL	32-A	201	-	34,34,34	0.97	1 (2%)	43,47,47	1.54	6 (13%)
3	NAP	22-A	202	-	50,52,52	3.29	14 (28%)	71,80,80	1.65	16 (22%)
2	FOL	13-A	201	-	34,34,34	1.10	2 (5%)	43,47,47	1.57	8 (18%)
3	NAP	34-A	202	-	50,52,52	3.19	12 (24%)	71,80,80	1.59	14 (19%)
2	FOL	17-A	201	-	34,34,34	1.08	2 (5%)	43,47,47	1.81	7 (16%)
3	NAP	29-A	202	-	50,52,52	3.27	11 (22%)	71,80,80	1.51	14 (19%)
3	NAP	44-A	202	-	50,52,52	3.30	13 (26%)	71,80,80	1.55	13 (18%)
2	FOL	20-A	201	-	34,34,34	0.97	1 (2%)	43,47,47	1.35	3 (6%)
2	FOL	31-A	201	-	34,34,34	1.03	1 (2%)	43,47,47	1.22	2 (4%)
2	FOL	12-A	201	-	34,34,34	1.01	1 (2%)	43,47,47	1.41	4 (9%)
3	NAP	3-A	202	-	50,52,52	3.35	15 (30%)	71,80,80	1.65	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAP	4-A	202	-	50,52,52	3.28	13 (26%)	71,80,80	1.57	15 (21%)
3	NAP	46-A	202	-	50,52,52	3.27	13 (26%)	71,80,80	1.58	16 (22%)
3	NAP	49-A	202	-	50,52,52	3.27	12 (24%)	71,80,80	1.57	13 (18%)
3	NAP	20-A	202	-	50,52,52	3.23	13 (26%)	71,80,80	1.59	14 (19%)
2	FOL	18-A	201	-	34,34,34	1.04	2 (5%)	43,47,47	1.76	14 (32%)
2	FOL	48-A	201	-	34,34,34	0.98	1 (2%)	43,47,47	1.43	2 (4%)
2	FOL	11-A	201	-	34,34,34	1.04	2 (5%)	43,47,47	1.41	3 (6%)
3	NAP	43-A	202	-	50,52,52	3.32	13 (26%)	71,80,80	1.59	17 (23%)
2	FOL	22-A	201	-	34,34,34	1.03	1 (2%)	43,47,47	1.22	3 (6%)
3	NAP	11-A	202	-	50,52,52	3.23	13 (26%)	71,80,80	1.52	13 (18%)
3	NAP	37-A	202	-	50,52,52	3.31	14 (28%)	71,80,80	1.54	14 (19%)
2	FOL	21-A	201	-	34,34,34	1.06	2 (5%)	43,47,47	1.30	3 (6%)
3	NAP	36-A	202	-	50,52,52	3.28	14 (28%)	71,80,80	1.68	16 (22%)
2	FOL	7-A	201	-	34,34,34	1.13	3 (8%)	43,47,47	1.95	11 (25%)
2	FOL	26-A	201	-	34,34,34	0.98	1 (2%)	43,47,47	1.71	6 (13%)
2	FOL	43-A	201	-	34,34,34	1.02	3 (8%)	43,47,47	1.31	2 (4%)
3	NAP	16-A	202	-	50,52,52	3.29	12 (24%)	71,80,80	1.54	14 (19%)
2	FOL	41-A	201	-	34,34,34	0.98	1 (2%)	43,47,47	1.38	3 (6%)
2	FOL	53-A	201	-	34,34,34	1.03	3 (8%)	43,47,47	1.28	3 (6%)
2	FOL	54-A	201	-	34,34,34	1.03	1 (2%)	43,47,47	1.41	3 (6%)
2	FOL	28-A	201	-	34,34,34	1.05	2 (5%)	43,47,47	1.28	2 (4%)
2	FOL	51-A	201	-	34,34,34	1.00	2 (5%)	43,47,47	1.39	3 (6%)
2	FOL	27-A	201	-	34,34,34	1.03	1 (2%)	43,47,47	1.25	3 (6%)
2	FOL	5-A	201	-	34,34,34	1.02	2 (5%)	43,47,47	1.59	8 (18%)
3	NAP	51-A	202	-	50,52,52	3.29	13 (26%)	71,80,80	1.52	13 (18%)
3	NAP	18-A	202	-	50,52,52	3.27	12 (24%)	71,80,80	1.54	13 (18%)
2	FOL	34-A	201	-	34,34,34	0.97	1 (2%)	43,47,47	1.57	6 (13%)
2	FOL	45-A	201	-	34,34,34	1.08	1 (2%)	43,47,47	1.75	4 (9%)
3	NAP	38-A	202	-	50,52,52	3.27	12 (24%)	71,80,80	1.48	11 (15%)
2	FOL	9-A	201	-	34,34,34	1.03	2 (5%)	43,47,47	1.33	4 (9%)
2	FOL	52-A	201	-	34,34,34	1.08	3 (8%)	43,47,47	1.43	7 (16%)
3	NAP	6-A	202	-	50,52,52	3.25	13 (26%)	71,80,80	1.60	14 (19%)
2	FOL	40-A	201	-	34,34,34	1.03	2 (5%)	43,47,47	1.63	7 (16%)
3	NAP	14-A	202	-	50,52,52	3.26	13 (26%)	71,80,80	1.53	14 (19%)
2	FOL	23-A	201	-	34,34,34	1.03	2 (5%)	43,47,47	1.27	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FOL	39-A	201	-	34,34,34	1.02	2 (5%)	43,47,47	1.32	3 (6%)
3	NAP	48-A	202	-	50,52,52	3.30	14 (28%)	71,80,80	1.49	11 (15%)
3	NAP	28-A	202	-	50,52,52	3.24	14 (28%)	71,80,80	1.52	14 (19%)
2	FOL	46-A	201	-	34,34,34	1.04	2 (5%)	43,47,47	1.34	4 (9%)
2	FOL	19-A	201	-	34,34,34	1.20	4 (11%)	43,47,47	2.18	18 (41%)
2	FOL	42-A	201	-	34,34,34	1.04	2 (5%)	43,47,47	1.43	4 (9%)
2	FOL	37-A	201	-	34,34,34	1.07	2 (5%)	43,47,47	1.47	4 (9%)
3	NAP	41-A	202	-	50,52,52	3.25	11 (22%)	71,80,80	1.50	11 (15%)
3	NAP	42-A	202	-	50,52,52	3.30	11 (22%)	71,80,80	1.55	13 (18%)
2	FOL	24-A	201	-	34,34,34	1.01	2 (5%)	43,47,47	1.30	2 (4%)
2	FOL	44-A	201	-	34,34,34	1.01	2 (5%)	43,47,47	1.45	4 (9%)
3	NAP	12-A	202	-	50,52,52	3.31	13 (26%)	71,80,80	1.52	14 (19%)
3	NAP	9-A	202	-	50,52,52	3.27	12 (24%)	71,80,80	1.56	12 (16%)
3	NAP	24-A	202	-	50,52,52	3.26	12 (24%)	71,80,80	1.52	13 (18%)
2	FOL	50-A	201	-	34,34,34	1.07	2 (5%)	43,47,47	1.47	6 (13%)
3	NAP	52-A	202	-	50,52,52	3.24	13 (26%)	71,80,80	1.61	17 (23%)
3	NAP	27-A	202	-	50,52,52	3.26	14 (28%)	71,80,80	1.53	14 (19%)
3	NAP	50-A	202	-	50,52,52	3.26	13 (26%)	71,80,80	1.50	11 (15%)
2	FOL	30-A	201	-	34,34,34	1.10	1 (2%)	43,47,47	1.28	3 (6%)
3	NAP	39-A	202	-	50,52,52	3.24	13 (26%)	71,80,80	1.63	14 (19%)
2	FOL	33-A	201	-	34,34,34	1.04	3 (8%)	43,47,47	1.36	4 (9%)
3	NAP	17-A	202	-	50,52,52	3.23	13 (26%)	71,80,80	1.53	13 (18%)
3	NAP	19-A	202	-	50,52,52	3.26	12 (24%)	71,80,80	1.52	14 (19%)
3	NAP	53-A	202	-	50,52,52	3.25	11 (22%)	71,80,80	1.68	14 (19%)
2	FOL	3-A	201	-	34,34,34	0.99	1 (2%)	43,47,47	1.57	8 (18%)
2	FOL	47-A	201	-	34,34,34	1.04	3 (8%)	43,47,47	1.48	7 (16%)
3	NAP	1-A	202	-	50,52,52	3.27	13 (26%)	71,80,80	1.54	12 (16%)
2	FOL	16-A	201	-	34,34,34	1.07	1 (2%)	43,47,47	1.65	6 (13%)
3	NAP	47-A	202	-	50,52,52	3.21	12 (24%)	71,80,80	1.55	15 (21%)
2	FOL	1-A	201	-	34,34,34	1.04	1 (2%)	43,47,47	1.34	3 (6%)

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	31-A	202	-	-	2/35/67/67	0/5/5/5
2	FOL	4-A	201	-	-	12/22/22/22	0/3/3/3
2	FOL	36-A	201	-	-	7/22/22/22	0/3/3/3
3	NAP	13-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	23-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	7-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	26-A	202	-	-	2/35/67/67	0/5/5/5
3	NAP	21-A	202	-	-	2/35/67/67	0/5/5/5
2	FOL	49-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	35-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	35-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	54-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	33-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	15-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	15-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	8-A	201	-	-	9/22/22/22	0/3/3/3
3	NAP	5-A	202	-	-	2/35/67/67	0/5/5/5
3	NAP	8-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	32-A	202	-	-	2/35/67/67	0/5/5/5
2	FOL	2-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	10-A	201	-	-	4/22/22/22	0/3/3/3
3	NAP	2-A	202	-	-	6/35/67/67	0/5/5/5
2	FOL	25-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	25-A	202	-	-	2/35/67/67	0/5/5/5
3	NAP	30-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	10-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	14-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	40-A	202	-	-	2/35/67/67	0/5/5/5
2	FOL	29-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	45-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	6-A	201	-	-	8/22/22/22	0/3/3/3
2	FOL	38-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	32-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	22-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	13-A	201	-	-	2/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	34-A	202	-	-	2/35/67/67	0/5/5/5
2	FOL	17-A	201	-	-	7/22/22/22	0/3/3/3
3	NAP	29-A	202	-	-	5/35/67/67	0/5/5/5
3	NAP	44-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	20-A	201	-	-	3/22/22/22	0/3/3/3
2	FOL	31-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	12-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	3-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	4-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	46-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	49-A	202	-	-	2/35/67/67	0/5/5/5
3	NAP	20-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	18-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	48-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	11-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	43-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	22-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	11-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	37-A	202	-	-	2/35/67/67	0/5/5/5
2	FOL	21-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	36-A	202	-	-	2/35/67/67	0/5/5/5
2	FOL	7-A	201	-	-	10/22/22/22	0/3/3/3
2	FOL	26-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	43-A	201	-	-	3/22/22/22	0/3/3/3
3	NAP	16-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	41-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	53-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	54-A	201	-	-	4/22/22/22	0/3/3/3
2	FOL	28-A	201	-	-	10/22/22/22	0/3/3/3
2	FOL	51-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	27-A	201	-	-	2/22/22/22	0/3/3/3
2	FOL	5-A	201	-	-	11/22/22/22	0/3/3/3
3	NAP	51-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	18-A	202	-	-	3/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FOL	34-A	201	-	-	6/22/22/22	0/3/3/3
2	FOL	45-A	201	-	-	8/22/22/22	0/3/3/3
3	NAP	38-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	9-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	52-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	6-A	202	-	-	4/35/67/67	0/5/5/5
2	FOL	40-A	201	-	-	9/22/22/22	0/3/3/3
3	NAP	14-A	202	-	-	2/35/67/67	0/5/5/5
2	FOL	23-A	201	-	-	5/22/22/22	0/3/3/3
2	FOL	39-A	201	-	-	5/22/22/22	0/3/3/3
3	NAP	48-A	202	-	-	2/35/67/67	0/5/5/5
3	NAP	28-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	46-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	19-A	201	-	-	9/22/22/22	0/3/3/3
2	FOL	42-A	201	-	-	11/22/22/22	0/3/3/3
2	FOL	37-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	41-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	42-A	202	-	-	2/35/67/67	0/5/5/5
2	FOL	24-A	201	-	-	0/22/22/22	0/3/3/3
2	FOL	44-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	12-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	9-A	202	-	-	2/35/67/67	0/5/5/5
3	NAP	24-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	50-A	201	-	-	6/22/22/22	0/3/3/3
3	NAP	52-A	202	-	-	2/35/67/67	0/5/5/5
3	NAP	27-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	50-A	202	-	-	3/35/67/67	0/5/5/5
2	FOL	30-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	39-A	202	-	-	1/35/67/67	0/5/5/5
2	FOL	33-A	201	-	-	2/22/22/22	0/3/3/3
3	NAP	17-A	202	-	-	3/35/67/67	0/5/5/5
3	NAP	19-A	202	-	-	4/35/67/67	0/5/5/5
3	NAP	53-A	202	-	-	6/35/67/67	0/5/5/5
2	FOL	3-A	201	-	-	7/22/22/22	0/3/3/3
2	FOL	47-A	201	-	-	2/22/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	1-A	202	-	-	2/35/67/67	0/5/5/5
2	FOL	16-A	201	-	-	13/22/22/22	0/3/3/3
3	NAP	47-A	202	-	-	2/35/67/67	0/5/5/5
2	FOL	1-A	201	-	-	5/22/22/22	0/3/3/3

The worst 5 of 789 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	16-A	202	NAP	O4D-C1D	14.55	1.60	1.40
3	15-A	202	NAP	O4D-C1D	14.37	1.59	1.40
3	3-A	202	NAP	O4D-C1D	14.35	1.59	1.40
3	42-A	202	NAP	O4D-C1D	14.34	1.59	1.40
3	40-A	202	NAP	O4D-C1D	14.32	1.59	1.40

The worst 5 of 1025 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	15-A	202	NAP	C2B-C1B-N9A	-8.27	100.14	113.75
2	19-A	201	FOL	C11-C-N	6.23	128.60	117.04
2	45-A	201	FOL	CB-CG-CD	-5.97	96.56	112.49
2	6-A	201	FOL	C8A-C4A-C4	-5.74	115.84	119.56
2	32-A	201	FOL	N1-C8A-N8	5.67	124.85	116.38

There are no chirality outliers.

5 of 431 torsion outliers are listed below:

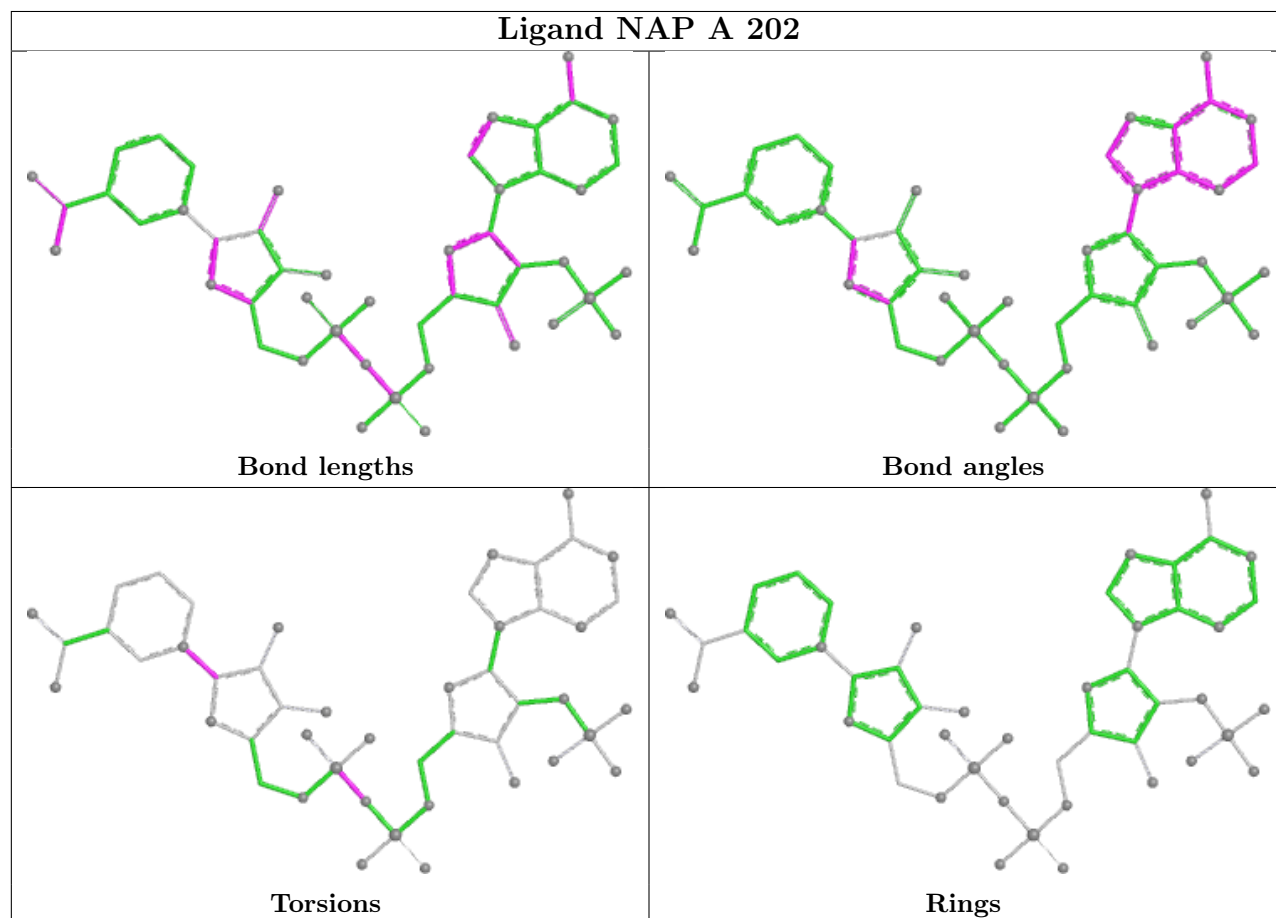
Mol	Chain	Res	Type	Atoms
2	3-A	201	FOL	N-CA-CB-CG
2	5-A	201	FOL	C6-C9-N10-C14
2	6-A	201	FOL	C11-C-N-CA
2	8-A	201	FOL	CB-CA-N-C
2	17-A	201	FOL	N-CA-CB-CG

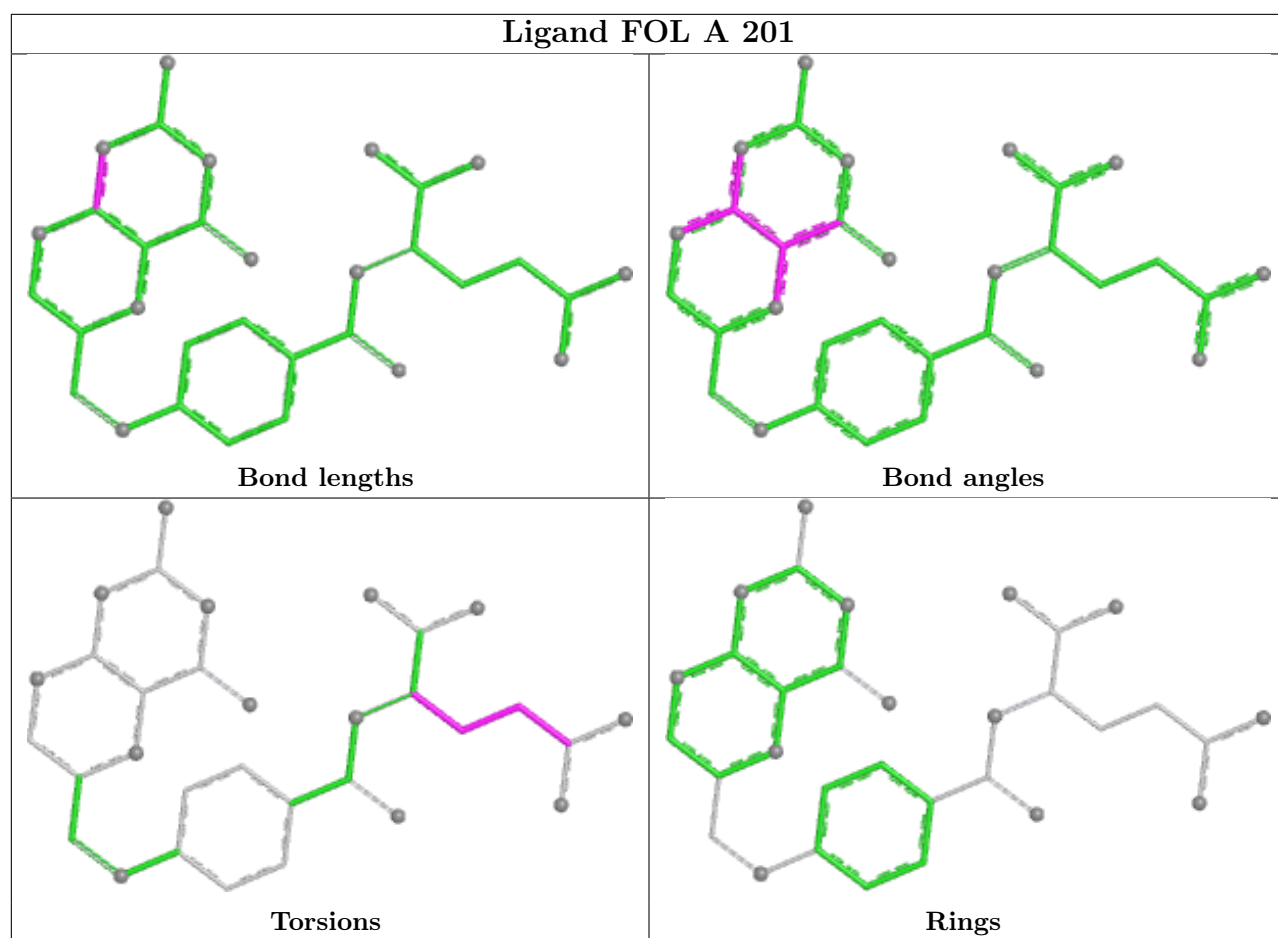
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1-A	159/159 (100%)	2.58	90 (56%) <b>0</b> <b>0</b>	0, 0, 0, 0	159 (100%)
1	2-A	0/159	-	-	-	-
1	3-A	0/159	-	-	-	-
1	4-A	0/159	-	-	-	-
1	5-A	0/159	-	-	-	-
1	6-A	0/159	-	-	-	-
1	7-A	0/159	-	-	-	-
1	8-A	0/159	-	-	-	-
1	9-A	0/159	-	-	-	-
1	10-A	0/159	-	-	-	-
1	11-A	0/159	-	-	-	-
1	12-A	0/159	-	-	-	-
1	13-A	0/159	-	-	-	-
1	14-A	0/159	-	-	-	-
1	15-A	0/159	-	-	-	-
1	16-A	0/159	-	-	-	-
1	17-A	0/159	-	-	-	-
1	18-A	0/159	-	-	-	-
1	19-A	0/159	-	-	-	-
1	20-A	0/159	-	-	-	-
1	21-A	0/159	-	-	-	-
1	22-A	0/159	-	-	-	-
1	23-A	0/159	-	-	-	-
1	24-A	0/159	-	-	-	-
1	25-A	0/159	-	-	-	-
1	26-A	0/159	-	-	-	-
1	27-A	0/159	-	-	-	-
1	28-A	0/159	-	-	-	-
1	29-A	0/159	-	-	-	-
1	30-A	0/159	-	-	-	-
1	31-A	0/159	-	-	-	-
1	32-A	0/159	-	-	-	-

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	33-A	0/159	-	-	-	-
1	34-A	0/159	-	-	-	-
1	35-A	0/159	-	-	-	-
1	36-A	0/159	-	-	-	-
1	37-A	0/159	-	-	-	-
1	38-A	0/159	-	-	-	-
1	39-A	0/159	-	-	-	-
1	40-A	0/159	-	-	-	-
1	41-A	0/159	-	-	-	-
1	42-A	0/159	-	-	-	-
1	43-A	0/159	-	-	-	-
1	44-A	0/159	-	-	-	-
1	45-A	0/159	-	-	-	-
1	46-A	0/159	-	-	-	-
1	47-A	0/159	-	-	-	-
1	48-A	0/159	-	-	-	-
1	49-A	0/159	-	-	-	-
1	50-A	0/159	-	-	-	-
1	51-A	0/159	-	-	-	-
1	52-A	0/159	-	-	-	-
1	53-A	0/159	-	-	-	-
1	54-A	0/159	-	-	-	-
All	All	159/8586 (1%)	2.58	90 (56%) <b>0</b> <b>0</b>	0, 0, 0, 0	159 (100%)

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	20	MET	11.7
1	1-A	130	PRO	9.0
1	1-A	119	VAL	7.4
1	1-A	128	TYR	5.6
1	1-A	21	PRO	5.6

## 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 oligosaccharides in this entry.

## 6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	FOL	1-A	201	32/32	0.68	0.18	14,15,18,18	32
2	FOL	2-A	201	32/32	-	-	14,15,18,18	32
2	FOL	3-A	201	32/32	-	-	14,15,18,19	32
2	FOL	4-A	201	32/32	-	-	14,15,19,19	32
2	FOL	5-A	201	32/32	-	-	14,15,18,19	32
2	FOL	6-A	201	32/32	-	-	14,15,17,18	32
2	FOL	7-A	201	32/32	-	-	14,15,19,19	32
2	FOL	8-A	201	32/32	-	-	14,15,19,19	32
2	FOL	9-A	201	32/32	-	-	14,15,17,18	32
2	FOL	10-A	201	32/32	-	-	14,15,17,18	32
2	FOL	11-A	201	32/32	-	-	14,15,17,18	32
2	FOL	12-A	201	32/32	-	-	14,15,17,18	32
2	FOL	13-A	201	32/32	-	-	14,15,17,18	32
2	FOL	14-A	201	32/32	-	-	14,15,17,18	32
2	FOL	15-A	201	32/32	-	-	14,15,17,17	32
2	FOL	16-A	201	32/32	-	-	14,15,18,19	32
2	FOL	17-A	201	32/32	-	-	14,15,19,19	32
2	FOL	18-A	201	32/32	-	-	14,15,18,19	32
2	FOL	19-A	201	32/32	-	-	14,15,18,19	32
2	FOL	20-A	201	32/32	-	-	14,15,18,18	32
2	FOL	21-A	201	32/32	-	-	14,15,18,18	32
2	FOL	22-A	201	32/32	-	-	14,15,17,18	32
2	FOL	23-A	201	32/32	-	-	14,15,17,18	32
2	FOL	24-A	201	32/32	-	-	14,15,17,18	32
2	FOL	25-A	201	32/32	-	-	14,15,17,18	32
2	FOL	26-A	201	32/32	-	-	14,15,18,18	32
2	FOL	27-A	201	32/32	-	-	14,15,18,18	32
2	FOL	28-A	201	32/32	-	-	14,15,18,19	32
2	FOL	29-A	201	32/32	-	-	14,15,17,18	32
2	FOL	30-A	201	32/32	-	-	14,15,17,18	32
2	FOL	31-A	201	32/32	-	-	14,15,17,18	32
2	FOL	32-A	201	32/32	-	-	14,15,17,18	32
2	FOL	33-A	201	32/32	-	-	14,15,17,18	32
2	FOL	34-A	201	32/32	-	-	14,15,17,18	32
2	FOL	35-A	201	32/32	-	-	14,15,18,18	32
2	FOL	36-A	201	32/32	-	-	14,15,18,19	32
2	FOL	37-A	201	32/32	-	-	14,15,17,18	32

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FOL	38-A	201	32/32	-	-	14,15,17,18	32
2	FOL	39-A	201	32/32	-	-	14,15,18,19	32
2	FOL	40-A	201	32/32	-	-	14,15,18,19	32
2	FOL	41-A	201	32/32	-	-	14,15,18,18	32
2	FOL	42-A	201	32/32	-	-	14,15,17,17	32
2	FOL	43-A	201	32/32	-	-	14,15,17,17	32
2	FOL	44-A	201	32/32	-	-	14,15,17,18	32
2	FOL	45-A	201	32/32	-	-	14,15,17,18	32
2	FOL	46-A	201	32/32	-	-	14,15,17,18	32
2	FOL	47-A	201	32/32	-	-	14,15,17,17	32
2	FOL	48-A	201	32/32	-	-	14,15,17,18	32
2	FOL	49-A	201	32/32	-	-	14,15,17,18	32
2	FOL	50-A	201	32/32	-	-	14,15,18,18	32
2	FOL	51-A	201	32/32	-	-	14,15,17,18	32
2	FOL	52-A	201	32/32	-	-	14,15,17,17	32
2	FOL	53-A	201	32/32	-	-	14,15,17,18	32
2	FOL	54-A	201	32/32	-	-	14,15,17,18	32
3	NAP	1-A	202	48/48	0.93	0.10	15,16,19,19	48
3	NAP	2-A	202	48/48	-	-	15,16,19,19	48
3	NAP	3-A	202	48/48	-	-	15,16,19,19	48
3	NAP	4-A	202	48/48	-	-	15,17,19,19	48
3	NAP	5-A	202	48/48	-	-	15,16,19,19	48
3	NAP	6-A	202	48/48	-	-	15,16,19,19	48
3	NAP	7-A	202	48/48	-	-	15,17,19,19	48
3	NAP	8-A	202	48/48	-	-	15,17,19,19	48
3	NAP	9-A	202	48/48	-	-	15,16,19,19	48
3	NAP	10-A	202	48/48	-	-	15,16,19,19	48
3	NAP	11-A	202	48/48	-	-	15,16,19,19	48
3	NAP	12-A	202	48/48	-	-	15,16,19,19	48
3	NAP	13-A	202	48/48	-	-	15,16,19,19	48
3	NAP	14-A	202	48/48	-	-	15,17,19,19	48
3	NAP	15-A	202	48/48	-	-	15,16,19,19	48
3	NAP	16-A	202	48/48	-	-	15,16,19,19	48
3	NAP	17-A	202	48/48	-	-	15,16,19,19	48
3	NAP	18-A	202	48/48	-	-	15,16,19,19	48
3	NAP	19-A	202	48/48	-	-	15,16,19,19	48
3	NAP	20-A	202	48/48	-	-	15,16,19,19	48
3	NAP	21-A	202	48/48	-	-	15,17,19,19	48
3	NAP	22-A	202	48/48	-	-	15,16,19,19	48
3	NAP	23-A	202	48/48	-	-	15,16,19,19	48
3	NAP	24-A	202	48/48	-	-	15,16,19,19	48
3	NAP	25-A	202	48/48	-	-	15,16,19,19	48

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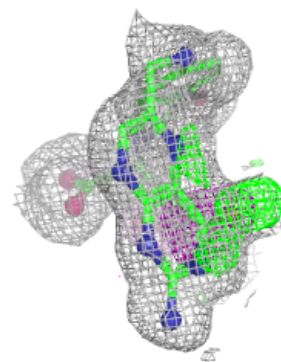
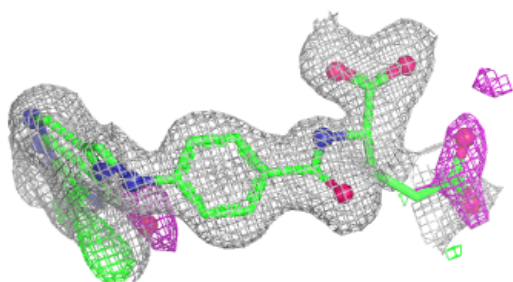
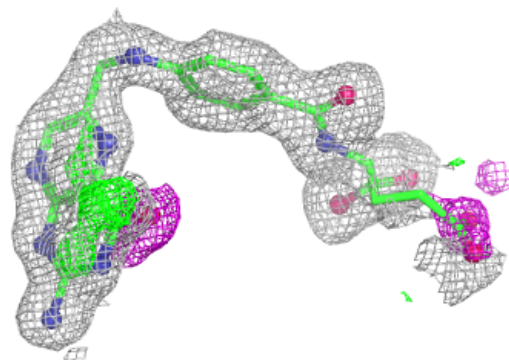
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAP	26-A	202	48/48	-	-	15,16,19,19	48
3	NAP	27-A	202	48/48	-	-	15,16,19,20	48
3	NAP	28-A	202	48/48	-	-	15,16,19,19	48
3	NAP	29-A	202	48/48	-	-	15,16,19,19	48
3	NAP	30-A	202	48/48	-	-	15,16,19,19	48
3	NAP	31-A	202	48/48	-	-	15,16,19,19	48
3	NAP	32-A	202	48/48	-	-	15,17,19,19	48
3	NAP	33-A	202	48/48	-	-	15,16,19,19	48
3	NAP	34-A	202	48/48	-	-	15,16,19,19	48
3	NAP	35-A	202	48/48	-	-	15,16,19,19	48
3	NAP	36-A	202	48/48	-	-	15,16,19,19	48
3	NAP	37-A	202	48/48	-	-	15,16,19,19	48
3	NAP	38-A	202	48/48	-	-	15,16,19,19	48
3	NAP	39-A	202	48/48	-	-	15,16,19,19	48
3	NAP	40-A	202	48/48	-	-	15,16,19,19	48
3	NAP	41-A	202	48/48	-	-	15,16,19,19	48
3	NAP	42-A	202	48/48	-	-	15,16,19,19	48
3	NAP	43-A	202	48/48	-	-	15,16,19,19	48
3	NAP	44-A	202	48/48	-	-	15,16,19,19	48
3	NAP	45-A	202	48/48	-	-	15,16,19,19	48
3	NAP	46-A	202	48/48	-	-	15,17,19,19	48
3	NAP	47-A	202	48/48	-	-	15,16,19,19	48
3	NAP	48-A	202	48/48	-	-	15,17,19,19	48
3	NAP	49-A	202	48/48	-	-	15,16,19,19	48
3	NAP	50-A	202	48/48	-	-	15,16,19,19	48
3	NAP	51-A	202	48/48	-	-	15,16,19,19	48
3	NAP	52-A	202	48/48	-	-	15,16,19,19	48
3	NAP	53-A	202	48/48	-	-	15,16,19,19	48
3	NAP	54-A	202	48/48	-	-	15,16,19,19	48

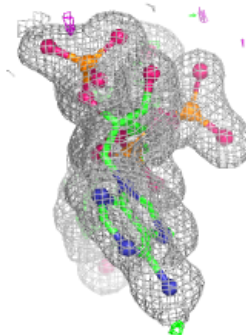
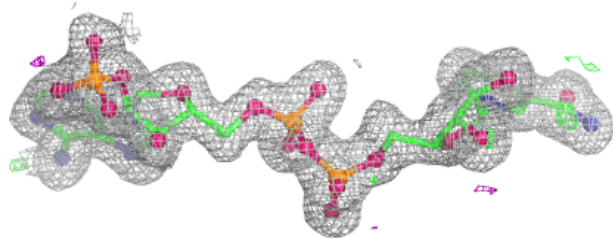
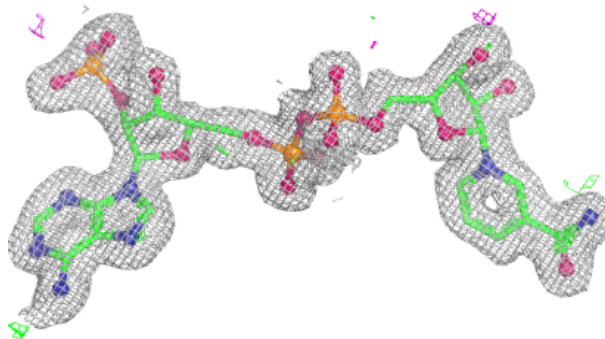
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FOL A 201:**

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

**Electron density around NAP A 202:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.