WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 08:10 PM JST

PDB ID	:	8JSY
Title	:	Dihydrofolate reductase-like enzyme from Leptospira interrogans
Authors	:	Wangkanont, K.
Deposited on	:	2023-06-20
Resolution	:	2.55 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

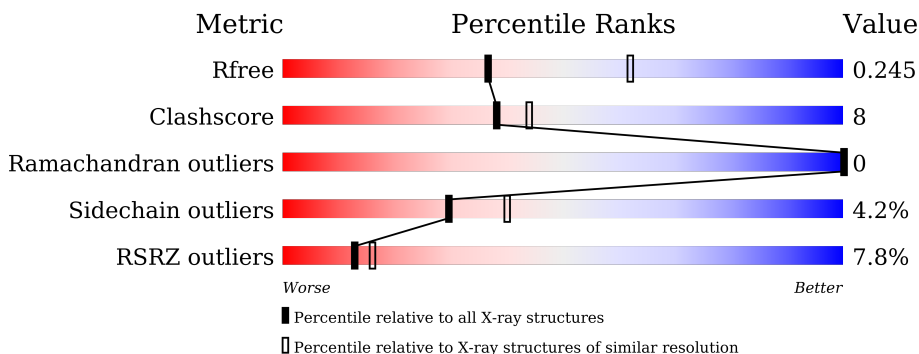|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.55 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	Percentile Ranks	Value
Rfree		0.245
Clashscore		8
Ramachandran outliers		0
Sidechain outliers		4.2%
RSRZ outliers		7.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

❏ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	A	203	10% — 68% — 26% · ·
1	B	203	11% — 73% — 22% · ·
1	C	203	10% — 79% — 19% ·
1	D	203	2% — 80% — 14% · ·
1	E	203	7% — 77% — 19% ·
1	F	203	3% — 80% — 16% ·

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Mol	Chain	Length	Quality of chain
1	G	203	3% 83% 11%
1	H	203	12% 85% 11%
1	I	203	10% 83% 16%
1	J	203	5% 84% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	G	307	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16770 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 family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1526	988	244	289	5			
1	B	195	Total	C	N	O	S	0	0	0
			1526	988	244	289	5			
1	C	202	Total	C	N	O	S	0	1	0
			1596	1032	262	297	5			
1	D	195	Total	C	N	O	S	0	0	0
			1526	988	244	289	5			
1	E	195	Total	C	N	O	S	0	0	0
			1526	988	244	289	5			
1	F	195	Total	C	N	O	S	0	0	0
			1526	988	244	289	5			
1	G	195	Total	C	N	O	S	0	0	0
			1526	988	244	289	5			
1	H	195	Total	C	N	O	S	0	1	0
			1537	997	245	290	5			
1	I	203	Total	C	N	O	S	0	0	0
			1596	1029	264	298	5			
1	J	202	Total	C	N	O	S	0	0	0
			1585	1023	261	296	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	HIS	-	expression tag	UNP A0A8I0PU34
A	199	HIS	-	expression tag	UNP A0A8I0PU34
A	200	HIS	-	expression tag	UNP A0A8I0PU34
A	201	HIS	-	expression tag	UNP A0A8I0PU34
A	202	HIS	-	expression tag	UNP A0A8I0PU34
A	203	HIS	-	expression tag	UNP A0A8I0PU34
B	198	HIS	-	expression tag	UNP A0A8I0PU34
B	199	HIS	-	expression tag	UNP A0A8I0PU34
B	200	HIS	-	expression tag	UNP A0A8I0PU34

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Chain	Residue	Modelled	Actual	Comment	Reference
B	201	HIS	-	expression tag	UNP A0A8I0PU34
B	202	HIS	-	expression tag	UNP A0A8I0PU34
B	203	HIS	-	expression tag	UNP A0A8I0PU34
C	198	HIS	-	expression tag	UNP A0A8I0PU34
C	199	HIS	-	expression tag	UNP A0A8I0PU34
C	200	HIS	-	expression tag	UNP A0A8I0PU34
C	201	HIS	-	expression tag	UNP A0A8I0PU34
C	202	HIS	-	expression tag	UNP A0A8I0PU34
C	203	HIS	-	expression tag	UNP A0A8I0PU34
D	198	HIS	-	expression tag	UNP A0A8I0PU34
D	199	HIS	-	expression tag	UNP A0A8I0PU34
D	200	HIS	-	expression tag	UNP A0A8I0PU34
D	201	HIS	-	expression tag	UNP A0A8I0PU34
D	202	HIS	-	expression tag	UNP A0A8I0PU34
D	203	HIS	-	expression tag	UNP A0A8I0PU34
E	198	HIS	-	expression tag	UNP A0A8I0PU34
E	199	HIS	-	expression tag	UNP A0A8I0PU34
E	200	HIS	-	expression tag	UNP A0A8I0PU34
E	201	HIS	-	expression tag	UNP A0A8I0PU34
E	202	HIS	-	expression tag	UNP A0A8I0PU34
E	203	HIS	-	expression tag	UNP A0A8I0PU34
F	198	HIS	-	expression tag	UNP A0A8I0PU34
F	199	HIS	-	expression tag	UNP A0A8I0PU34
F	200	HIS	-	expression tag	UNP A0A8I0PU34
F	201	HIS	-	expression tag	UNP A0A8I0PU34
F	202	HIS	-	expression tag	UNP A0A8I0PU34
F	203	HIS	-	expression tag	UNP A0A8I0PU34
G	198	HIS	-	expression tag	UNP A0A8I0PU34
G	199	HIS	-	expression tag	UNP A0A8I0PU34
G	200	HIS	-	expression tag	UNP A0A8I0PU34
G	201	HIS	-	expression tag	UNP A0A8I0PU34
G	202	HIS	-	expression tag	UNP A0A8I0PU34
G	203	HIS	-	expression tag	UNP A0A8I0PU34
H	198	HIS	-	expression tag	UNP A0A8I0PU34
H	199	HIS	-	expression tag	UNP A0A8I0PU34
H	200	HIS	-	expression tag	UNP A0A8I0PU34
H	201	HIS	-	expression tag	UNP A0A8I0PU34
H	202	HIS	-	expression tag	UNP A0A8I0PU34
H	203	HIS	-	expression tag	UNP A0A8I0PU34
I	198	HIS	-	expression tag	UNP A0A8I0PU34
I	199	HIS	-	expression tag	UNP A0A8I0PU34
I	200	HIS	-	expression tag	UNP A0A8I0PU34

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Chain	Residue	Modelled	Actual	Comment	Reference
I	201	HIS	-	expression tag	UNP A0A8I0PU34
I	202	HIS	-	expression tag	UNP A0A8I0PU34
I	203	HIS	-	expression tag	UNP A0A8I0PU34
J	198	HIS	-	expression tag	UNP A0A8I0PU34
J	199	HIS	-	expression tag	UNP A0A8I0PU34
J	200	HIS	-	expression tag	UNP A0A8I0PU34
J	201	HIS	-	expression tag	UNP A0A8I0PU34
J	202	HIS	-	expression tag	UNP A0A8I0PU34
J	203	HIS	-	expression tag	UNP A0A8I0PU34

- Molecule 2 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).
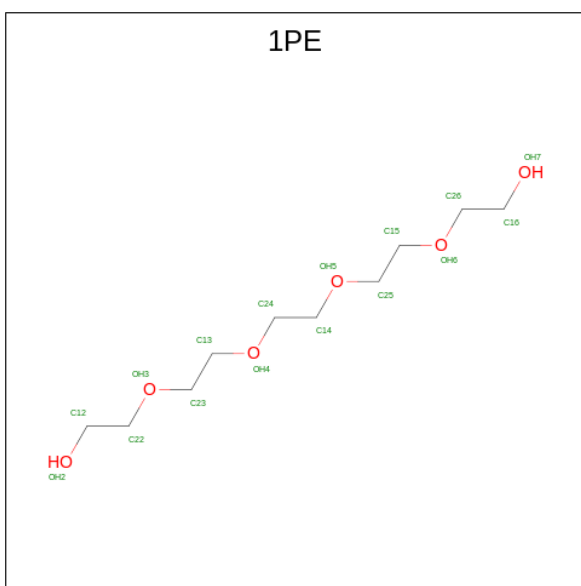
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			16	10	6		
2	C	1	Total	C	O	0	0
			16	10	6		
2	D	1	Total	C	O	0	0
			16	10	6		
2	E	1	Total	C	O	0	0
			16	10	6		
2	F	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total 16	C 10	O 6	0	0
2	G	1	Total 16	C 10	O 6	0	0
2	G	1	Total 10	C 6	O 4	0	0
2	H	1	Total 16	C 10	O 6	0	0
2	H	1	Total 16	C 10	O 6	0	0
2	I	1	Total 13	C 8	O 5	0	0
2	I	1	Total 10	C 6	O 4	0	0
2	J	1	Total 16	C 10	O 6	0	0
2	J	1	Total 16	C 10	O 6	0	0
2	J	1	Total 7	C 4	O 3	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).
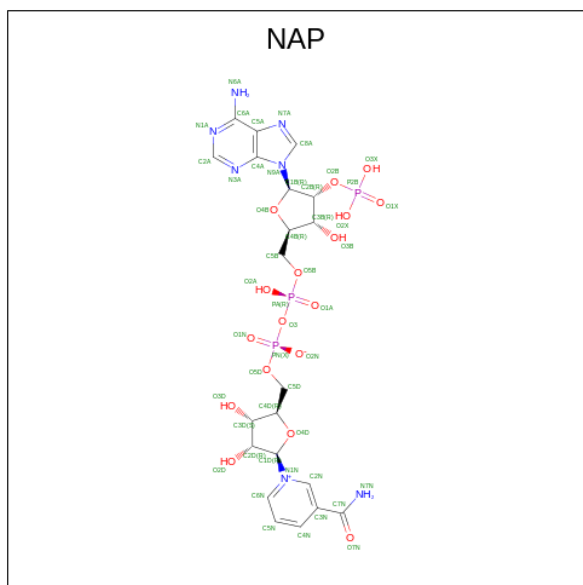
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
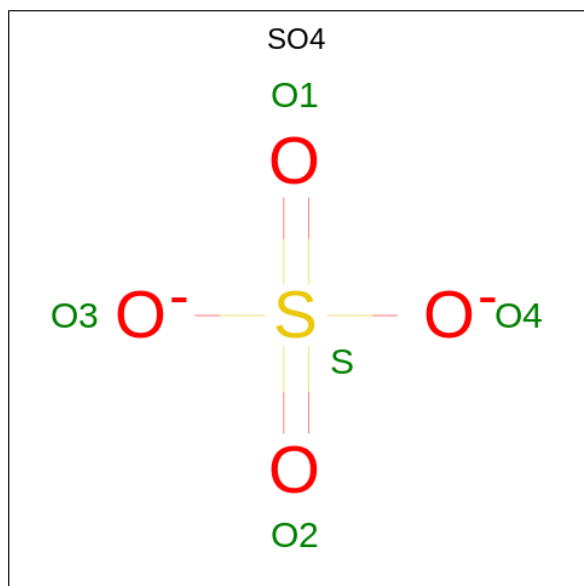
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 5	O 4	S 1	0	0
4	C	1	Total 5	O 4	S 1	0	0
4	C	1	Total 5	O 4	S 1	0	0
4	C	1	Total 5	O 4	S 1	0	0
4	C	1	Total 5	O 4	S 1	0	0
4	C	1	Total 5	O 4	S 1	0	0
4	D	1	Total 5	O 4	S 1	0	0
4	D	1	Total 5	O 4	S 1	0	0
4	E	1	Total 5	O 4	S 1	0	0
4	E	1	Total 5	O 4	S 1	0	0
4	E	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0
4	G	1	Total 5	O 4	S 1	0	0
4	G	1	Total 5	O 4	S 1	0	0
4	G	1	Total 5	O 4	S 1	0	0
4	G	1	Total 5	O 4	S 1	0	0
4	G	1	Total 5	O 4	S 1	0	0
4	H	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total 5	O 4	S 1	0	0
4	I	1	Total 5	O 4	S 1	0	0
4	I	1	Total 5	O 4	S 1	0	0
4	I	1	Total 5	O 4	S 1	0	0
4	I	1	Total 5	O 4	S 1	0	0
4	I	1	Total 5	O 4	S 1	0	0
4	J	1	Total 5	O 4	S 1	0	0
4	J	1	Total 5	O 4	S 1	0	0
4	J	1	Total 5	O 4	S 1	0	0
4	J	1	Total 5	O 4	S 1	0	0
4	J	1	Total 5	O 4	S 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
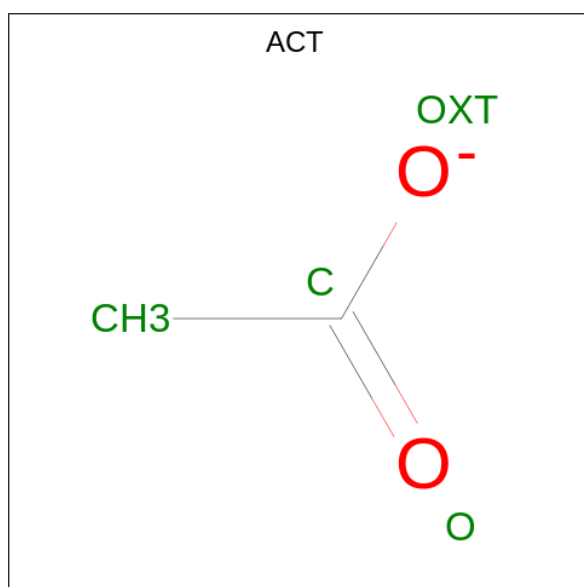
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total 4	C 2	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total 18	O 18	0	0
6	B	23	Total 23	O 23	0	0
6	C	45	Total 45	O 45	0	0
6	D	54	Total 54	O 54	0	0
6	E	41	Total 41	O 41	0	0
6	F	60	Total 60	O 60	0	0
6	G	52	Total 52	O 52	0	0
6	H	23	Total 23	O 23	0	0
6	I	59	Total 59	O 59	0	0
6	J	38	Total 38	O 38	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.
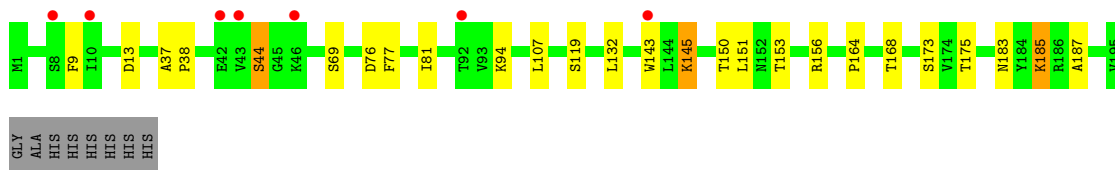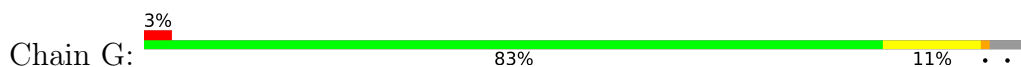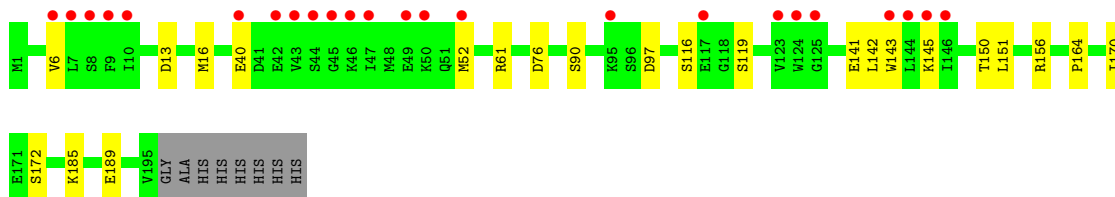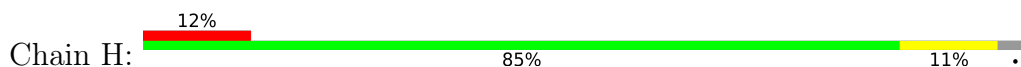
- Molecule 1: Dihydrofolate reductase family protein
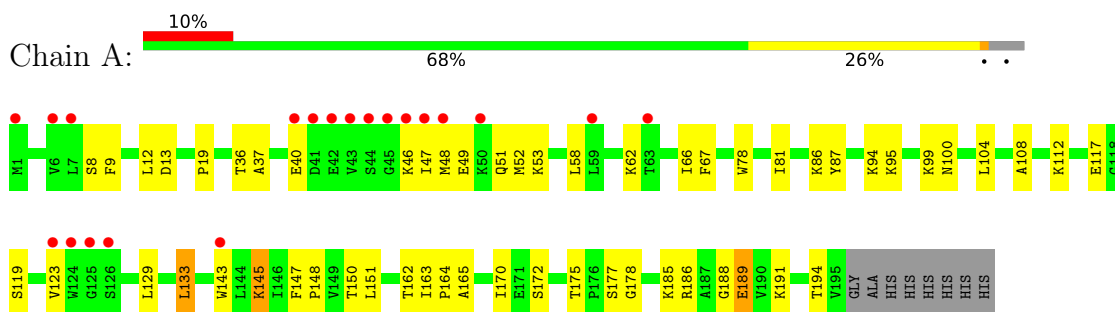
Chain A:

- Molecule 1: Dihydrofolate reductase family protein

Chain B:

- Molecule 1: Dihydrofolate reductase family protein

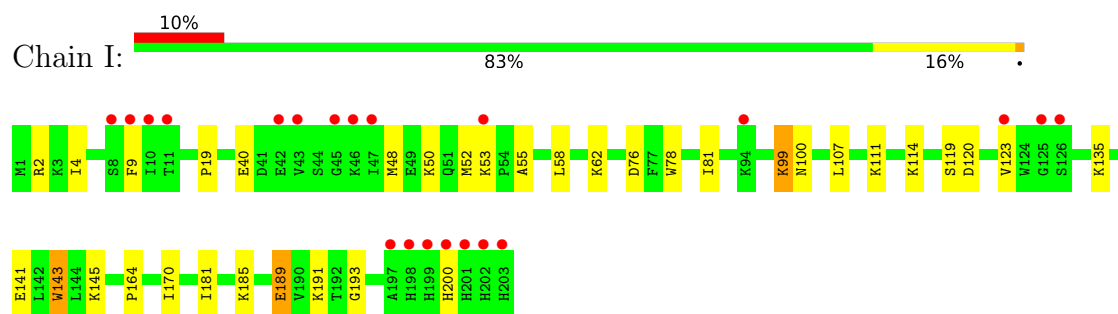Chain C:

- Molecule 1: Dihydrofolate reductase family protein

Chain D:

- Molecule 1: Dihydrofolate reductase family protein

Chain E:

- Molecule 1: Dihydrofolate reductase family protein
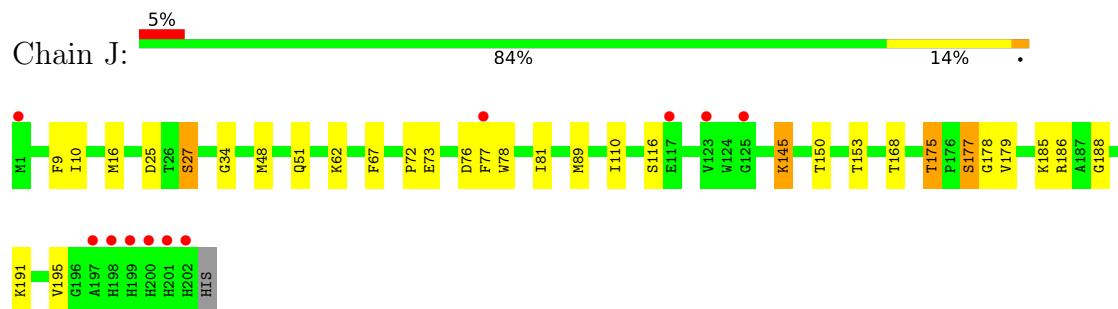
Chain F:

- Molecule 1: Dihydrofolate reductase family protein

Chain G:

- Molecule 1: Dihydrofolate reductase family protein

Chain H:

- Molecule 1: Dihydrofolate reductase family protein

Chain I:

10%

83% 16%

M1 R2 K3 I4 S8 F9 I10 T11 P19 E40 D41 E42 V43 S44 G45 K46 I47 M48 E49 K50 Q51 M52 K53 P54 A55 L58 K62 D76 F77 W78 I81 K94 K99 N100 L107 K111 K114 S119 D120 V123 W124 G125 S126 K135

E141 L142 W143 L144 K145 P164 I170 I181 K185 E189 V190 K191 T192 G193 A197 H198 H199 H200 H201 H202 H203

• Molecule 1: Dihydrofolate reductase family protein

Chain J:

5%

84% 14%

M1 F9 I10 M16 D25 T26 S27 G34 M48 Q51 K62 F67 P72 E73 D76 F77 W78 I81 M89 I110 S116 E117 V123 W124 G125 K145 T150 T153 T168 T175 P176 S177 G178 V179 K185 R186 A187 G188

K191 V195 G196 A197 H198 H199 H200 H201 H202 HIS
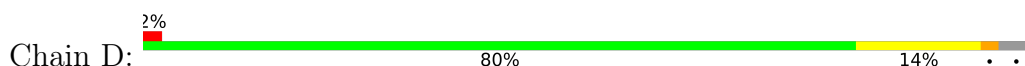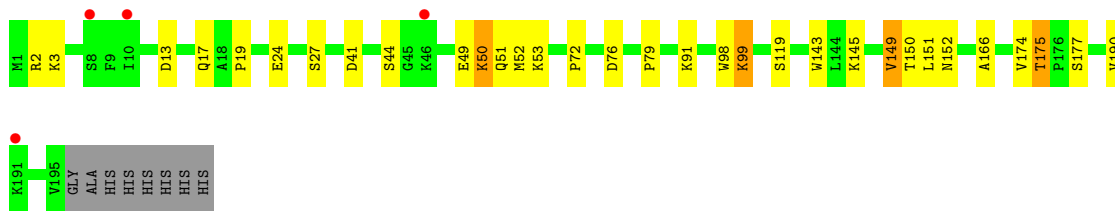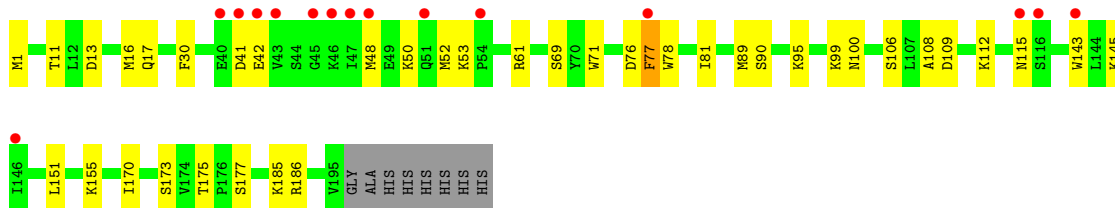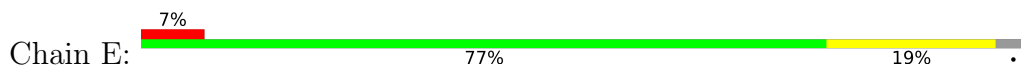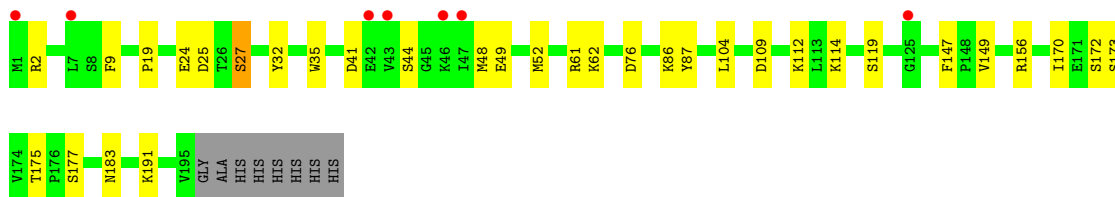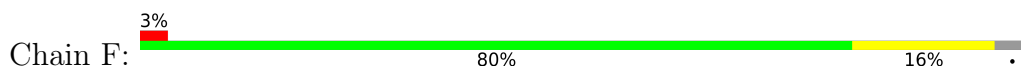
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.24Å 137.36Å 236.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.55 29.90 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.90-2.55) 99.7 (29.90-2.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.197 , 0.247 0.196 , 0.245	Depositor DCC
R_{free} test set	4372 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.8	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16770	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, 1PE, ACT, SO4

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	A	0.42	0/1563	0.63	0/2114
1	B	0.42	0/1563	0.64	0/2114
1	C	0.44	0/1639	0.65	0/2217
1	D	0.51	0/1563	0.68	0/2114
1	E	0.48	0/1563	0.63	0/2114
1	F	0.49	0/1563	0.69	0/2114
1	G	0.49	0/1563	0.69	0/2114
1	H	0.47	0/1575	0.66	0/2130
1	I	0.49	0/1639	0.64	0/2216
1	J	0.50	0/1627	0.65	0/2201
All	All	0.47	0/15858	0.66	0/21448

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	1526	0	1528	34	0
1	B	1526	0	1528	40	0
1	C	1596	0	1579	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1526	0	1528	21	0
1	E	1526	0	1528	21	0
1	F	1526	0	1528	23	0
1	G	1526	0	1528	20	0
1	H	1537	0	1536	9	0
1	I	1596	0	1578	29	0
1	J	1585	0	1571	23	0
2	A	23	0	30	1	0
2	B	16	0	22	0	0
2	C	16	0	22	2	0
2	D	16	0	22	0	0
2	E	16	0	22	4	0
2	F	26	0	35	4	0
2	G	26	0	35	5	0
2	H	32	0	44	0	0
2	I	23	0	30	6	0
2	J	39	0	53	3	0
3	A	48	0	23	1	0
3	B	48	0	23	3	0
3	C	48	0	23	2	0
3	D	48	0	25	0	0
3	E	48	0	24	2	0
3	F	48	0	24	2	0
3	G	48	0	24	4	0
3	H	48	0	23	1	0
3	I	48	0	24	1	0
3	J	48	0	23	2	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	25	0	0	0	0
4	D	10	0	0	1	0
4	E	15	0	0	0	0
4	F	20	0	0	1	0
4	G	25	0	0	4	0
4	H	10	0	0	0	0
4	I	25	0	0	0	0
4	J	25	0	0	1	0
5	D	4	0	3	1	0
6	A	18	0	0	0	0
6	B	23	0	0	1	0
6	C	45	0	0	2	0
6	D	54	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	41	0	0	0	0
6	F	60	0	0	1	0
6	G	52	0	0	0	0
6	H	23	0	0	0	0
6	I	59	0	0	2	0
6	J	38	0	0	1	0
All	All	16770	0	15986	245	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 245 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:SER:HB2	2:G:302:1PE:H121	1.50	0.91
1:I:40:GLU:HB3	2:I:302:1PE:H152	1.55	0.87
1:E:170:ILE:HD11	1:E:185:LYS:HE2	1.56	0.84
1:J:62:LYS:HD2	3:J:304:NAP:H51A	1.59	0.82
1:F:104:LEU:HD22	1:F:109:ASP:HB3	1.62	0.82

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	A	193/203 (95%)	186 (96%)	7 (4%)	0	100	100
1	B	193/203 (95%)	186 (96%)	7 (4%)	0	100	100
1	C	201/203 (99%)	197 (98%)	4 (2%)	0	100	100
1	D	193/203 (95%)	187 (97%)	6 (3%)	0	100	100
1	E	193/203 (95%)	191 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	193/203 (95%)	187 (97%)	6 (3%)	0	100	100
1	G	193/203 (95%)	187 (97%)	6 (3%)	0	100	100
1	H	194/203 (96%)	188 (97%)	6 (3%)	0	100	100
1	I	201/203 (99%)	195 (97%)	6 (3%)	0	100	100
1	J	200/203 (98%)	193 (96%)	7 (4%)	0	100	100
All	All	1954/2030 (96%)	1897 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	165/171 (96%)	155 (94%)	10 (6%)	18	24
1	B	165/171 (96%)	163 (99%)	2 (1%)	71	81
1	C	171/171 (100%)	163 (95%)	8 (5%)	26	35
1	D	165/171 (96%)	159 (96%)	6 (4%)	35	47
1	E	165/171 (96%)	157 (95%)	8 (5%)	25	34
1	F	165/171 (96%)	159 (96%)	6 (4%)	35	47
1	G	165/171 (96%)	157 (95%)	8 (5%)	25	34
1	H	166/171 (97%)	157 (95%)	9 (5%)	22	29
1	I	171/171 (100%)	165 (96%)	6 (4%)	36	49
1	J	170/171 (99%)	163 (96%)	7 (4%)	30	41
All	All	1668/1710 (98%)	1598 (96%)	70 (4%)	30	40

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	76	ASP
1	I	135	LYS

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Mol	Chain	Res	Type
1	J	116	SER
1	D	149	VAL
1	D	99	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	152	ASN
1	E	115	ASN
1	G	183	ASN
1	J	51	GLN

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 ⓘ

62 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	$\#|Z|>2$
4	SO4	J	306	-	4,4,4	0.21	0	6,6,6	0.27	0
4	SO4	J	309	-	4,4,4	0.25	0	6,6,6	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NAP	A	303	-	45,52,52	4.43	14 (31%)	56,80,80	1.22	3 (5%)
4	SO4	D	305	-	4,4,4	0.22	0	6,6,6	0.60	0
4	SO4	B	304	-	4,4,4	0.15	0	6,6,6	0.26	0
4	SO4	I	305	-	4,4,4	0.15	0	6,6,6	0.47	0
4	SO4	F	304	-	4,4,4	0.13	0	6,6,6	0.12	0
2	1PE	G	302	-	9,9,15	0.94	0	8,8,14	0.96	0
2	1PE	J	301	-	15,15,15	0.81	0	14,14,14	0.75	0
2	1PE	A	301	-	9,9,15	0.79	0	8,8,14	0.84	0
2	1PE	H	302	-	15,15,15	0.90	0	14,14,14	0.72	0
5	ACT	D	302	-	3,3,3	2.06	1 (33%)	3,3,3	1.42	0
2	1PE	H	301	-	15,15,15	0.89	1 (6%)	14,14,14	0.81	0
2	1PE	B	301	-	15,15,15	0.75	0	14,14,14	0.82	0
4	SO4	F	307	-	4,4,4	0.18	0	6,6,6	0.13	0
2	1PE	A	302	-	12,12,15	0.81	0	11,11,14	0.87	0
4	SO4	H	304	-	4,4,4	0.12	0	6,6,6	0.08	0
4	SO4	J	307	-	4,4,4	0.12	0	6,6,6	0.23	0
4	SO4	G	306	-	4,4,4	0.16	0	6,6,6	0.22	0
4	SO4	J	308	-	4,4,4	0.15	0	6,6,6	0.30	0
2	1PE	F	302	-	15,15,15	0.71	0	14,14,14	0.75	0
4	SO4	C	306	-	4,4,4	0.10	0	6,6,6	0.12	0
2	1PE	I	302	-	9,9,15	0.82	0	8,8,14	0.84	0
2	1PE	I	301	-	12,12,15	0.96	0	11,11,14	0.82	0
2	1PE	J	302	-	15,15,15	0.73	0	14,14,14	0.85	0
4	SO4	E	303	-	4,4,4	0.13	0	6,6,6	0.26	0
4	SO4	E	305	-	4,4,4	0.11	0	6,6,6	0.28	0
3	NAP	I	303	-	45,52,52	4.43	15 (33%)	56,80,80	1.20	2 (3%)
3	NAP	G	303	-	45,52,52	4.34	13 (28%)	56,80,80	1.21	4 (7%)
2	1PE	C	301	-	15,15,15	0.82	0	14,14,14	0.81	0
2	1PE	G	301	-	15,15,15	0.82	0	14,14,14	0.89	0
4	SO4	B	303	-	4,4,4	0.17	0	6,6,6	0.30	0
4	SO4	G	304	-	4,4,4	0.15	0	6,6,6	0.31	0
3	NAP	J	304	-	45,52,52	4.39	14 (31%)	56,80,80	1.28	4 (7%)
4	SO4	C	304	-	4,4,4	0.21	0	6,6,6	0.30	0
4	SO4	H	305	-	4,4,4	0.19	0	6,6,6	0.17	0
4	SO4	J	305	-	4,4,4	0.16	0	6,6,6	0.34	0
4	SO4	G	308	-	4,4,4	0.24	0	6,6,6	0.17	0
4	SO4	C	303	-	4,4,4	0.20	0	6,6,6	0.32	0
4	SO4	A	304	-	4,4,4	0.17	0	6,6,6	0.43	0
4	SO4	F	305	-	4,4,4	0.09	0	6,6,6	0.23	0
4	SO4	G	307	-	4,4,4	0.17	0	6,6,6	0.25	0
3	NAP	H	303	-	45,52,52	4.30	13 (28%)	56,80,80	1.51	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	SO4	D	304	-	4,4,4	0.18	0	6,6,6	0.41	0
4	SO4	C	305	-	4,4,4	0.14	0	6,6,6	0.13	0
4	SO4	I	307	-	4,4,4	0.16	0	6,6,6	0.20	0
2	1PE	D	301	-	15,15,15	1.38	3 (20%)	14,14,14	0.76	0
3	NAP	B	302	-	45,52,52	4.38	15 (33%)	56,80,80	1.20	3 (5%)
4	SO4	I	308	-	4,4,4	0.14	0	6,6,6	0.18	0
4	SO4	I	306	-	4,4,4	0.19	0	6,6,6	0.15	0
2	1PE	F	301	-	9,9,15	0.76	0	8,8,14	0.74	0
4	SO4	I	304	-	4,4,4	0.22	0	6,6,6	0.31	0
4	SO4	G	305	-	4,4,4	0.19	0	6,6,6	0.22	0
3	NAP	D	303	-	45,52,52	4.33	14 (31%)	56,80,80	1.26	5 (8%)
3	NAP	E	302	-	45,52,52	4.43	14 (31%)	56,80,80	1.25	4 (7%)
3	NAP	F	303	-	45,52,52	4.37	15 (33%)	56,80,80	1.32	7 (12%)
4	SO4	F	306	-	4,4,4	0.18	0	6,6,6	0.37	0
2	1PE	J	303	-	6,6,15	0.64	0	5,5,14	0.68	0
2	1PE	E	301	-	15,15,15	0.85	0	14,14,14	0.77	0
4	SO4	E	304	-	4,4,4	0.13	0	6,6,6	0.34	0
3	NAP	C	302	-	45,52,52	4.49	15 (33%)	56,80,80	1.34	6 (10%)
4	SO4	C	307	-	4,4,4	0.17	0	6,6,6	0.14	0

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	A	303	-	-	11/31/67/67	0/5/5/5
2	1PE	G	302	-	-	3/7/7/13	-
2	1PE	J	301	-	-	7/13/13/13	-
2	1PE	A	301	-	-	6/7/7/13	-
2	1PE	H	302	-	-	6/13/13/13	-
2	1PE	H	301	-	-	7/13/13/13	-
2	1PE	B	301	-	-	10/13/13/13	-
2	1PE	A	302	-	-	6/10/10/13	-
2	1PE	F	302	-	-	7/13/13/13	-
2	1PE	I	302	-	-	6/7/7/13	-
2	1PE	I	301	-	-	7/10/10/13	-
2	1PE	J	302	-	-	6/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAP	I	303	-	-	11/31/67/67	0/5/5/5
3	NAP	G	303	-	-	8/31/67/67	0/5/5/5
2	1PE	C	301	-	-	7/13/13/13	-
2	1PE	G	301	-	-	9/13/13/13	-
3	NAP	J	304	-	-	14/31/67/67	0/5/5/5
3	NAP	H	303	-	-	9/31/67/67	0/5/5/5
2	1PE	D	301	-	-	7/13/13/13	-
3	NAP	B	302	-	-	13/31/67/67	0/5/5/5
2	1PE	F	301	-	-	6/7/7/13	-
3	NAP	D	303	-	-	7/31/67/67	0/5/5/5
3	NAP	E	302	-	-	9/31/67/67	0/5/5/5
3	NAP	F	303	-	-	9/31/67/67	0/5/5/5
2	1PE	J	303	-	-	1/4/4/13	-
2	1PE	E	301	-	-	7/13/13/13	-
3	NAP	C	302	-	-	11/31/67/67	0/5/5/5

The worst 5 of 147 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302	NAP	O4B-C1B	15.85	1.63	1.41
3	C	302	NAP	C2D-C1D	-15.63	1.30	1.53
3	D	303	NAP	O4B-C1B	15.61	1.62	1.41
3	I	303	NAP	O4B-C1B	15.48	1.62	1.41
3	E	302	NAP	C2D-C1D	-15.41	1.30	1.53

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	NAP	N3A-C2A-N1A	-5.86	119.52	128.68
3	E	302	NAP	N3A-C2A-N1A	-5.72	119.74	128.68
3	J	304	NAP	N3A-C2A-N1A	-5.65	119.84	128.68
3	C	302	NAP	N3A-C2A-N1A	-5.60	119.92	128.68
3	H	303	NAP	N3A-C2A-N1A	-5.48	120.11	128.68

There are no chirality outliers.

5 of 210 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	NAP	C5B-O5B-PA-O1A
3	A	303	NAP	C5D-O5D-PN-O1N
3	A	303	NAP	O4D-C1D-N1N-C2N
3	A	303	NAP	O4D-C1D-N1N-C6N
3	A	303	NAP	C2D-C1D-N1N-C2N

There are no ring outliers.

26 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	NAP	1	0
4	F	304	SO4	1	0
2	G	302	1PE	3	0
2	J	301	1PE	1	0
5	D	302	ACT	1	0
2	A	302	1PE	1	0
4	G	306	SO4	1	0
4	J	308	SO4	1	0
2	I	302	1PE	5	0
2	I	301	1PE	2	0
2	J	302	1PE	2	0
3	I	303	NAP	1	0
3	G	303	NAP	4	0
2	C	301	1PE	2	0
2	G	301	1PE	3	0
3	J	304	NAP	2	0
4	G	308	SO4	1	0
4	G	307	SO4	2	0
3	H	303	NAP	1	0
4	D	304	SO4	1	0
3	B	302	NAP	3	0
2	F	301	1PE	4	0
3	E	302	NAP	2	0
3	F	303	NAP	2	0
2	E	301	1PE	4	0
3	C	302	NAP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NAP A 303

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP I 303

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP G 303

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP J 304

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP H 303

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 302

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP D 303

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP E 302

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP F 303

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP C 302

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	195/203 (96%)	0.45	20 (10%)	6	8	52, 73, 107, 131	0
1	B	195/203 (96%)	0.56	23 (11%)	4	6	55, 76, 108, 119	0
1	C	202/203 (99%)	0.31	21 (10%)	6	8	47, 62, 98, 120	0
1	D	195/203 (96%)	-0.14	4 (2%)	63	70	42, 52, 72, 86	0
1	E	195/203 (96%)	0.25	15 (7%)	13	17	48, 64, 106, 124	0
1	F	195/203 (96%)	0.11	7 (3%)	42	49	43, 56, 86, 96	0
1	G	195/203 (96%)	-0.02	7 (3%)	42	49	44, 57, 81, 99	0
1	H	195/203 (96%)	0.36	24 (12%)	4	5	49, 63, 106, 118	0
1	I	203/203 (100%)	0.35	21 (10%)	6	8	44, 58, 98, 117	0
1	J	202/203 (99%)	0.17	11 (5%)	25	30	42, 62, 84, 102	0
All	All	1972/2030 (97%)	0.24	153 (7%)	13	16	42, 62, 96, 131	0

The worst 5 of 153 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	47	ILE	7.5
1	A	47	ILE	7.4
1	I	200	HIS	5.9
1	E	77	PHE	5.3
1	E	43	VAL	5.2

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

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(Å^2)	Q<0.9
2	1PE	H	302	16/16	0.65	0.38	81,89,102,103	0
4	SO4	D	305	5/5	0.68	0.37	74,77,86,95	5
4	SO4	H	305	5/5	0.70	0.40	76,80,86,91	5
4	SO4	F	307	5/5	0.71	0.38	69,71,87,87	5
2	1PE	F	302	16/16	0.75	0.29	61,81,90,92	0
4	SO4	B	304	5/5	0.77	0.28	84,90,95,98	5
2	1PE	D	301	16/16	0.77	0.29	64,72,85,85	0
2	1PE	E	301	16/16	0.78	0.28	80,89,98,101	0
4	SO4	G	308	5/5	0.78	0.31	67,76,84,92	5
2	1PE	J	301	16/16	0.78	0.38	78,91,104,105	0
4	SO4	E	305	5/5	0.80	0.39	70,73,80,85	5
4	SO4	I	306	5/5	0.80	0.34	77,80,87,90	5
4	SO4	G	305	5/5	0.81	0.29	75,75,87,89	5
4	SO4	I	305	5/5	0.82	0.26	65,68,74,76	5
4	SO4	J	305	5/5	0.82	0.20	88,91,93,93	5
4	SO4	J	308	5/5	0.82	0.32	78,82,89,91	5
4	SO4	H	304	5/5	0.83	0.33	76,79,86,93	5
4	SO4	I	308	5/5	0.83	0.38	68,69,75,87	5
4	SO4	B	303	5/5	0.84	0.26	62,68,74,75	5
4	SO4	J	307	5/5	0.84	0.19	94,97,106,108	5
2	1PE	B	301	16/16	0.84	0.24	80,84,90,95	0
2	1PE	H	301	16/16	0.85	0.26	66,76,90,91	0
4	SO4	G	307	5/5	0.86	0.39	76,76,83,84	5
4	SO4	E	304	5/5	0.86	0.37	68,71,75,75	5
4	SO4	I	304	5/5	0.86	0.23	71,72,82,83	5
2	1PE	F	301	10/16	0.87	0.36	70,76,81,89	0
4	SO4	C	305	5/5	0.87	0.48	84,89,96,99	5
4	SO4	F	305	5/5	0.88	0.39	61,67,70,72	5
4	SO4	F	306	5/5	0.88	0.21	52,57,61,63	5
4	SO4	C	306	5/5	0.88	0.36	84,86,91,91	5
4	SO4	G	306	5/5	0.89	0.29	71,72,81,84	5
2	1PE	A	302	13/16	0.89	0.34	68,77,83,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	1PE	G	302	10/16	0.89	0.22	73,79,85,88	0
2	1PE	A	301	10/16	0.90	0.24	80,85,91,93	0
2	1PE	C	301	16/16	0.90	0.17	69,78,85,86	0
4	SO4	C	304	5/5	0.90	0.23	63,69,74,74	5
4	SO4	J	309	5/5	0.90	0.36	47,50,56,57	5
4	SO4	E	303	5/5	0.91	0.14	70,76,79,80	5
2	1PE	J	302	16/16	0.91	0.19	63,70,84,85	0
4	SO4	J	306	5/5	0.91	0.16	68,72,80,82	5
4	SO4	A	304	5/5	0.91	0.17	65,71,77,79	5
2	1PE	I	302	10/16	0.91	0.13	75,80,86,89	0
2	1PE	I	301	13/16	0.91	0.29	64,67,78,84	0
5	ACT	D	302	4/4	0.91	0.15	54,55,70,71	0
4	SO4	C	307	5/5	0.92	0.19	73,75,81,83	5
4	SO4	C	303	5/5	0.93	0.16	72,73,74,75	5
2	1PE	G	301	16/16	0.93	0.18	65,73,82,84	0
3	NAP	B	302	48/48	0.94	0.17	53,65,83,85	0
2	1PE	J	303	7/16	0.94	0.17	55,61,66,68	0
3	NAP	I	303	48/48	0.95	0.17	42,51,66,69	0
4	SO4	I	307	5/5	0.95	0.18	78,82,85,87	5
3	NAP	D	303	48/48	0.95	0.15	38,51,57,65	0
3	NAP	E	302	48/48	0.95	0.16	48,58,64,66	0
4	SO4	F	304	5/5	0.95	0.16	77,77,88,92	5
3	NAP	G	303	48/48	0.95	0.15	42,52,57,60	0
4	SO4	D	304	5/5	0.95	0.19	58,61,68,74	5
3	NAP	H	303	48/48	0.95	0.15	45,57,68,71	0
4	SO4	G	304	5/5	0.95	0.11	68,75,80,82	5
3	NAP	J	304	48/48	0.96	0.14	47,57,76,79	0
3	NAP	C	302	48/48	0.96	0.14	43,60,67,68	0
3	NAP	A	303	48/48	0.96	0.16	54,62,74,76	0
3	NAP	F	303	48/48	0.98	0.16	42,47,52,54	0

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 NAP B 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
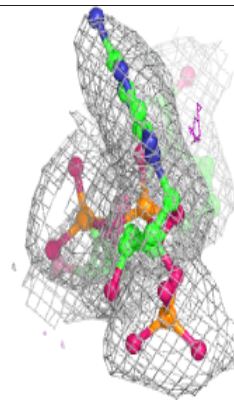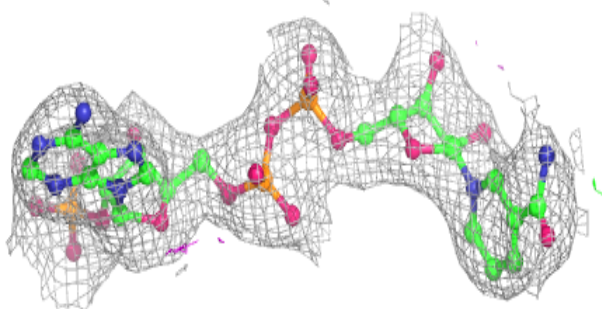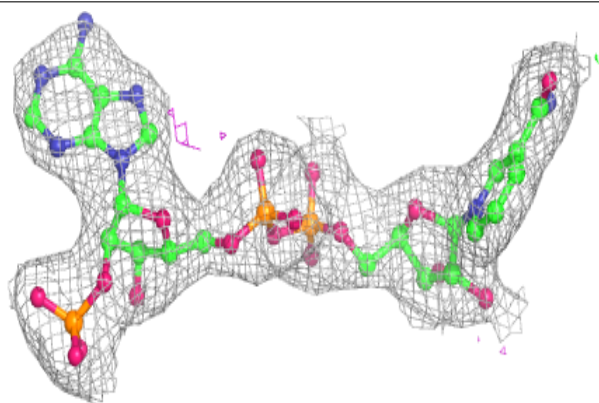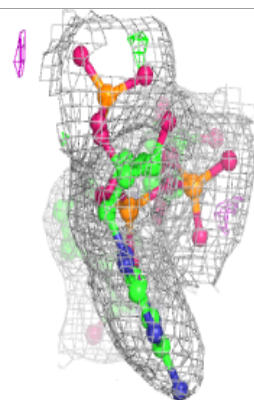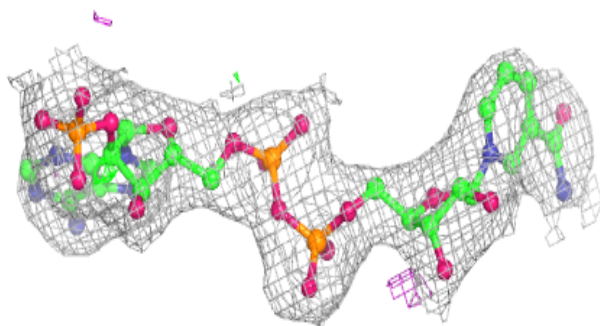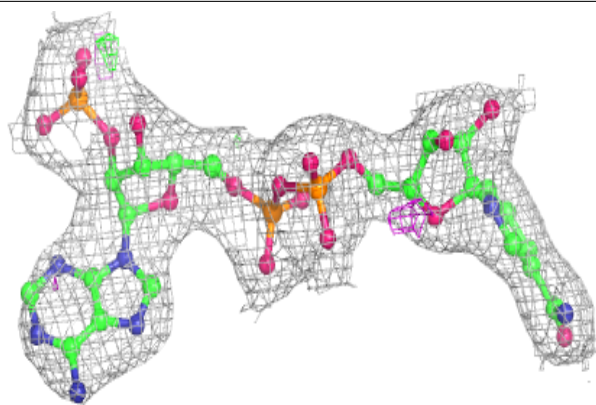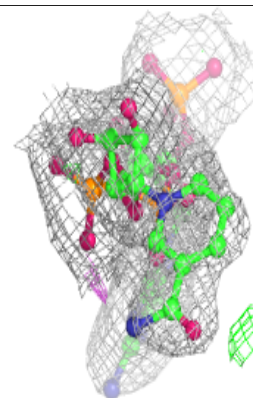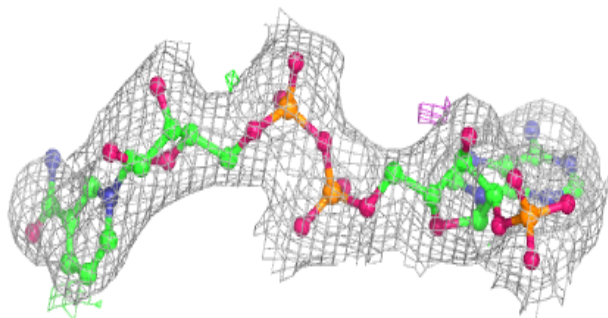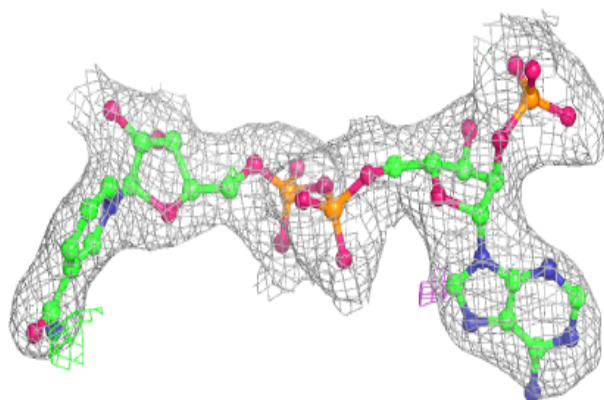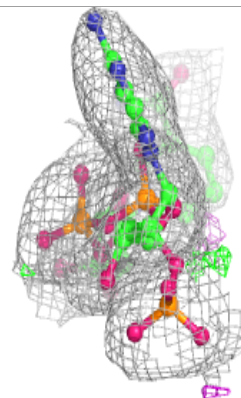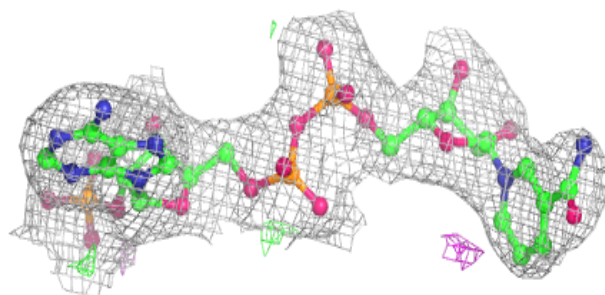mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
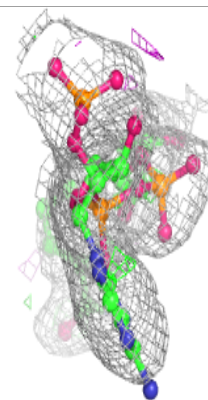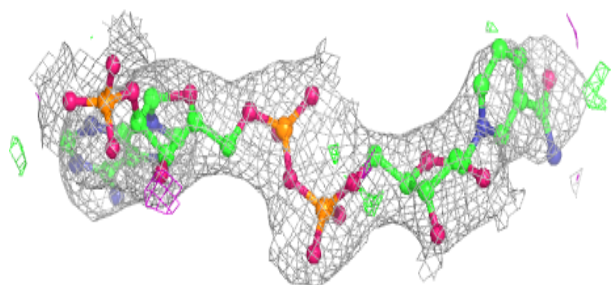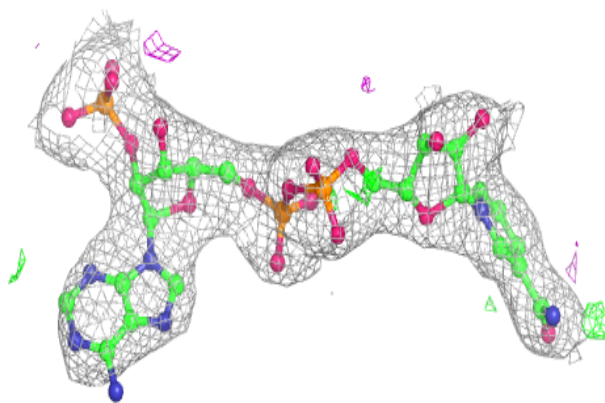
Electron density around NAP I 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
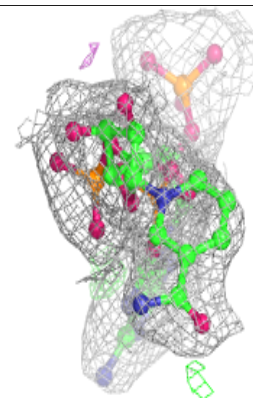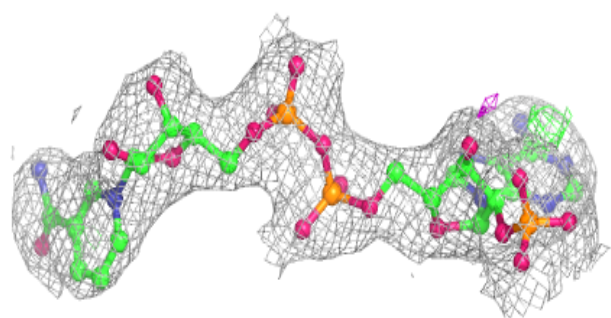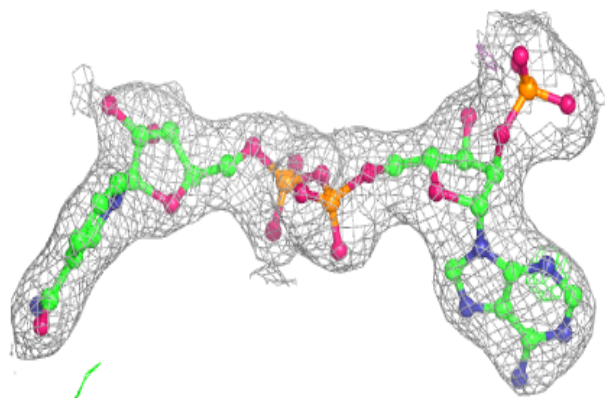
Electron density around NAP D 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
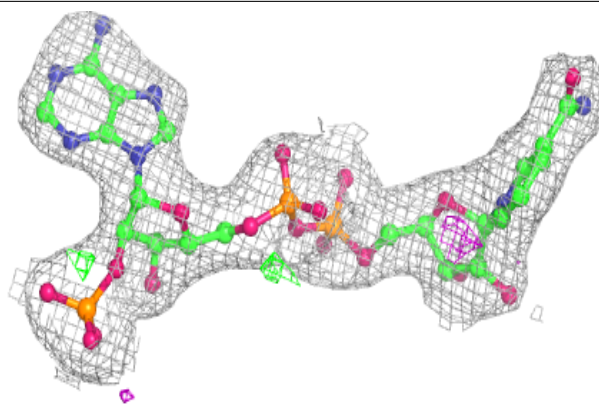and green (positive)
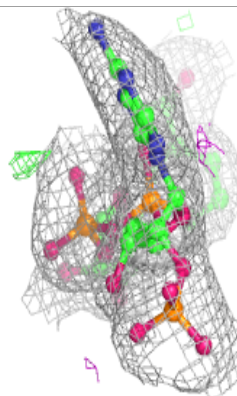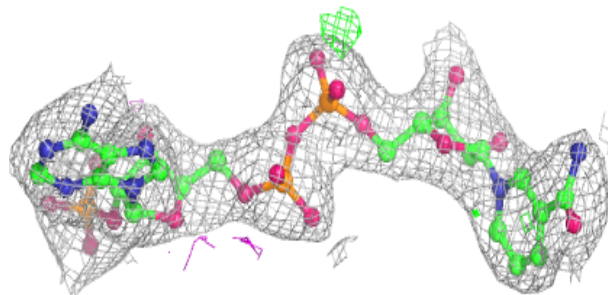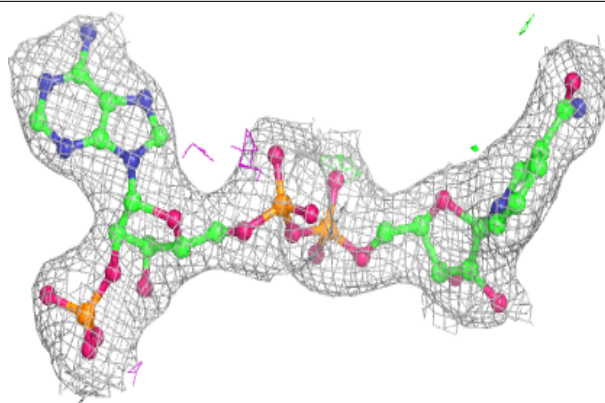
Electron density around NAP E 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
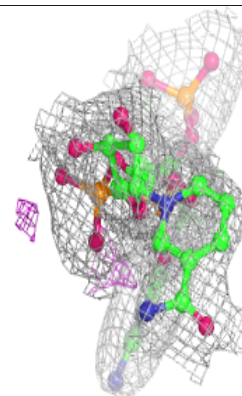and green (positive)
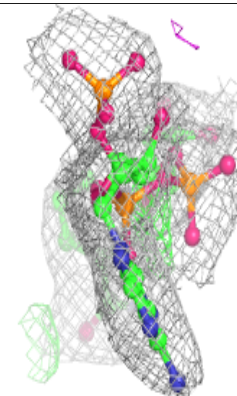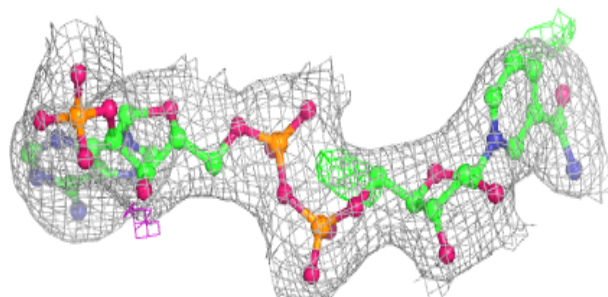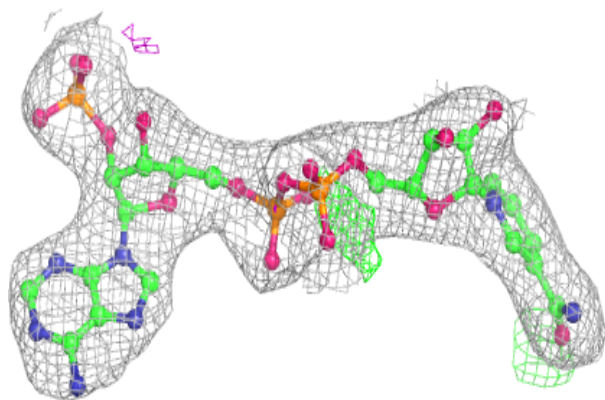
Electron density around NAP G 303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
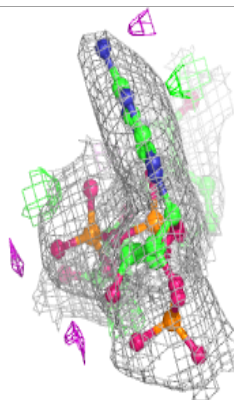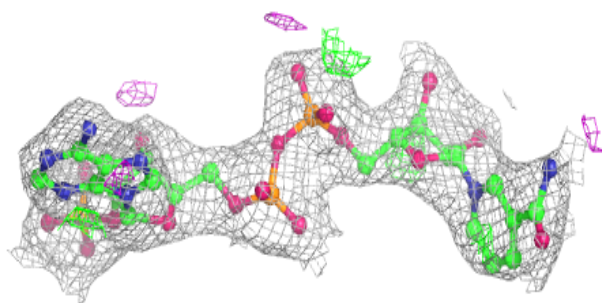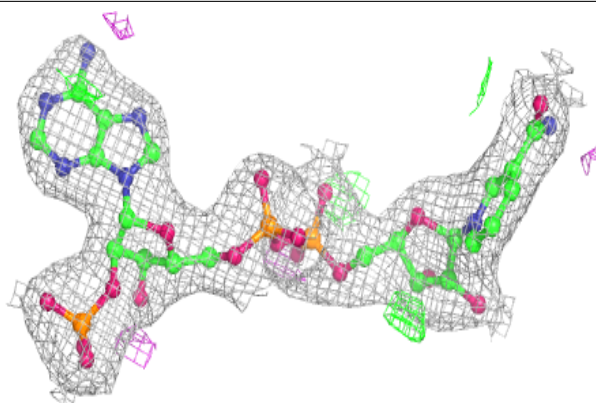
Electron density around NAP H 303:

$2mF_o$-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 J 304:

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 C 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

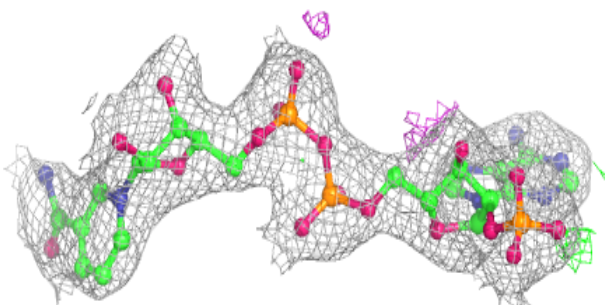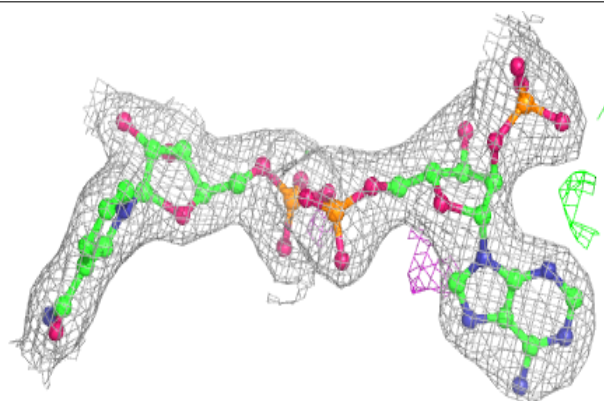**Electron density around NAP A 303:**

$2mF_o$-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 F 303:

$2mF_o$-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.