Full wwPDB X-ray Structure Validation Report (i)

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 Full wwPDB X-ray Structure Validation 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 (i) 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 (i)) were used in the production of this report:

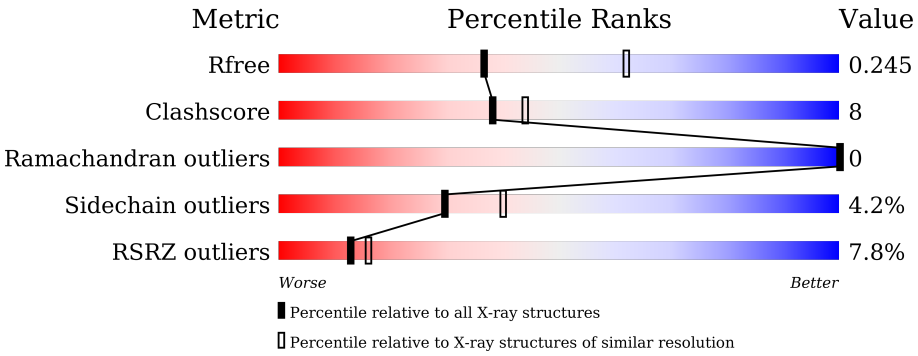
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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	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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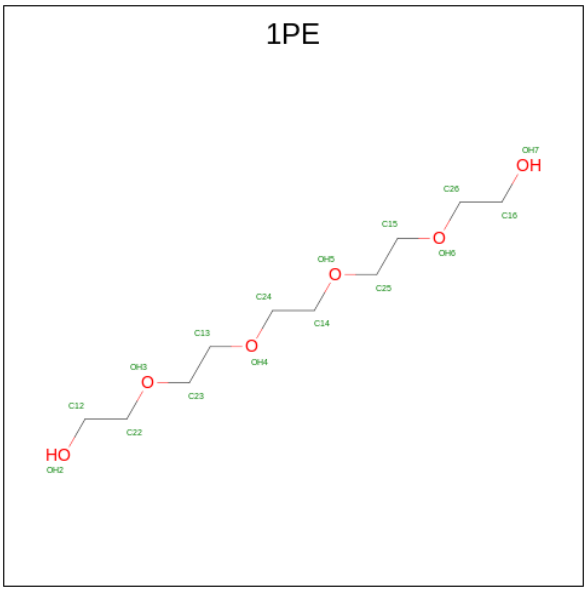
Chain	Residue	Modelled	Actual	Comment	Reference
I	201	HIS	-	expression tag	UNP A0A8I0PU34
I	202	HIS	-	expression tag	UNP A0A8I0PU34
I	203	HIS	-	expression tag	UNP A0A8I0PU34
J	198	HIS	-	expression tag	UNP A0A8I0PU34
J	199	HIS	-	expression tag	UNP A0A8I0PU34
J	200	HIS	-	expression tag	UNP A0A8I0PU34
J	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 10 6 4	0	0
2	A	1	Total C O 13 8 5	0	0
2	B	1	Total C O 16 10 6	0	0
2	C	1	Total C O 16 10 6	0	0
2	D	1	Total C O 16 10 6	0	0
2	E	1	Total C O 16 10 6	0	0
2	F	1	Total C O 10 6 4	0	0

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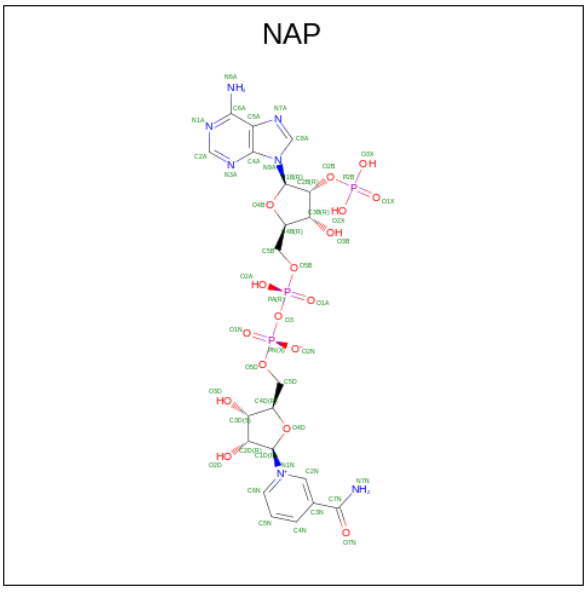
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O 16 10 6	0	0
2	G	1	Total C O 16 10 6	0	0
2	G	1	Total C O 10 6 4	0	0
2	H	1	Total C O 16 10 6	0	0
2	H	1	Total C O 16 10 6	0	0
2	I	1	Total C O 13 8 5	0	0
2	I	1	Total C O 10 6 4	0	0
2	J	1	Total C O 16 10 6	0	0
2	J	1	Total C O 16 10 6	0	0
2	J	1	Total C O 7 4 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 C N O P 48 21 7 17 3	0	0

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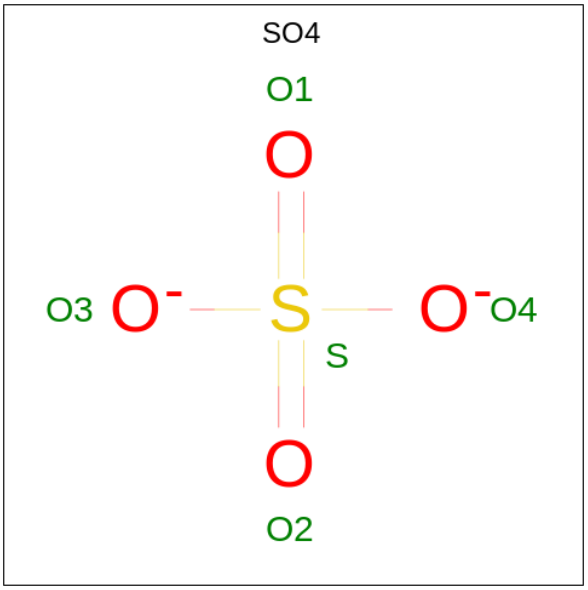
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	H	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 O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0

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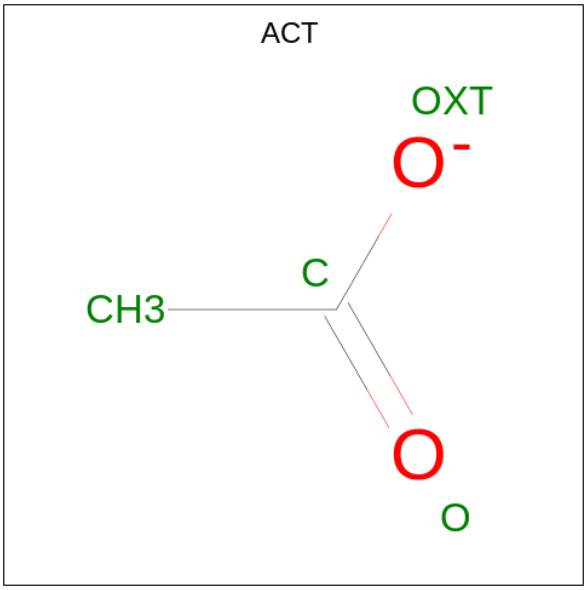
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 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 C O 4 2 2	0	0

- Molecule 6 is water.

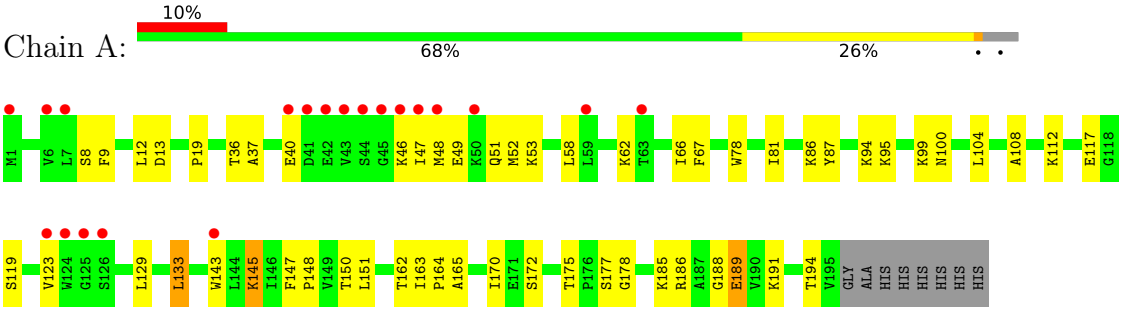
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	18	Total O 18 18	0	0
6	B	23	Total O 23 23	0	0
6	C	45	Total O 45 45	0	0
6	D	54	Total O 54 54	0	0
6	E	41	Total O 41 41	0	0
6	F	60	Total O 60 60	0	0
6	G	52	Total O 52 52	0	0
6	H	23	Total O 23 23	0	0
6	I	59	Total O 59 59	0	0
6	J	38	Total O 38 38	0	0

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.

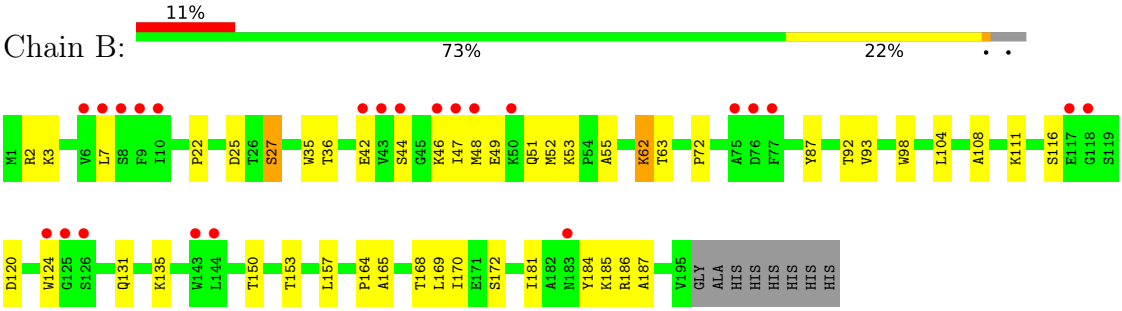
• Molecule 1: Dihydrofolate reductase family protein

Chain A:



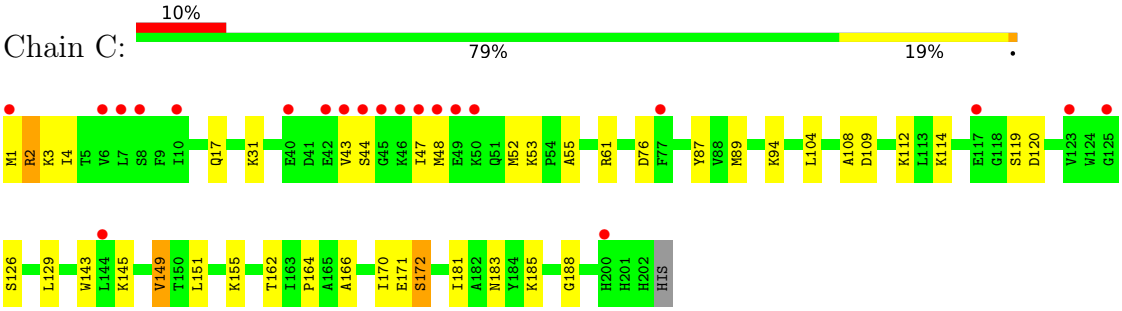
• Molecule 1: Dihydrofolate reductase family protein

Chain B:



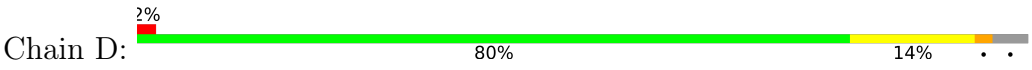
• Molecule 1: Dihydrofolate reductase family protein

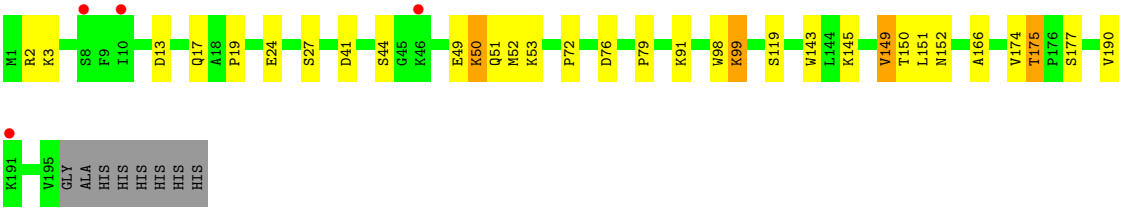
Chain C:



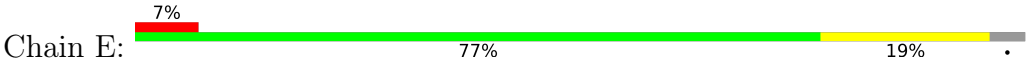
• Molecule 1: Dihydrofolate reductase family protein

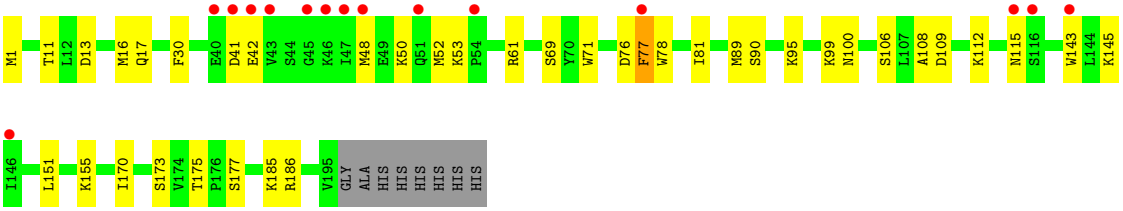
Chain D:



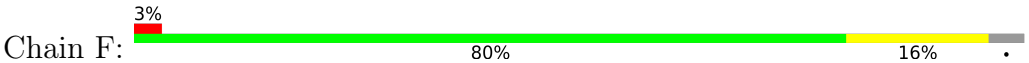


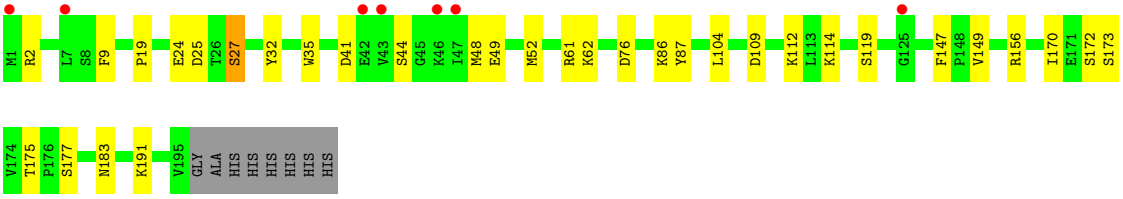
• Molecule 1: Dihydrofolate reductase family protein



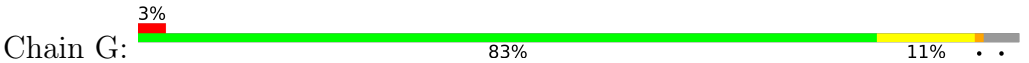


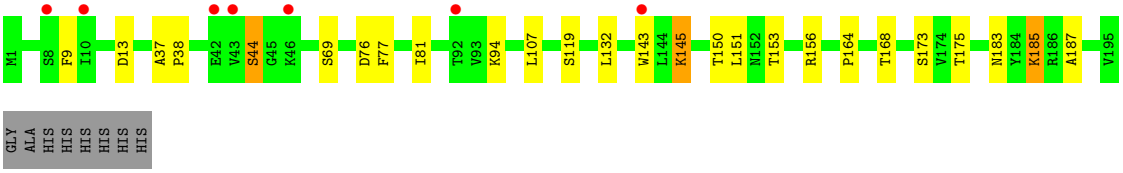
• Molecule 1: Dihydrofolate reductase family protein



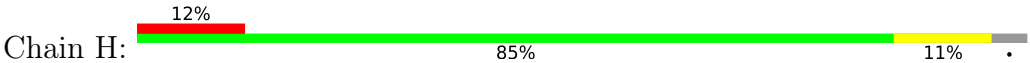


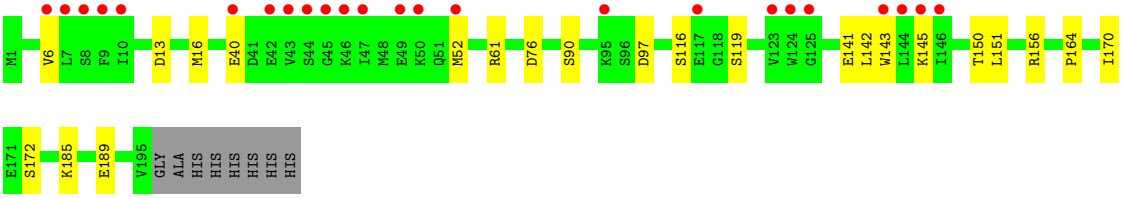
• Molecule 1: Dihydrofolate reductase family protein





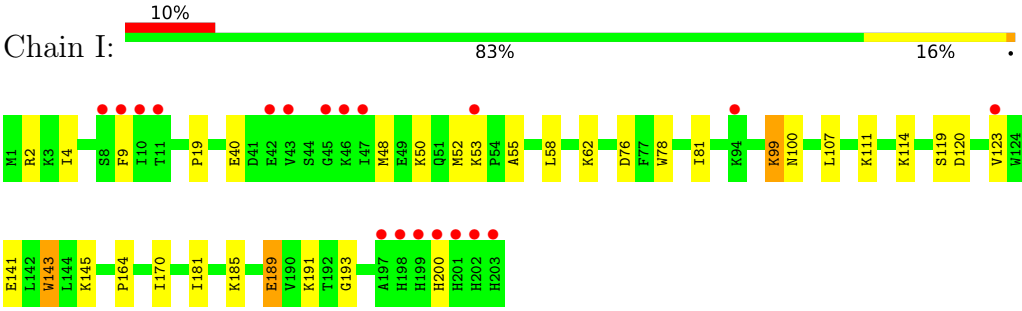
• Molecule 1: Dihydrofolate reductase family protein





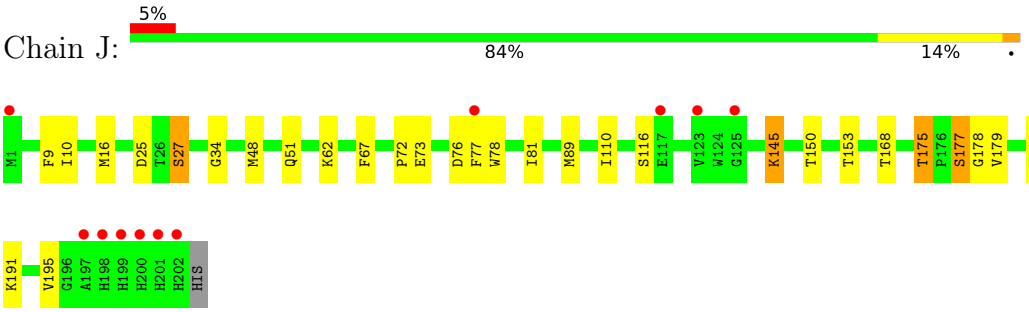
• Molecule 1: Dihydrofolate reductase family protein

Chain I:



• Molecule 1: Dihydrofolate reductase family protein

Chain J:



4 Data and refinement statistics (i)

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.*

[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.

All (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
1:H:170:ILE:HD11	1:H:185:LYS:HB2	1.63	0.81
1:C:48:MET:HE1	1:C:145:LYS:HD2	1.64	0.77
1:C:2:ARG:HD3	1:C:119:SER:O	1.85	0.75
1:A:170:ILE:HD11	1:A:185:LYS:HB2	1.67	0.74
1:E:175:THR:HG22	1:E:177:SER:H	1.52	0.73
1:I:170:ILE:HD11	1:I:185:LYS:HB2	1.72	0.71
2:G:301:1PE:H242	3:G:303:NAP:H5N	1.73	0.71
1:C:170:ILE:HD11	1:C:185:LYS:HB2	1.73	0.70
1:B:48:MET:O	1:B:52:MET:HG3	1.93	0.68
1:I:189:GLU:HG2	1:I:191:LYS:HE3	1.76	0.67
1:A:108:ALA:O	1:A:112:LYS:HG3	1.95	0.66
1:C:149:VAL:HG23	1:D:166:ALA:HA	1.77	0.66
1:D:145:LYS:NZ	6:D:401:HOH:O	2.28	0.66
1:A:62:LYS:O	1:A:66:ILE:HG13	1.95	0.66
1:E:48:MET:O	1:E:52:MET:HG3	1.96	0.65
1:B:62:LYS:HD3	3:B:302:NAP:H51A	1.79	0.64
1:E:11:THR:HG21	1:E:151:LEU:HD12	1.80	0.64
1:B:172:SER:HA	1:B:181:ILE:O	1.98	0.63
1:E:99:LYS:HG3	1:E:100:ASN:OD1	1.98	0.63
1:F:2:ARG:HD3	1:F:119:SER:O	1.98	0.63
1:A:175:THR:HG22	1:A:177:SER:H	1.63	0.62
1:I:189:GLU:CD	1:I:189:GLU:H	2.02	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:186:ARG:NH1	1:J:188:GLY:O	2.27	0.62
1:C:108:ALA:O	1:C:112:LYS:HD3	2.00	0.62
1:I:48:MET:O	1:I:52:MET:HG3	2.00	0.61
1:I:141:GLU:HB3	1:I:143:TRP:HZ3	1.65	0.61
1:G:9:PHE:HE2	1:G:145:LYS:HD2	1.64	0.61
1:A:9:PHE:CE1	1:A:145:LYS:HD3	2.34	0.61
1:A:19:PRO:O	1:A:36:THR:HG22	2.00	0.60
1:F:49:GLU:HA	1:F:52:MET:HG3	1.83	0.60
1:I:48:MET:HG2	2:I:302:1PE:H241	1.84	0.60
1:B:87:TYR:HB3	1:B:104:LEU:HD11	1.84	0.60
1:J:175:THR:HG23	1:J:177:SER:H	1.66	0.60
1:F:9:PHE:HB3	1:F:147:PHE:CE1	2.36	0.60
1:D:99:LYS:HG2	6:D:438:HOH:O	2.01	0.59
1:A:37:ALA:O	1:A:40:GLU:HG2	2.03	0.59
1:G:153:THR:OG1	4:G:308:SO4:O1	2.20	0.58
1:J:51:GLN:HE22	1:J:145:LYS:NZ	2.01	0.58
1:F:104:LEU:HD21	2:F:301:1PE:H252	1.84	0.58
1:B:72:PRO:HG3	1:B:98:TRP:CE2	2.38	0.58
1:C:162:THR:O	1:D:152:ASN:ND2	2.36	0.57
1:A:87:TYR:HB3	1:A:104:LEU:HD11	1.86	0.57
1:E:76:ASP:OD1	1:E:77:PHE:N	2.37	0.57
1:C:31:LYS:NZ	6:C:401:HOH:O	2.37	0.57
2:E:301:1PE:H141	3:E:302:NAP:C5N	2.34	0.57
1:I:141:GLU:HB3	1:I:143:TRP:CZ3	2.40	0.57
1:G:9:PHE:CE2	1:G:145:LYS:HD2	2.40	0.56
1:B:25:ASP:OD1	1:B:27:SER:OG	2.23	0.56
1:F:61:ARG:NE	3:F:303:NAP:O2X	2.35	0.56
1:A:62:LYS:HD2	3:A:303:NAP:H51A	1.88	0.55
1:B:47:ILE:HG22	1:B:51:GLN:NE2	2.21	0.54
1:A:150:THR:O	1:B:164:PRO:HA	2.08	0.54
1:C:44:SER:OG	1:C:145:LYS:NZ	2.40	0.54
1:C:48:MET:O	1:C:52:MET:HG3	2.07	0.54
1:B:47:ILE:HG22	1:B:51:GLN:HE21	1.73	0.54
1:B:170:ILE:HG21	1:B:185:LYS:HE2	1.90	0.54
1:J:48:MET:HE3	1:J:145:LYS:HE2	1.90	0.53
2:E:301:1PE:H141	3:E:302:NAP:H5N	1.89	0.53
1:G:94:LYS:HB2	1:G:94:LYS:NZ	2.24	0.53
1:E:78:TRP:CE2	1:E:81:ILE:HB	2.44	0.53
2:G:301:1PE:OH7	2:G:302:1PE:H142	2.08	0.53
1:I:48:MET:CE	1:I:145:LYS:HZ3	2.22	0.52
1:J:175:THR:HG22	1:J:179:VAL:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:301:1PE:H242	3:G:303:NAP:C5N	2.40	0.52
1:I:99:LYS:HG3	1:I:100:ASN:OD1	2.09	0.52
1:I:2:ARG:HD3	1:I:119:SER:O	2.10	0.52
1:D:91:LYS:NZ	5:D:302:ACT:O	2.42	0.52
1:B:49:GLU:O	1:B:53:LYS:HE3	2.10	0.52
1:E:48:MET:SD	1:E:145:LYS:HE2	2.49	0.51
1:J:153:THR:HG22	6:J:432:HOH:O	2.10	0.51
1:B:108:ALA:HA	1:B:111:LYS:HZ2	1.75	0.51
1:F:48:MET:HA	1:F:48:MET:HE3	1.91	0.51
1:I:111:LYS:HD3	6:I:453:HOH:O	2.10	0.51
1:I:55:ALA:HB1	1:I:120:ASP:O	2.11	0.51
1:I:9:PHE:HE1	1:I:145:LYS:HD3	1.76	0.50
1:B:35:TRP:CZ3	1:B:36:THR:HG22	2.45	0.50
1:B:108:ALA:HA	1:B:111:LYS:NZ	2.26	0.50
1:C:89:MET:HG3	1:C:129:LEU:HD13	1.93	0.50
1:A:129:LEU:O	1:A:133:LEU:HD12	2.12	0.50
1:B:63:THR:OG1	3:B:302:NAP:O2A	2.23	0.50
1:D:41:ASP:OD1	1:D:177:SER:OG	2.29	0.50
1:E:17:GLN:HB2	1:E:155:LYS:HB2	1.94	0.50
1:F:175:THR:HG22	1:F:177:SER:H	1.77	0.50
1:J:78:TRP:CD2	1:J:81:ILE:HB	2.47	0.50
1:J:25:ASP:OD1	1:J:27:SER:OG	2.24	0.50
2:J:302:1PE:H142	3:J:304:NAP:H4N	1.93	0.50
1:E:17:GLN:HG2	1:E:30:PHE:CD2	2.47	0.50
1:G:13:ASP:OD2	1:G:151:LEU:O	2.30	0.50
1:C:151:LEU:HD21	1:D:190:VAL:HG11	1.93	0.49
1:B:2:ARG:NH2	1:B:116:SER:OG	2.40	0.49
1:C:43:VAL:O	1:C:47:ILE:HG22	2.12	0.49
1:H:141:GLU:HG2	1:H:143:TRP:HE1	1.76	0.49
1:B:168:THR:OG1	1:B:187:ALA:HB2	2.13	0.49
1:B:153:THR:HG22	6:B:421:HOH:O	2.11	0.49
1:A:67:PHE:HE1	2:A:302:1PE:H131	1.77	0.49
1:J:72:PRO:HG2	1:J:73:GLU:OE1	2.12	0.49
1:J:9:PHE:CE1	1:J:145:LYS:HD3	2.48	0.49
1:F:61:ARG:HE	3:F:303:NAP:P2B	2.36	0.48
1:A:12:LEU:HD23	1:A:147:PHE:O	2.13	0.48
1:I:9:PHE:CE1	1:I:145:LYS:HD3	2.48	0.48
1:I:53:LYS:HD2	1:I:53:LYS:HA	1.56	0.48
1:F:41:ASP:H	1:F:44:SER:HG	1.61	0.48
1:B:165:ALA:HB1	1:B:186:ARG:CZ	2.44	0.48
1:E:106:SER:OG	1:E:109:ASP:OD1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:150:THR:O	1:H:164:PRO:HA	2.14	0.48
1:B:48:MET:O	1:B:51:GLN:N	2.47	0.48
1:I:50:LYS:HD2	1:I:50:LYS:N	2.28	0.47
1:D:53:LYS:HE2	1:D:53:LYS:HA	1.95	0.47
1:I:62:LYS:HD2	3:I:303:NAP:H51A	1.96	0.47
1:B:92:THR:HB	3:B:302:NAP:O1X	2.13	0.47
1:J:48:MET:CE	1:J:145:LYS:HE2	2.44	0.47
1:A:47:ILE:HG22	1:A:51:GLN:HE21	1.78	0.47
1:D:51:GLN:HG2	1:D:143:TRP:CZ3	2.50	0.47
1:E:175:THR:HG22	1:E:177:SER:N	2.24	0.47
1:G:168:THR:HG23	1:G:187:ALA:CB	2.45	0.47
1:C:171:GLU:HG2	1:C:172:SER:N	2.28	0.47
1:G:164:PRO:HA	1:H:150:THR:O	2.15	0.47
1:C:61:ARG:HE	3:C:302:NAP:P2B	2.38	0.47
1:D:174:VAL:HG22	1:D:175:THR:H	1.80	0.47
1:B:111:LYS:HZ2	1:B:111:LYS:HB2	1.79	0.47
1:F:32:TYR:O	1:F:35:TRP:HD1	1.98	0.47
1:C:145:LYS:HB3	1:C:145:LYS:HE3	1.67	0.46
1:F:191:LYS:HD2	1:F:191:LYS:HA	1.69	0.46
1:A:86:LYS:HE2	1:A:100:ASN:O	2.15	0.46
1:A:164:PRO:HA	1:B:150:THR:O	2.14	0.46
1:D:49:GLU:HA	1:D:52:MET:HE2	1.97	0.46
1:F:9:PHE:HB3	1:F:147:PHE:HE1	1.80	0.46
1:G:77:PHE:N	4:G:307:SO4:O3	2.42	0.46
1:A:48:MET:O	1:A:52:MET:HG3	2.16	0.46
1:I:40:GLU:HB3	2:I:302:1PE:C15	2.36	0.46
1:G:37:ALA:HB3	1:G:38:PRO:HD3	1.98	0.46
1:B:169:LEU:HD11	1:B:172:SER:HB3	1.98	0.46
1:E:41:ASP:OD2	1:E:42:GLU:N	2.47	0.46
1:C:87:TYR:HB3	1:C:104:LEU:HD11	1.98	0.46
1:F:175:THR:HG22	1:F:177:SER:N	2.30	0.46
1:G:44:SER:CB	2:G:302:1PE:H121	2.33	0.46
1:A:163:ILE:O	1:B:150:THR:HG23	2.16	0.45
1:G:185:LYS:HE2	1:G:185:LYS:HB3	1.36	0.45
1:A:78:TRP:O	1:A:81:ILE:HG22	2.16	0.45
1:B:44:SER:O	1:B:48:MET:HG2	2.16	0.45
1:D:50:LYS:HE2	1:D:50:LYS:HB2	1.73	0.45
1:C:143:TRP:CZ3	1:C:183:ASN:HB2	2.52	0.45
1:E:13:ASP:OD2	1:E:151:LEU:O	2.35	0.45
2:E:301:1PE:H142	2:E:301:1PE:H152	1.62	0.45
1:F:104:LEU:HD21	2:F:301:1PE:C25	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:302:1PE:H251	1:J:195:VAL:HG11	1.97	0.45
1:F:2:ARG:HG3	1:F:114:LYS:O	2.17	0.45
2:C:301:1PE:H142	3:C:302:NAP:H4N	1.98	0.45
1:A:186:ARG:NH2	1:A:188:GLY:O	2.39	0.44
1:A:99:LYS:HA	1:A:99:LYS:HD2	1.55	0.44
1:A:194:THR:HG22	1:B:22:PRO:CD	2.48	0.44
1:A:58:LEU:HB3	1:A:123:VAL:HG22	1.99	0.44
1:H:6:VAL:HB	1:H:142:LEU:HD23	2.00	0.44
1:E:61:ARG:HB2	1:E:90:SER:HB2	1.98	0.44
1:F:112:LYS:HG2	2:F:301:1PE:H151	2.00	0.44
1:F:25:ASP:OD1	1:F:27:SER:HB3	2.17	0.44
1:B:55:ALA:HB1	1:B:120:ASP:O	2.18	0.44
1:E:1:MET:SD	1:E:115:ASN:ND2	2.91	0.44
1:J:76:ASP:HB2	4:J:308:SO4:O2	2.18	0.44
1:J:185:LYS:HB3	1:J:185:LYS:HE2	1.86	0.44
1:J:191:LYS:HA	1:J:191:LYS:HD2	1.88	0.44
1:B:7:LEU:HD22	1:B:124:TRP:CZ2	2.53	0.43
1:C:143:TRP:CE3	1:C:183:ASN:HB2	2.53	0.43
1:H:61:ARG:HB2	1:H:90:SER:HB2	2.00	0.43
1:C:143:TRP:HZ3	1:C:181:ILE:HG22	1.83	0.43
1:A:148:PRO:HD3	1:A:178:GLY:O	2.19	0.43
1:D:13:ASP:OD2	1:D:151:LEU:O	2.35	0.43
1:F:170:ILE:HD11	1:F:183:ASN:ND2	2.33	0.43
1:G:13:ASP:OD1	1:G:150:THR:HA	2.18	0.43
1:A:46:LYS:HD2	1:A:46:LYS:HA	1.90	0.43
1:B:53:LYS:HD3	1:B:53:LYS:HA	1.69	0.43
1:C:4:ILE:HD11	1:C:114:LYS:HG3	2.01	0.43
1:D:17:GLN:HE22	1:D:27:SER:HB2	1.84	0.43
1:G:107:LEU:N	4:G:306:SO4:O2	2.39	0.43
1:I:4:ILE:CD1	1:I:114:LYS:HD2	2.48	0.43
1:I:58:LEU:HB3	1:I:123:VAL:HG22	2.01	0.43
1:I:193:GLY:O	1:J:34:GLY:HA3	2.19	0.43
1:B:35:TRP:CE3	1:B:36:THR:HG22	2.54	0.42
1:G:168:THR:HG23	1:G:187:ALA:HB2	2.01	0.42
1:A:51:GLN:HG2	1:A:143:TRP:CZ3	2.54	0.42
1:C:104:LEU:HB3	1:C:109:ASP:HB3	2.00	0.42
2:C:301:1PE:H231	2:C:301:1PE:H242	1.87	0.42
1:D:2:ARG:HD3	1:D:119:SER:O	2.19	0.42
1:B:169:LEU:HA	1:B:184:TYR:HD1	1.84	0.42
1:C:55:ALA:HB1	1:C:120:ASP:O	2.19	0.42
1:C:166:ALA:HA	1:D:149:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:16:MET:HG2	3:H:303:NAP:N7N	2.35	0.42
1:I:19:PRO:HG2	2:I:301:1PE:H141	2.01	0.42
1:J:51:GLN:HE22	1:J:145:LYS:CE	2.32	0.42
1:G:132:LEU:HD22	3:G:303:NAP:N6A	2.34	0.42
1:B:3:LYS:HB3	1:B:120:ASP:CG	2.40	0.42
1:I:145:LYS:HE3	1:I:145:LYS:HB3	1.73	0.42
1:J:10:ILE:HG22	1:J:16:MET:HB3	2.00	0.42
1:B:72:PRO:HG3	1:B:98:TRP:NE1	2.35	0.42
1:C:94:LYS:HD2	1:C:94:LYS:HA	1.83	0.42
1:A:49:GLU:HA	1:A:52:MET:HE2	2.02	0.42
1:A:53:LYS:HD2	1:A:53:LYS:N	2.35	0.42
1:A:194:THR:HG22	1:B:22:PRO:HD3	2.01	0.42
1:B:2:ARG:HH21	1:B:116:SER:HG	1.64	0.42
1:E:50:LYS:HB2	1:E:50:LYS:HE2	1.67	0.42
1:C:188:GLY:N	6:C:406:HOH:O	2.51	0.42
1:E:78:TRP:CD2	1:E:81:ILE:HB	2.55	0.42
1:F:62:LYS:NZ	6:F:406:HOH:O	2.47	0.42
1:J:175:THR:HG22	1:J:178:GLY:N	2.35	0.41
1:A:13:ASP:OD2	1:A:151:LEU:O	2.37	0.41
1:C:164:PRO:HA	1:D:150:THR:O	2.20	0.41
1:F:87:TYR:OH	2:F:301:1PE:H161	2.21	0.41
1:I:78:TRP:O	1:I:81:ILE:HG22	2.21	0.41
1:I:145:LYS:HG2	1:I:181:ILE:HD13	2.03	0.41
1:G:143:TRP:HA	1:G:183:ASN:ND2	2.34	0.41
1:I:48:MET:HE3	1:I:48:MET:HB2	1.82	0.41
2:I:301:1PE:OH3	2:I:302:1PE:H242	2.19	0.41
1:B:42:GLU:HG2	1:B:46:LYS:HE2	2.03	0.41
1:C:17:GLN:HB2	1:C:155:LYS:HB2	2.01	0.41
1:F:76:ASP:HB2	4:F:304:SO4:S	2.59	0.41
1:G:76:ASP:HB2	4:G:307:SO4:O3	2.20	0.41
1:I:164:PRO:HA	1:J:150:THR:O	2.19	0.41
2:J:301:1PE:H241	2:J:301:1PE:H231	1.83	0.41
1:B:92:THR:HG22	1:B:93:VAL:HG23	2.01	0.41
1:D:19:PRO:HD2	1:D:24:GLU:OE2	2.21	0.41
1:D:76:ASP:HB2	4:D:304:SO4:O3	2.21	0.41
1:F:19:PRO:HD2	1:F:24:GLU:OE2	2.21	0.41
1:A:175:THR:HG22	1:A:177:SER:N	2.30	0.41
1:H:156:ARG:HH11	1:H:156:ARG:HG2	1.85	0.41
1:J:67:PHE:HE1	2:J:302:1PE:H131	1.85	0.41
1:D:41:ASP:HB2	1:D:44:SER:H	1.84	0.41
1:E:71:TRP:CZ2	2:E:301:1PE:H221	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:303:NAP:H2D	3:G:303:NAP:H6N	1.79	0.41
1:A:51:GLN:OE1	1:A:143:TRP:HE3	2.04	0.41
1:B:131:GLN:NE2	1:B:157:LEU:O	2.44	0.41
1:A:189:GLU:HG2	1:A:191:LYS:HE2	2.02	0.40
1:B:135:LYS:HB2	1:B:135:LYS:HE2	1.82	0.40
1:J:89:MET:HG3	1:J:110:ILE:HD11	2.03	0.40
1:D:72:PRO:HG3	1:D:98:TRP:CD1	2.56	0.40
1:A:165:ALA:HB1	1:A:186:ARG:CZ	2.51	0.40
1:I:107:LEU:HD23	6:I:454:HOH:O	2.21	0.40
1:G:81:ILE:HD12	1:G:81:ILE:HA	1.85	0.40
1:H:13:ASP:OD2	1:H:151:LEU:O	2.40	0.40
1:E:53:LYS:HA	1:E:53:LYS:HD2	1.89	0.40
1:E:108:ALA:O	1:E:112:LYS:HG3	2.21	0.40

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	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1954/2030 (96%)	1897 (97%)	57 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	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

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	94	LYS
1	A	95	LYS
1	A	117	GLU
1	A	119	SER
1	A	133	LEU
1	A	145	LYS
1	A	162	THR
1	A	172	SER

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Mol	Chain	Res	Type
1	A	189	GLU
1	B	27	SER
1	B	62	LYS
1	C	1	MET
1	C	2	ARG
1	C	3	LYS
1	C	53	LYS
1	C	76	ASP
1	C	126	SER
1	C	149	VAL
1	C	172	SER
1	D	3	LYS
1	D	50	LYS
1	D	79	PRO
1	D	99	LYS
1	D	149	VAL
1	D	175	THR
1	E	16	MET
1	E	69	SER
1	E	77	PHE
1	E	89	MET
1	E	95	LYS
1	E	143	TRP
1	E	173	SER
1	E	186	ARG
1	F	27	SER
1	F	86	LYS
1	F	149	VAL
1	F	156	ARG
1	F	172	SER
1	F	173	SER
1	G	44	SER
1	G	69	SER
1	G	119	SER
1	G	145	LYS
1	G	156	ARG
1	G	173	SER
1	G	175	THR
1	G	185	LYS
1	H	40	GLU
1	H	52	MET
1	H	76	ASP

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Mol	Chain	Res	Type
1	H	97	ASP
1	H	116	SER
1	H	119	SER
1	H	145	LYS
1	H	172	SER
1	H	189	GLU
1	I	76	ASP
1	I	99	LYS
1	I	135	LYS
1	I	143	TRP
1	I	189	GLU
1	I	200	HIS
1	J	27	SER
1	J	77	PHE
1	J	116	SER
1	J	145	LYS
1	J	168	THR
1	J	175	THR
1	J	177	SER

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 (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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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%)
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

All (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
3	A	303	NAP	C2D-C1D	-15.19	1.30	1.53
3	E	302	NAP	O4B-C1B	15.05	1.62	1.41
3	B	302	NAP	O4D-C1D	15.02	1.62	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	303	NAP	O4B-C1B	15.00	1.62	1.41
3	F	303	NAP	O4D-C1D	14.98	1.62	1.41
3	A	303	NAP	O4B-C1B	14.97	1.62	1.41
3	G	303	NAP	C2D-C1D	-14.96	1.31	1.53
3	I	303	NAP	C2D-C1D	-14.91	1.31	1.53
3	J	304	NAP	C2D-C1D	-14.87	1.31	1.53
3	J	304	NAP	O4B-C1B	14.84	1.61	1.41
3	J	304	NAP	O4D-C1D	14.77	1.61	1.41
3	B	302	NAP	C2D-C1D	-14.75	1.31	1.53
3	H	303	NAP	O4D-C1D	14.70	1.61	1.41
3	D	303	NAP	C2D-C1D	-14.70	1.31	1.53
3	B	302	NAP	O4B-C1B	14.59	1.61	1.41
3	H	303	NAP	O4B-C1B	14.56	1.61	1.41
3	I	303	NAP	O4D-C1D	14.51	1.61	1.41
3	F	303	NAP	C2D-C1D	-14.51	1.31	1.53
3	H	303	NAP	C2D-C1D	-14.45	1.31	1.53
3	A	303	NAP	O4D-C1D	14.34	1.61	1.41
3	F	303	NAP	O4B-C1B	14.33	1.61	1.41
3	E	302	NAP	O4D-C1D	14.18	1.60	1.41
3	G	303	NAP	O4D-C1D	13.96	1.60	1.41
3	C	302	NAP	O4D-C1D	13.76	1.60	1.41
3	D	303	NAP	O4D-C1D	13.34	1.59	1.41
3	G	303	NAP	C7N-N7N	7.06	1.46	1.33
3	E	302	NAP	O4D-C4D	-6.97	1.29	1.45
3	B	302	NAP	C7N-N7N	6.96	1.46	1.33
3	H	303	NAP	C7N-N7N	6.88	1.46	1.33
3	C	302	NAP	C7N-N7N	6.84	1.46	1.33
3	F	303	NAP	C7N-N7N	6.73	1.45	1.33
3	A	303	NAP	O4D-C4D	-6.72	1.30	1.45
3	D	303	NAP	C7N-N7N	6.70	1.45	1.33
3	J	304	NAP	C7N-N7N	6.68	1.45	1.33
3	E	302	NAP	C7N-N7N	6.64	1.45	1.33
3	A	303	NAP	C7N-N7N	6.59	1.45	1.33
3	A	303	NAP	O4B-C4B	-6.31	1.30	1.45
3	D	303	NAP	O4D-C4D	-6.26	1.31	1.45
3	I	303	NAP	O4D-C4D	-6.25	1.31	1.45
3	F	303	NAP	O4D-C4D	-6.25	1.31	1.45
3	F	303	NAP	O4B-C4B	-6.22	1.31	1.45
3	C	302	NAP	O4D-C4D	-6.15	1.31	1.45
3	I	303	NAP	C7N-N7N	6.08	1.44	1.33
3	G	303	NAP	O4B-C4B	-6.05	1.31	1.45
3	B	302	NAP	O4D-C4D	-6.03	1.31	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	303	NAP	O4B-C4B	-6.01	1.31	1.45
3	J	304	NAP	O4B-C4B	-5.95	1.31	1.45
3	D	303	NAP	O4B-C4B	-5.92	1.31	1.45
3	E	302	NAP	O4B-C4B	-5.91	1.31	1.45
3	J	304	NAP	O4D-C4D	-5.90	1.31	1.45
3	H	303	NAP	O4B-C4B	-5.77	1.32	1.45
3	C	302	NAP	O4B-C4B	-5.68	1.32	1.45
3	B	302	NAP	O4B-C4B	-5.61	1.32	1.45
3	G	303	NAP	O4D-C4D	-5.49	1.32	1.45
3	H	303	NAP	O4D-C4D	-4.97	1.33	1.45
3	I	303	NAP	P2B-O2B	3.97	1.66	1.59
3	C	302	NAP	P2B-O2B	3.76	1.66	1.59
3	F	303	NAP	P2B-O2B	3.54	1.66	1.59
3	E	302	NAP	P2B-O2B	3.45	1.65	1.59
3	H	303	NAP	P2B-O2B	3.41	1.65	1.59
3	J	304	NAP	P2B-O2B	3.39	1.65	1.59
3	A	303	NAP	P2B-O2B	3.38	1.65	1.59
5	D	302	ACT	CH3-C	3.30	1.63	1.49
3	B	302	NAP	P2B-O2B	3.23	1.65	1.59
3	D	303	NAP	C6A-N6A	3.21	1.45	1.34
3	A	303	NAP	O2D-C2D	3.20	1.50	1.43
3	B	302	NAP	C6A-N6A	3.19	1.45	1.34
3	G	303	NAP	O3B-C3B	-3.14	1.35	1.43
3	I	303	NAP	O3D-C3D	-3.13	1.35	1.43
3	J	304	NAP	C6A-N6A	3.11	1.45	1.34
3	G	303	NAP	C6A-N6A	3.11	1.45	1.34
3	C	302	NAP	O2D-C2D	3.10	1.50	1.43
3	F	303	NAP	O2D-C2D	3.07	1.50	1.43
3	H	303	NAP	C6A-N6A	3.06	1.45	1.34
3	G	303	NAP	P2B-O2B	3.05	1.65	1.59
3	J	304	NAP	O2D-C2D	3.04	1.50	1.43
3	J	304	NAP	O3B-C3B	-3.04	1.35	1.43
3	D	303	NAP	O2D-C2D	3.03	1.50	1.43
3	C	302	NAP	C6A-N6A	3.01	1.45	1.34
3	I	303	NAP	C6A-N6A	3.01	1.45	1.34
3	E	302	NAP	C6A-N6A	2.99	1.44	1.34
3	G	303	NAP	O2D-C2D	2.98	1.50	1.43
3	C	302	NAP	O3D-C3D	-2.96	1.36	1.43
3	C	302	NAP	C3N-C7N	2.95	1.55	1.50
3	C	302	NAP	O7N-C7N	-2.93	1.18	1.24
3	C	302	NAP	O3B-C3B	-2.93	1.36	1.43
3	A	303	NAP	C6A-N6A	2.92	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	303	NAP	O2D-C2D	2.92	1.49	1.43
3	F	303	NAP	O3B-C3B	-2.92	1.36	1.43
3	E	302	NAP	C3N-C7N	2.90	1.54	1.50
3	D	303	NAP	O7N-C7N	-2.87	1.18	1.24
3	I	303	NAP	O2D-C2D	2.85	1.49	1.43
3	J	304	NAP	O3D-C3D	-2.84	1.36	1.43
3	B	302	NAP	O3B-C3B	-2.82	1.36	1.43
3	H	303	NAP	O3B-C3B	-2.81	1.36	1.43
3	B	302	NAP	O2D-C2D	2.81	1.49	1.43
3	E	302	NAP	O2D-C2D	2.78	1.49	1.43
3	A	303	NAP	O7N-C7N	-2.77	1.18	1.24
3	J	304	NAP	O7N-C7N	-2.73	1.18	1.24
3	E	302	NAP	O3B-C3B	-2.69	1.36	1.43
3	B	302	NAP	O3D-C3D	-2.69	1.36	1.43
3	F	303	NAP	C5A-C4A	-2.69	1.33	1.40
3	D	303	NAP	P2B-O2B	2.68	1.64	1.59
3	H	303	NAP	O3D-C3D	-2.67	1.36	1.43
3	A	303	NAP	O3D-C3D	-2.66	1.36	1.43
3	F	303	NAP	C6A-N6A	2.65	1.43	1.34
3	A	303	NAP	O3B-C3B	-2.61	1.36	1.43
3	F	303	NAP	C2A-N3A	2.57	1.36	1.32
3	D	303	NAP	O3B-C3B	-2.55	1.37	1.43
3	B	302	NAP	C2A-N3A	2.54	1.36	1.32
3	I	303	NAP	O3B-C3B	-2.51	1.37	1.43
3	D	303	NAP	C3N-C7N	2.50	1.54	1.50
3	D	303	NAP	C5A-C4A	-2.50	1.34	1.40
3	J	304	NAP	C2A-N3A	2.49	1.36	1.32
3	E	302	NAP	C5A-C4A	-2.48	1.34	1.40
3	C	302	NAP	C5A-C4A	-2.47	1.34	1.40
3	B	302	NAP	C5A-C4A	-2.47	1.34	1.40
2	D	301	1PE	C22-C12	2.46	1.62	1.49
3	E	302	NAP	O3D-C3D	-2.46	1.37	1.43
3	H	303	NAP	C5A-C4A	-2.45	1.34	1.40
3	G	303	NAP	C5A-C4A	-2.41	1.34	1.40
3	A	303	NAP	C5A-C4A	-2.36	1.34	1.40
3	A	303	NAP	C2A-N3A	2.35	1.35	1.32
3	I	303	NAP	O7N-C7N	-2.31	1.19	1.24
3	D	303	NAP	O3D-C3D	-2.31	1.37	1.43
3	I	303	NAP	C2A-N3A	2.31	1.35	1.32
3	F	303	NAP	O7N-C7N	-2.30	1.19	1.24
3	C	302	NAP	C2A-N3A	2.28	1.35	1.32
3	H	303	NAP	C2A-N3A	2.27	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	302	NAP	O7N-C7N	-2.26	1.19	1.24
2	D	301	1PE	C23-C13	2.24	1.60	1.49
3	I	303	NAP	C5A-C4A	-2.23	1.35	1.40
3	J	304	NAP	C5A-C4A	-2.22	1.35	1.40
3	B	302	NAP	C3N-C7N	2.20	1.53	1.50
3	B	302	NAP	O7N-C7N	-2.17	1.20	1.24
3	G	303	NAP	C4N-C3N	-2.12	1.35	1.39
2	D	301	1PE	C25-C15	2.11	1.59	1.49
3	F	303	NAP	O3D-C3D	-2.10	1.38	1.43
3	I	303	NAP	C3N-C7N	2.09	1.53	1.50
3	G	303	NAP	C2A-N3A	2.05	1.35	1.32
2	H	301	1PE	C25-C15	2.05	1.59	1.49
3	F	303	NAP	C3N-C7N	2.01	1.53	1.50

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
3	B	302	NAP	N3A-C2A-N1A	-5.48	120.12	128.68
3	I	303	NAP	N3A-C2A-N1A	-5.45	120.16	128.68
3	F	303	NAP	N3A-C2A-N1A	-5.43	120.19	128.68
3	D	303	NAP	N3A-C2A-N1A	-5.02	120.83	128.68
3	G	303	NAP	N3A-C2A-N1A	-5.02	120.83	128.68
3	H	303	NAP	C5D-C4D-C3D	-3.78	101.02	115.18
3	C	302	NAP	O7N-C7N-N7N	-3.36	117.81	122.58
3	F	303	NAP	O4D-C1D-C2D	-3.32	102.07	106.93
3	E	302	NAP	O4D-C1D-C2D	-3.09	102.41	106.93
3	H	303	NAP	O4D-C1D-C2D	-3.07	102.44	106.93
3	H	303	NAP	PN-O3-PA	-3.03	122.42	132.83
3	F	303	NAP	O4B-C1B-C2B	-2.66	101.97	106.59
3	A	303	NAP	C6N-N1N-C2N	-2.66	119.55	121.97
3	F	303	NAP	O7N-C7N-N7N	-2.60	118.88	122.58
3	I	303	NAP	O4D-C1D-C2D	-2.57	103.18	106.93
3	H	303	NAP	C6N-N1N-C2N	-2.54	119.66	121.97
3	D	303	NAP	O7N-C7N-N7N	-2.54	118.97	122.58
3	H	303	NAP	O2N-PN-O5D	2.51	119.40	107.75
3	C	302	NAP	C4A-C5A-N7A	-2.47	106.83	109.40
3	C	302	NAP	C3N-C7N-N7N	2.46	120.70	117.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	303	NAP	C2N-C3N-C4N	2.43	121.01	118.26
3	D	303	NAP	C1B-N9A-C4A	-2.38	122.45	126.64
3	C	302	NAP	C1B-N9A-C4A	-2.37	122.47	126.64
3	J	304	NAP	C2B-C3B-C4B	-2.36	96.87	101.99
3	G	303	NAP	O7N-C7N-C3N	2.36	122.45	119.63
3	J	304	NAP	C1B-N9A-C4A	-2.35	122.51	126.64
3	D	303	NAP	O4B-C1B-C2B	-2.28	102.64	106.59
3	G	303	NAP	O4B-C1B-C2B	-2.26	102.67	106.59
3	E	302	NAP	PN-O3-PA	-2.24	125.13	132.83
3	J	304	NAP	O2B-C2B-C3B	-2.24	103.56	111.68
3	B	302	NAP	O4D-C1D-C2D	-2.24	103.66	106.93
3	F	303	NAP	O5D-PN-O1N	2.19	117.61	109.07
3	C	302	NAP	O4D-C1D-C2D	-2.12	103.83	106.93
3	B	302	NAP	C6N-N1N-C2N	-2.11	120.05	121.97
3	F	303	NAP	C6N-N1N-C2N	-2.11	120.06	121.97
3	H	303	NAP	C5B-C4B-C3B	-2.09	107.34	115.18
3	E	302	NAP	C1B-N9A-C4A	-2.04	123.06	126.64
3	G	303	NAP	C2B-C3B-C4B	-2.03	97.59	101.99
3	D	303	NAP	O7N-C7N-C3N	2.02	122.05	119.63
3	F	303	NAP	C2B-C3B-C4B	-2.02	97.61	101.99
3	H	303	NAP	O7N-C7N-C3N	2.02	122.05	119.63

There are no chirality outliers.

All (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
3	A	303	NAP	C2D-C1D-N1N-C6N
3	B	302	NAP	C5B-O5B-PA-O3
3	B	302	NAP	O4D-C1D-N1N-C2N
3	B	302	NAP	O4D-C1D-N1N-C6N
3	B	302	NAP	C2D-C1D-N1N-C2N
3	B	302	NAP	C2D-C1D-N1N-C6N
3	C	302	NAP	C2B-O2B-P2B-O2X
3	C	302	NAP	O4D-C1D-N1N-C2N
3	C	302	NAP	O4D-C1D-N1N-C6N
3	C	302	NAP	C2D-C1D-N1N-C2N
3	C	302	NAP	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	D	303	NAP	O4D-C1D-N1N-C2N
3	D	303	NAP	O4D-C1D-N1N-C6N
3	D	303	NAP	C2D-C1D-N1N-C2N
3	D	303	NAP	C2D-C1D-N1N-C6N
3	E	302	NAP	C5B-O5B-PA-O1A
3	E	302	NAP	C5B-O5B-PA-O3
3	E	302	NAP	O4D-C1D-N1N-C2N
3	E	302	NAP	O4D-C1D-N1N-C6N
3	E	302	NAP	C2D-C1D-N1N-C2N
3	E	302	NAP	C2D-C1D-N1N-C6N
3	F	303	NAP	O4D-C1D-N1N-C2N
3	F	303	NAP	O4D-C1D-N1N-C6N
3	F	303	NAP	C2D-C1D-N1N-C2N
3	F	303	NAP	C2D-C1D-N1N-C6N
3	G	303	NAP	O4D-C1D-N1N-C2N
3	G	303	NAP	O4D-C1D-N1N-C6N
3	G	303	NAP	C2D-C1D-N1N-C2N
3	G	303	NAP	C2D-C1D-N1N-C6N
3	H	303	NAP	C5D-O5D-PN-O1N
3	H	303	NAP	C5D-O5D-PN-O2N
3	H	303	NAP	O4D-C1D-N1N-C2N
3	H	303	NAP	O4D-C1D-N1N-C6N
3	H	303	NAP	C2D-C1D-N1N-C2N
3	H	303	NAP	C2D-C1D-N1N-C6N
3	I	303	NAP	O4D-C1D-N1N-C2N
3	I	303	NAP	O4D-C1D-N1N-C6N
3	I	303	NAP	C2D-C1D-N1N-C2N
3	I	303	NAP	C2D-C1D-N1N-C6N
3	J	304	NAP	C5B-O5B-PA-O3
3	J	304	NAP	C5D-O5D-PN-O1N
3	J	304	NAP	O4D-C1D-N1N-C2N
3	J	304	NAP	O4D-C1D-N1N-C6N
3	J	304	NAP	C2D-C1D-N1N-C2N
3	J	304	NAP	C2D-C1D-N1N-C6N
3	J	304	NAP	C3B-C4B-C5B-O5B
2	B	301	1PE	OH5-C14-C24-OH4
2	G	301	1PE	OH6-C15-C25-OH5
2	B	301	1PE	OH6-C15-C25-OH5
2	J	301	1PE	C23-C13-OH4-C24
2	F	302	1PE	OH4-C13-C23-OH3
2	B	301	1PE	C13-C23-OH3-C22
2	G	301	1PE	C23-C13-OH4-C24

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Mol	Chain	Res	Type	Atoms
2	G	301	1PE	OH4-C13-C23-OH3
2	C	301	1PE	OH4-C13-C23-OH3
2	F	302	1PE	OH5-C14-C24-OH4
2	H	301	1PE	OH5-C14-C24-OH4
2	J	302	1PE	OH4-C13-C23-OH3
2	A	302	1PE	OH2-C12-C22-OH3
2	B	301	1PE	OH2-C12-C22-OH3
2	B	301	1PE	OH7-C16-C26-OH6
2	E	301	1PE	OH7-C16-C26-OH6
2	F	301	1PE	OH7-C16-C26-OH6
2	E	301	1PE	OH5-C14-C24-OH4
2	B	301	1PE	OH4-C13-C23-OH3
2	E	301	1PE	C14-C24-OH4-C13
2	C	301	1PE	C23-C13-OH4-C24
2	F	302	1PE	OH6-C15-C25-OH5
2	J	302	1PE	OH2-C12-C22-OH3
2	J	302	1PE	OH7-C16-C26-OH6
2	A	302	1PE	OH4-C13-C23-OH3
2	H	302	1PE	OH4-C13-C23-OH3
2	E	301	1PE	OH6-C15-C25-OH5
2	E	301	1PE	OH2-C12-C22-OH3
2	F	301	1PE	OH5-C14-C24-OH4
2	I	301	1PE	OH4-C13-C23-OH3
2	J	302	1PE	OH5-C14-C24-OH4
2	F	302	1PE	C25-C15-OH6-C26
2	I	301	1PE	OH7-C16-C26-OH6
2	C	301	1PE	OH5-C14-C24-OH4
3	J	304	NAP	O4B-C4B-C5B-O5B
2	H	302	1PE	OH6-C15-C25-OH5
2	G	301	1PE	C13-C23-OH3-C22
2	E	301	1PE	OH4-C13-C23-OH3
2	I	302	1PE	OH6-C15-C25-OH5
2	E	301	1PE	C15-C25-OH5-C14
2	A	301	1PE	OH2-C12-C22-OH3
2	D	301	1PE	OH2-C12-C22-OH3
2	I	302	1PE	OH7-C16-C26-OH6
2	F	301	1PE	OH6-C15-C25-OH5
2	A	301	1PE	C14-C24-OH4-C13
3	B	302	NAP	C3B-C4B-C5B-O5B
2	J	302	1PE	C14-C24-OH4-C13
3	D	303	NAP	C4D-C5D-O5D-PN
3	G	303	NAP	C4D-C5D-O5D-PN

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Mol	Chain	Res	Type	Atoms
3	I	303	NAP	C4D-C5D-O5D-PN
3	H	303	NAP	PA-O3-PN-O5D
2	D	301	1PE	OH5-C14-C24-OH4
2	D	301	1PE	C15-C25-OH5-C14
2	I	302	1PE	C24-C14-OH5-C25
2	H	301	1PE	OH7-C16-C26-OH6
2	J	301	1PE	OH7-C16-C26-OH6
2	C	301	1PE	C13-C23-OH3-C22
2	H	301	1PE	C24-C14-OH5-C25
2	A	302	1PE	C12-C22-OH3-C23
2	G	301	1PE	C12-C22-OH3-C23
2	G	302	1PE	C14-C24-OH4-C13
3	B	302	NAP	C4D-C5D-O5D-PN
3	H	303	NAP	C4D-C5D-O5D-PN
2	A	301	1PE	C12-C22-OH3-C23
2	D	301	1PE	C13-C23-OH3-C22
2	I	302	1PE	C15-C25-OH5-C14
2	F	302	1PE	C15-C25-OH5-C14
2	J	301	1PE	C25-C15-OH6-C26
2	C	301	1PE	C15-C25-OH5-C14
2	H	301	1PE	C23-C13-OH4-C24
3	A	303	NAP	C5B-O5B-PA-O3
3	A	303	NAP	C5D-O5D-PN-O3
3	F	303	NAP	C5D-O5D-PN-O3
3	G	303	NAP	C5D-O5D-PN-O3
3	I	303	NAP	C5D-O5D-PN-O3
3	J	304	NAP	C5D-O5D-PN-O3
2	H	302	1PE	OH2-C12-C22-OH3
2	A	301	1PE	C13-C23-OH3-C22
2	H	302	1PE	C15-C25-OH5-C14
2	I	301	1PE	C15-C25-OH5-C14
3	A	303	NAP	C4D-C5D-O5D-PN
3	F	303	NAP	C4D-C5D-O5D-PN
3	J	304	NAP	C4D-C5D-O5D-PN
2	J	302	1PE	C23-C13-OH4-C24
3	A	303	NAP	C5D-O5D-PN-O2N
3	B	302	NAP	C5B-O5B-PA-O1A
3	B	302	NAP	C5B-O5B-PA-O2A
3	C	302	NAP	C5D-O5D-PN-O2N
3	E	302	NAP	C5B-O5B-PA-O2A
3	J	304	NAP	C5B-O5B-PA-O1A
3	J	304	NAP	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	J	304	NAP	C5D-O5D-PN-O2N
2	J	303	1PE	OH4-C13-C23-OH3
2	G	301	1PE	C14-C24-OH4-C13
2	G	302	1PE	C23-C13-OH4-C24
2	H	301	1PE	C16-C26-OH6-C15
2	H	302	1PE	C12-C22-OH3-C23
2	F	301	1PE	C25-C15-OH6-C26
2	D	301	1PE	C25-C15-OH6-C26
2	A	302	1PE	OH6-C15-C25-OH5
2	B	301	1PE	C15-C25-OH5-C14
2	F	301	1PE	C16-C26-OH6-C15
2	J	301	1PE	C24-C14-OH5-C25
3	E	302	NAP	C4D-C5D-O5D-PN
2	A	302	1PE	OH5-C14-C24-OH4
3	G	303	NAP	O4D-C4D-C5D-O5D
2	I	301	1PE	C14-C24-OH4-C13
2	B	301	1PE	C14-C24-OH4-C13
3	C	302	NAP	C4D-C5D-O5D-PN
2	F	301	1PE	C15-C25-OH5-C14
2	G	301	1PE	OH5-C14-C24-OH4
2	I	301	1PE	C25-C15-OH6-C26
3	I	303	NAP	O4D-C4D-C5D-O5D
2	I	301	1PE	C23-C13-OH4-C24
2	B	301	1PE	C25-C15-OH6-C26
2	A	301	1PE	C23-C13-OH4-C24
2	C	301	1PE	C24-C14-OH5-C25
2	A	302	1PE	C15-C25-OH5-C14
2	I	302	1PE	C25-C15-OH6-C26
2	F	302	1PE	C12-C22-OH3-C23
2	H	301	1PE	C14-C24-OH4-C13
2	H	301	1PE	OH4-C13-C23-OH3
2	I	302	1PE	C16-C26-OH6-C15
2	F	302	1PE	C14-C24-OH4-C13
3	E	302	NAP	O4D-C4D-C5D-O5D
2	J	301	1PE	C15-C25-OH5-C14
2	A	301	1PE	OH4-C13-C23-OH3
3	I	303	NAP	C1B-C2B-O2B-P2B
3	C	302	NAP	C3B-C4B-C5B-O5B
3	I	303	NAP	C3D-C4D-C5D-O5D
2	G	302	1PE	C12-C22-OH3-C23
3	B	302	NAP	O4B-C4B-C5B-O5B
3	B	302	NAP	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
3	C	302	NAP	C5D-O5D-PN-O3
3	D	303	NAP	C5D-O5D-PN-O3
3	H	303	NAP	C5D-O5D-PN-O3
2	C	301	1PE	C16-C26-OH6-C15
2	G	301	1PE	C25-C15-OH6-C26
3	C	302	NAP	O4D-C4D-C5D-O5D
3	D	303	NAP	O4D-C4D-C5D-O5D
2	B	301	1PE	C24-C14-OH5-C25
2	D	301	1PE	OH4-C13-C23-OH3
3	B	302	NAP	C5D-O5D-PN-O2N
3	C	302	NAP	C5B-O5B-PA-O1A
3	F	303	NAP	C5B-O5B-PA-O1A
3	F	303	NAP	C5D-O5D-PN-O2N
3	G	303	NAP	C5B-O5B-PA-O1A
3	I	303	NAP	C5B-O5B-PA-O1A
3	A	303	NAP	O4D-C4D-C5D-O5D
3	B	302	NAP	O4D-C4D-C5D-O5D
3	F	303	NAP	O4D-C4D-C5D-O5D
3	J	304	NAP	O4D-C4D-C5D-O5D
2	J	301	1PE	C13-C23-OH3-C22
2	G	301	1PE	C24-C14-OH5-C25
3	I	303	NAP	C3B-C2B-O2B-P2B
2	H	302	1PE	C14-C24-OH4-C13
2	J	301	1PE	OH4-C13-C23-OH3
2	I	301	1PE	C24-C14-OH5-C25
2	D	301	1PE	OH6-C15-C25-OH5

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

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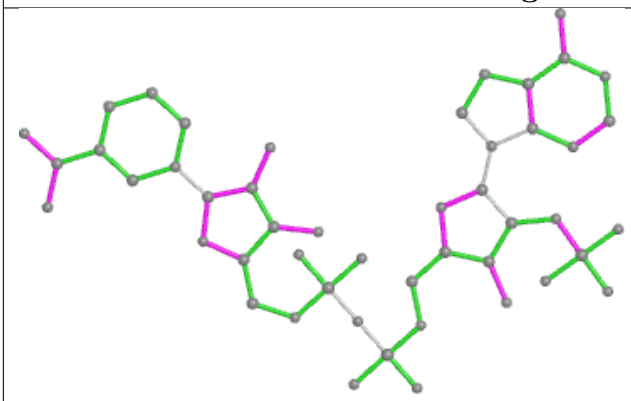
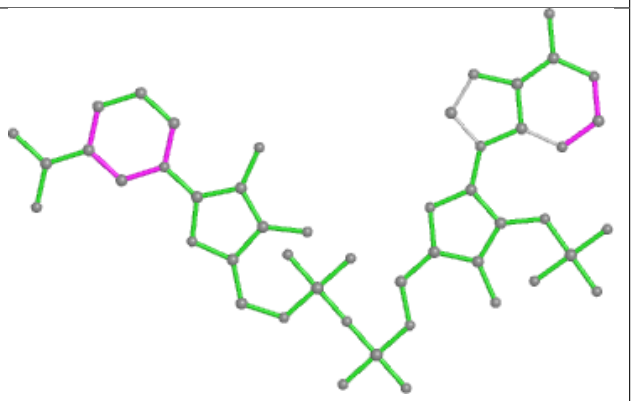
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	303	NAP	1	0
3	G	303	NAP	4	0
2	C	301	1PE	2	0
2	G	301	1PE	3	0
3	J	304	NAP	2	0
4	G	308	SO4	1	0
4	G	307	SO4	2	0
3	H	303	NAP	1	0
4	D	304	SO4	1	0
3	B	302	NAP	3	0
2	F	301	1PE	4	0
3	E	302	NAP	2	0
3	F	303	NAP	2	0
2	E	301	1PE	4	0
3	C	302	NAP	2	0

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.

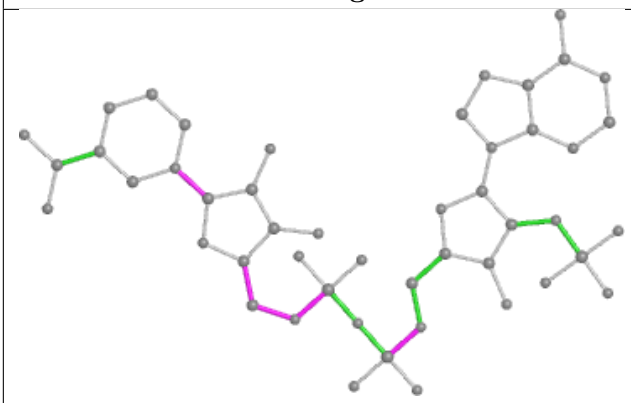
Ligand NAP A 303



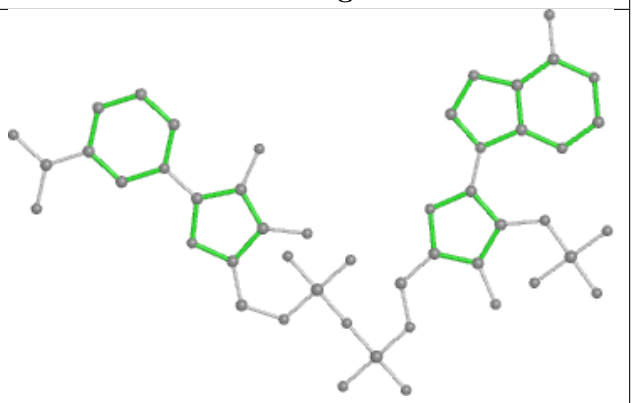
Bond lengths



Bond angles

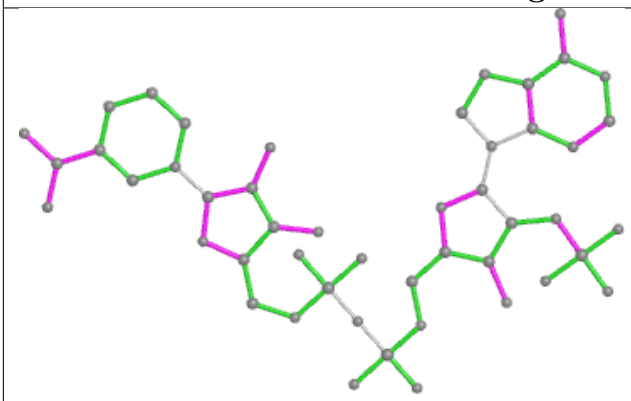


Torsions

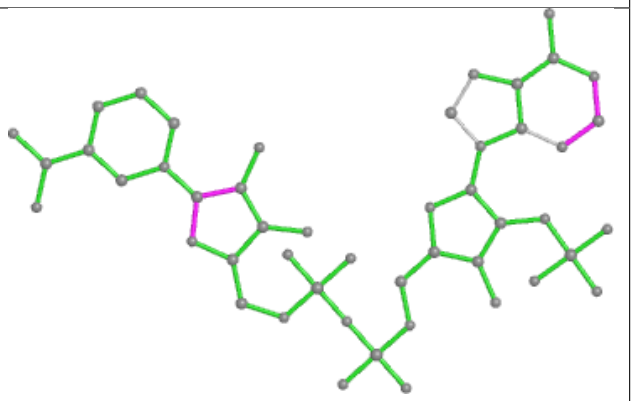


Rings

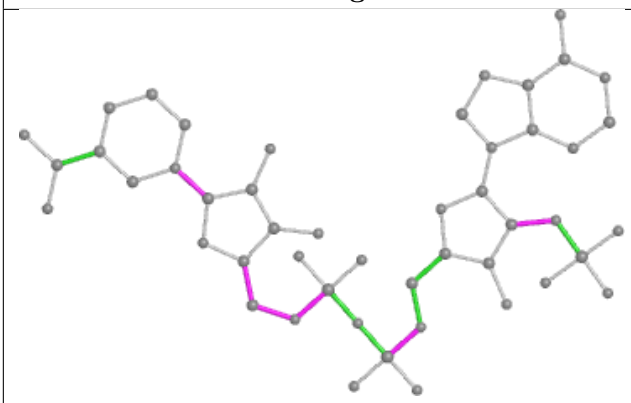
Ligand NAP I 303



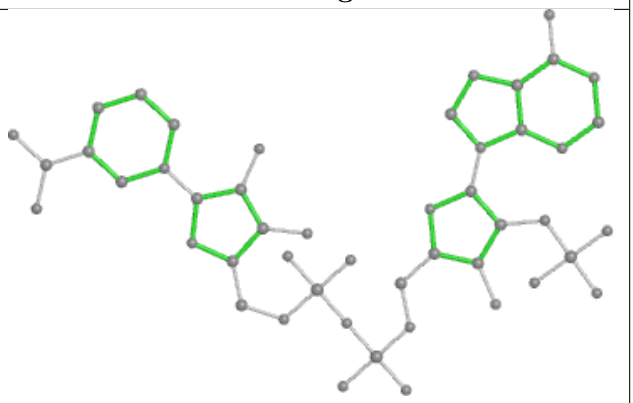
Bond lengths



Bond angles

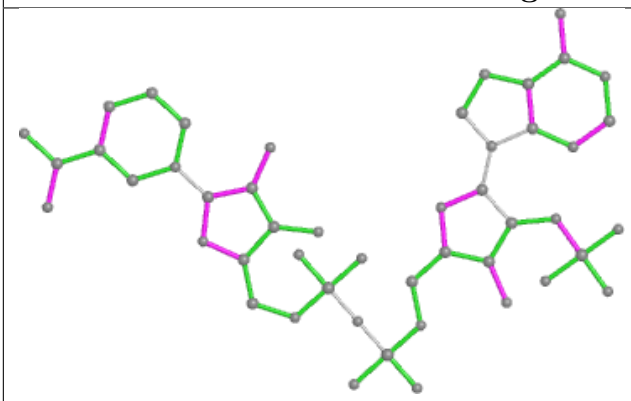


Torsions

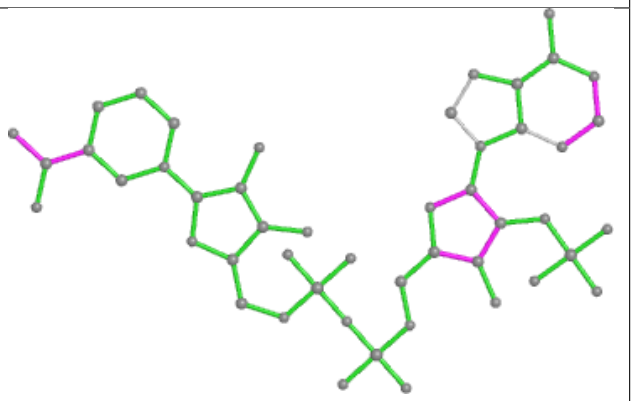


Rings

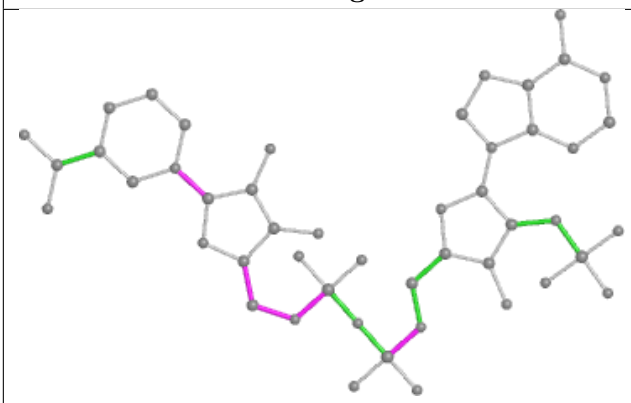
Ligand NAP G 303



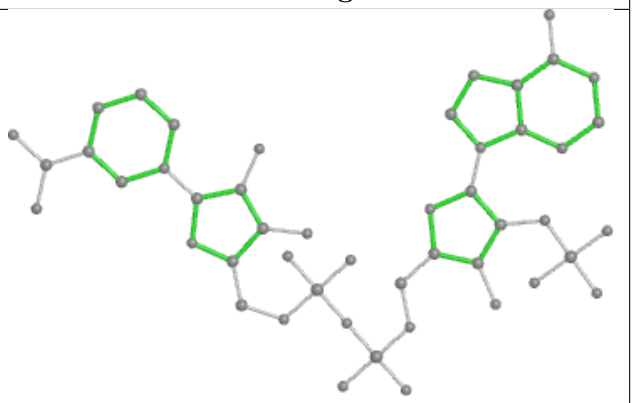
Bond lengths



Bond angles

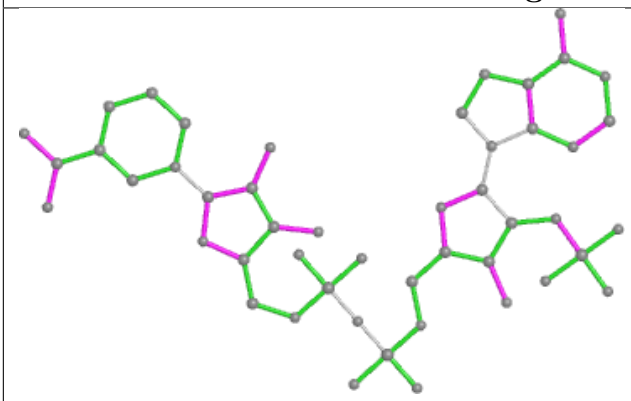


Torsions

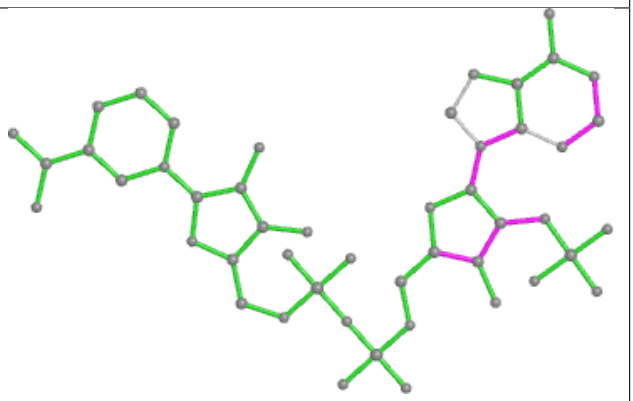


Rings

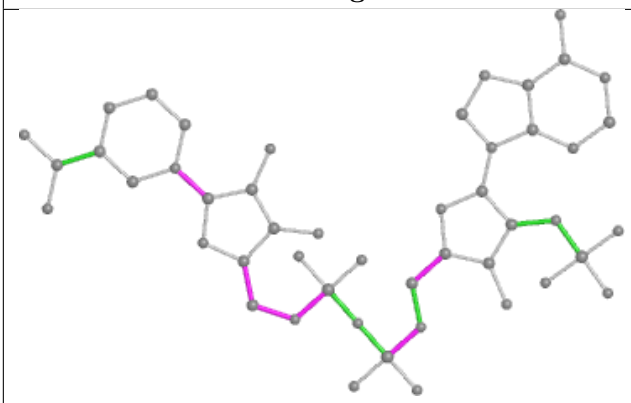
Ligand NAP J 304



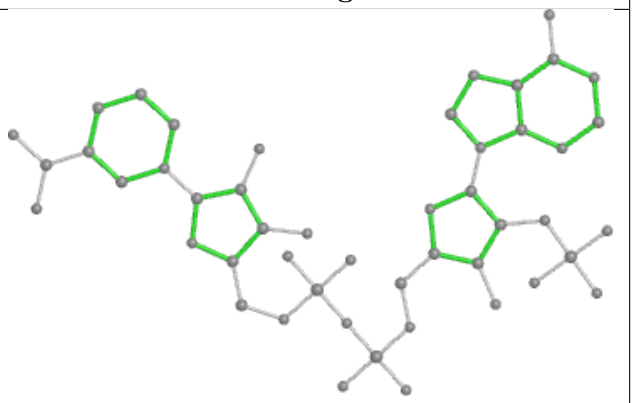
Bond lengths



Bond angles

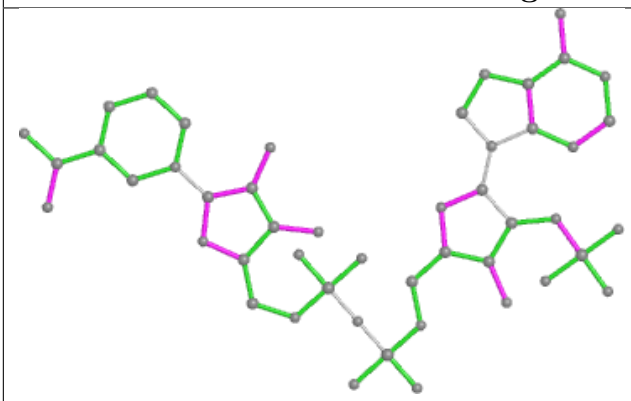


Torsions

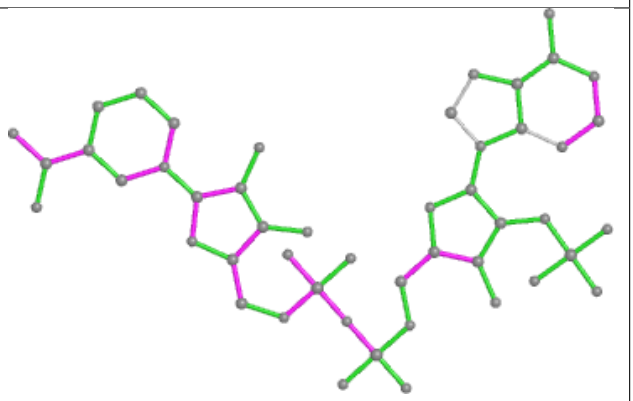


Rings

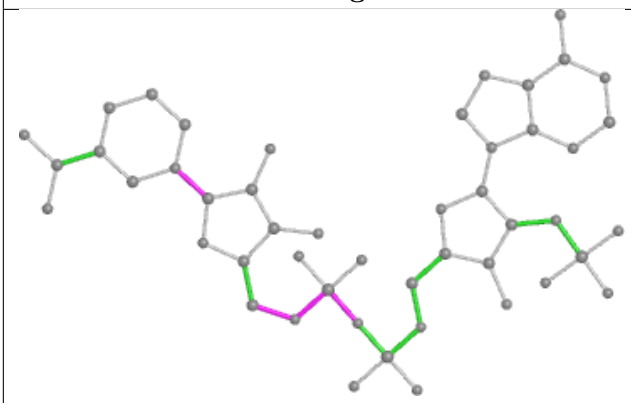
Ligand NAP H 303



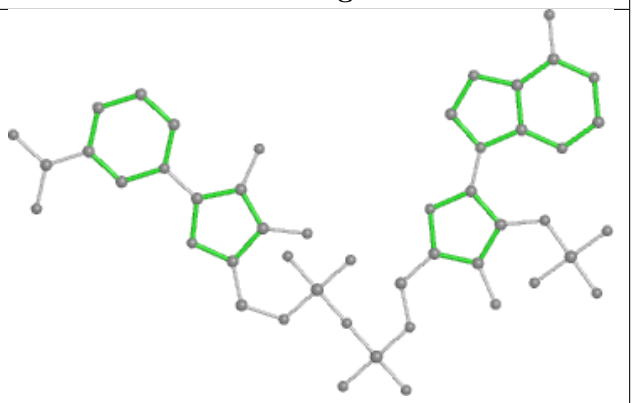
Bond lengths



Bond angles

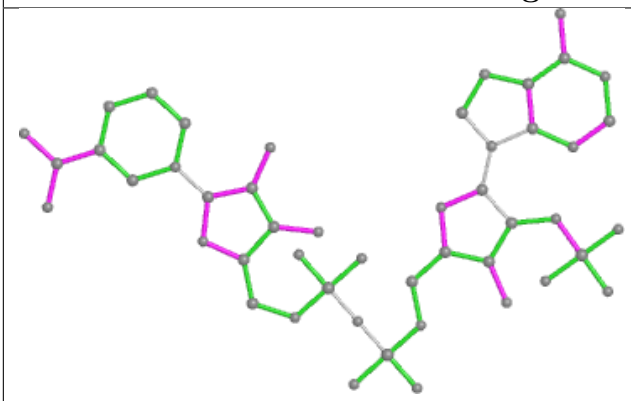


Torsions

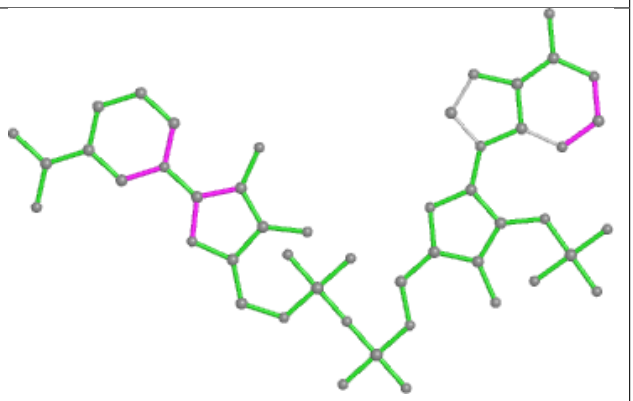


Rings

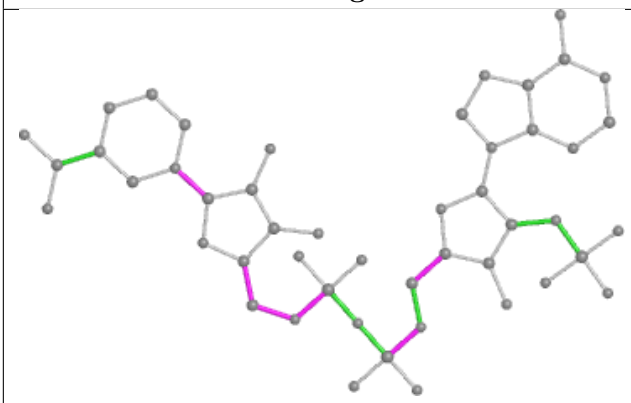
Ligand NAP B 302



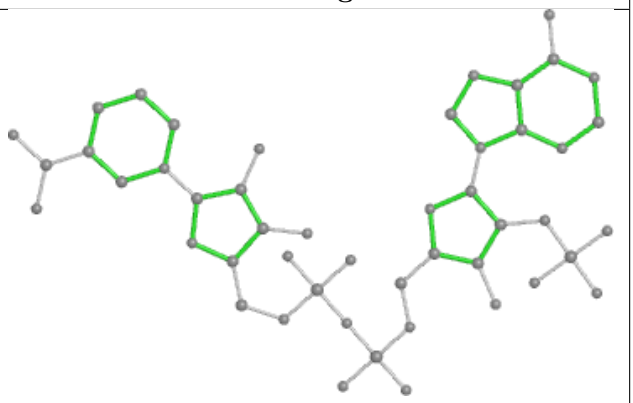
Bond lengths



Bond angles

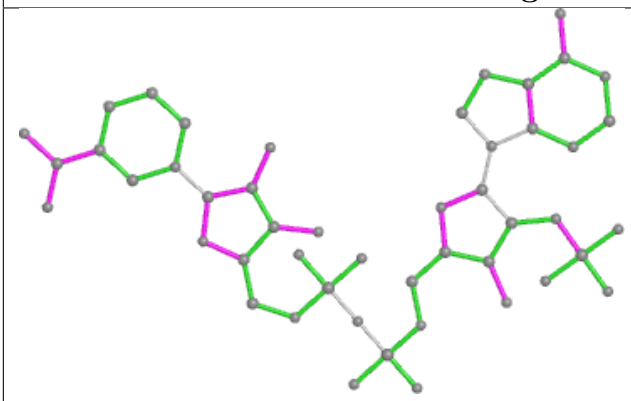


Torsions

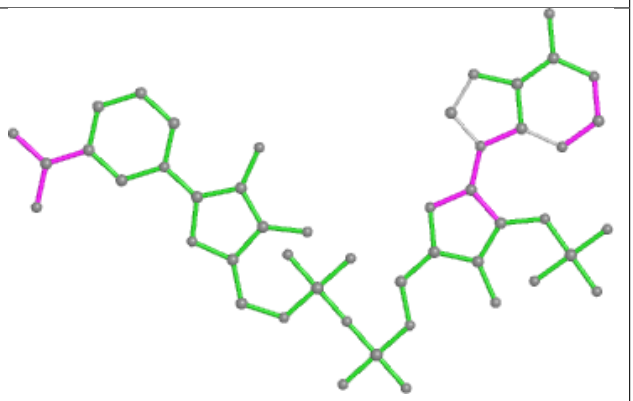


Rings

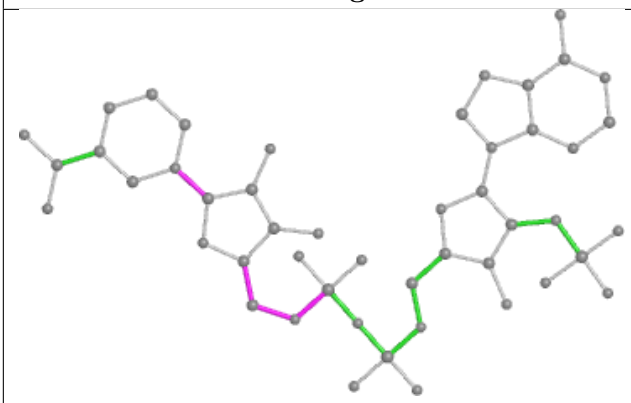
Ligand NAP D 303



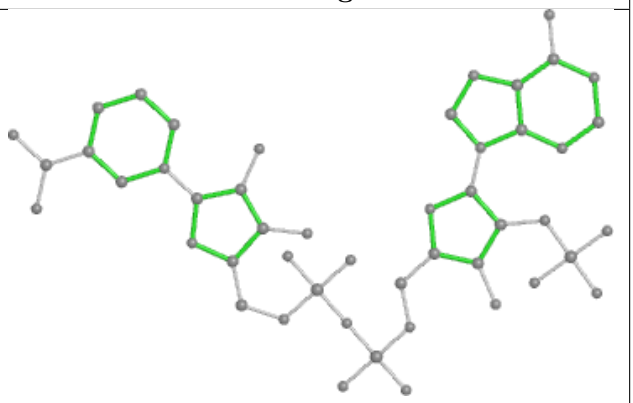
Bond lengths



Bond angles

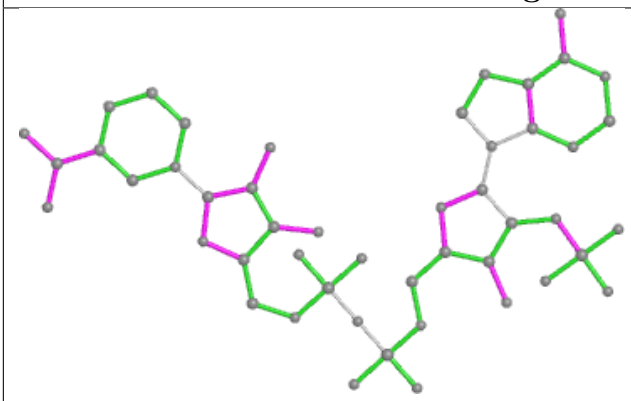


Torsions

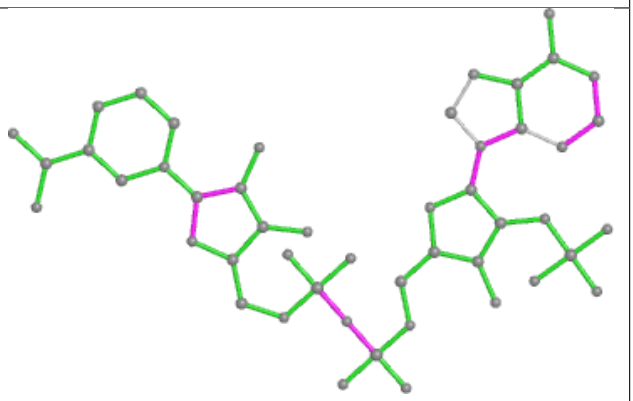


Rings

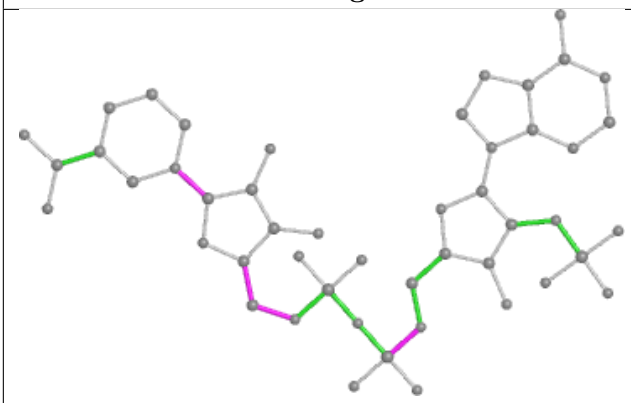
Ligand NAP E 302



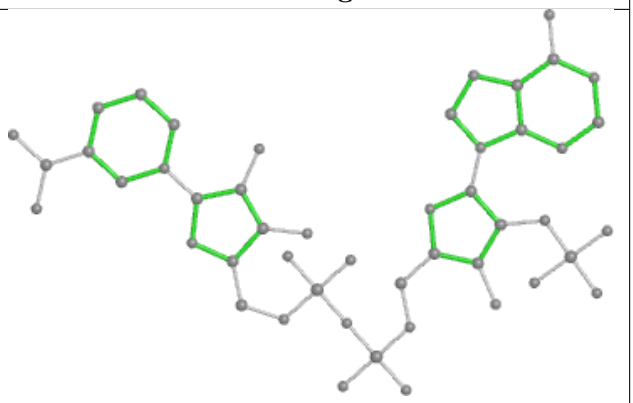
Bond lengths



Bond angles

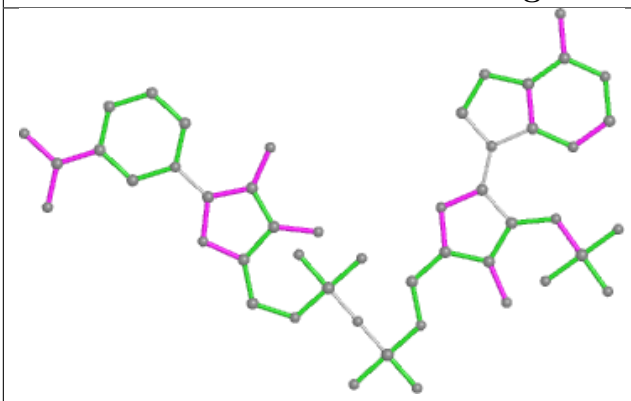


Torsions

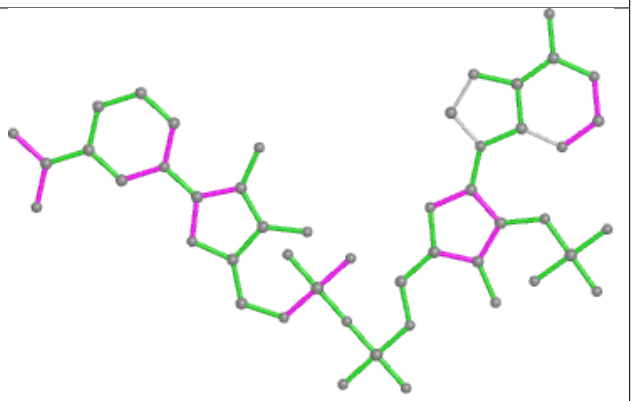


Rings

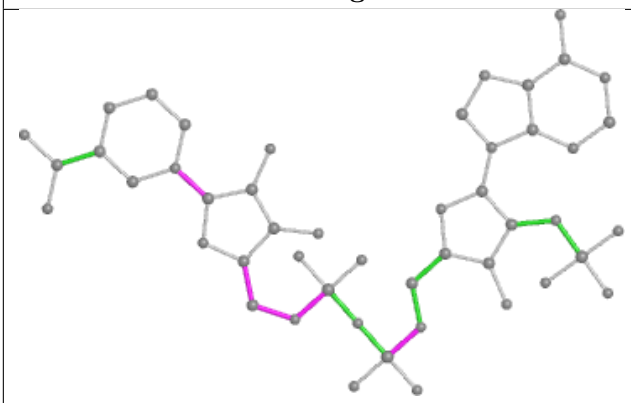
Ligand NAP F 303



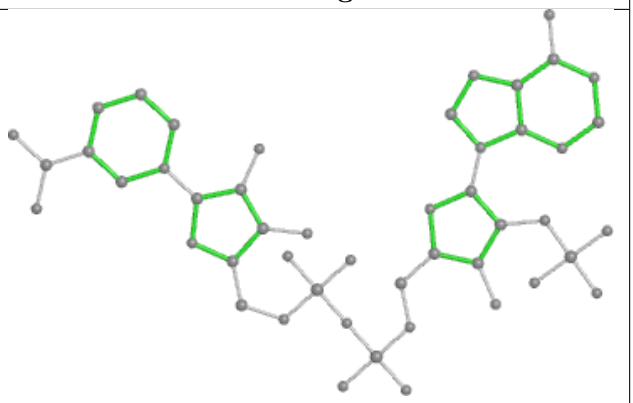
Bond lengths



Bond angles

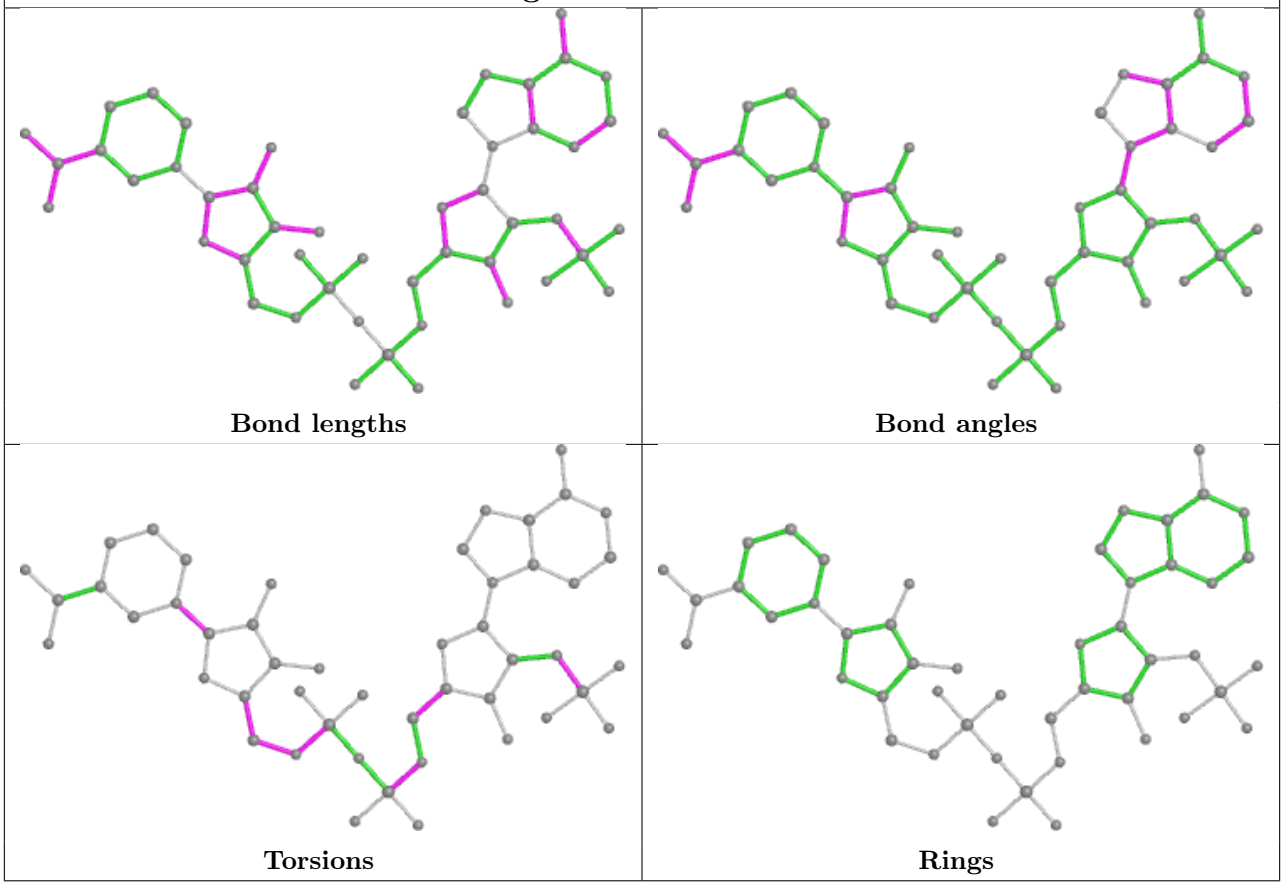


Torsions



Rings

Ligand NAP C 302



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^{th} 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

All (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
1	J	200	HIS	5.0
1	J	201	HIS	4.8
1	A	42	GLU	4.7
1	I	199	HIS	4.5
1	H	46	LYS	4.5
1	A	43	VAL	4.5
1	J	197	ALA	4.3
1	I	202	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	44	SER	4.2
1	I	201	HIS	4.2
1	H	8	SER	4.2
1	C	42	GLU	4.2
1	B	46	LYS	4.1
1	H	43	VAL	4.1
1	A	46	LYS	4.1
1	B	47	ILE	4.0
1	H	7	LEU	4.0
1	H	50	LYS	3.9
1	B	43	VAL	3.9
1	C	43	VAL	3.9
1	I	203	HIS	3.8
1	A	44	SER	3.7
1	I	43	VAL	3.7
1	J	202	HIS	3.7
1	H	9	PHE	3.7
1	G	43	VAL	3.6
1	C	48	MET	3.5
1	C	123	VAL	3.5
1	A	125	GLY	3.5
1	H	117	GLU	3.4
1	A	48	MET	3.4
1	I	46	LYS	3.4
1	C	125	GLY	3.3
1	B	8	SER	3.3
1	J	123	VAL	3.3
1	A	45	GLY	3.3
1	H	44	SER	3.2
1	I	125	GLY	3.2
1	I	47	ILE	3.2
1	I	42	GLU	3.2
1	E	47	ILE	3.2
1	G	42	GLU	3.1
1	J	77	PHE	3.1
1	H	10	ILE	3.1
1	J	198	HIS	3.0
1	A	123	VAL	3.0
1	H	42	GLU	3.0
1	B	76	ASP	3.0
1	B	77	PHE	3.0
1	H	49	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	124	TRP	3.0
1	H	47	ILE	2.9
1	G	8	SER	2.9
1	B	125	GLY	2.9
1	I	45	GLY	2.9
1	H	125	GLY	2.9
1	C	46	LYS	2.9
1	H	124	TRP	2.9
1	H	143	TRP	2.9
1	E	42	GLU	2.8
1	I	197	ALA	2.8
1	B	143	TRP	2.8
1	F	46	LYS	2.8
1	B	48	MET	2.8
1	F	1	MET	2.8
1	E	54	PRO	2.8
1	E	51	GLN	2.8
1	E	41	ASP	2.8
1	I	198	HIS	2.8
1	B	144	LEU	2.8
1	J	199	HIS	2.7
1	B	44	SER	2.7
1	I	8	SER	2.7
1	C	1	MET	2.7
1	C	45	GLY	2.7
1	G	46	LYS	2.7
1	E	45	GLY	2.6
1	C	6	VAL	2.6
1	F	43	VAL	2.6
1	C	7	LEU	2.6
1	I	123	VAL	2.6
1	B	42	GLU	2.6
1	C	49	GLU	2.6
1	H	144	LEU	2.6
1	F	42	GLU	2.6
1	A	143	TRP	2.6
1	D	191	LYS	2.6
1	C	8	SER	2.6
1	H	45	GLY	2.5
1	A	63	THR	2.5
1	A	1	MET	2.5
1	H	6	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	125	GLY	2.5
1	A	124	TRP	2.5
1	I	53	LYS	2.5
1	F	47	ILE	2.4
1	B	50	LYS	2.4
1	C	77[A]	PHE	2.4
1	B	6	VAL	2.4
1	G	10	ILE	2.4
1	B	9	PHE	2.4
1	A	40	GLU	2.4
1	E	46	LYS	2.4
1	G	92	THR	2.4
1	A	41	ASP	2.3
1	B	10	ILE	2.3
1	J	1	MET	2.3
1	B	7	LEU	2.3
1	G	143	TRP	2.3
1	D	46	LYS	2.3
1	I	94	LYS	2.3
1	A	7	LEU	2.3
1	A	126	SER	2.3
1	C	200	HIS	2.3
1	A	6	VAL	2.3
1	I	10	ILE	2.3
1	C	117	GLU	2.3
1	E	143	TRP	2.2
1	I	126	SER	2.2
1	E	116	SER	2.2
1	D	10	ILE	2.2
1	B	183	ASN	2.2
1	E	40	GLU	2.2
1	B	126	SER	2.2
1	H	123	VAL	2.2
1	E	146	ILE	2.2
1	E	115	ASN	2.2
1	J	117	GLU	2.2
1	C	50	LYS	2.2
1	B	75	ALA	2.2
1	H	40	GLU	2.2
1	I	11	THR	2.1
1	A	59	LEU	2.1
1	F	7	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	8	SER	2.1
1	B	117	GLU	2.1
1	C	144	LEU	2.1
1	I	9	PHE	2.1
1	H	95	LYS	2.1
1	C	40	GLU	2.0
1	A	50	LYS	2.0
1	E	48	MET	2.0
1	H	52	MET	2.0
1	B	118	GLY	2.0
1	F	125	GLY	2.0
1	H	145	LYS	2.0
1	C	10	ILE	2.0
1	H	146	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
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

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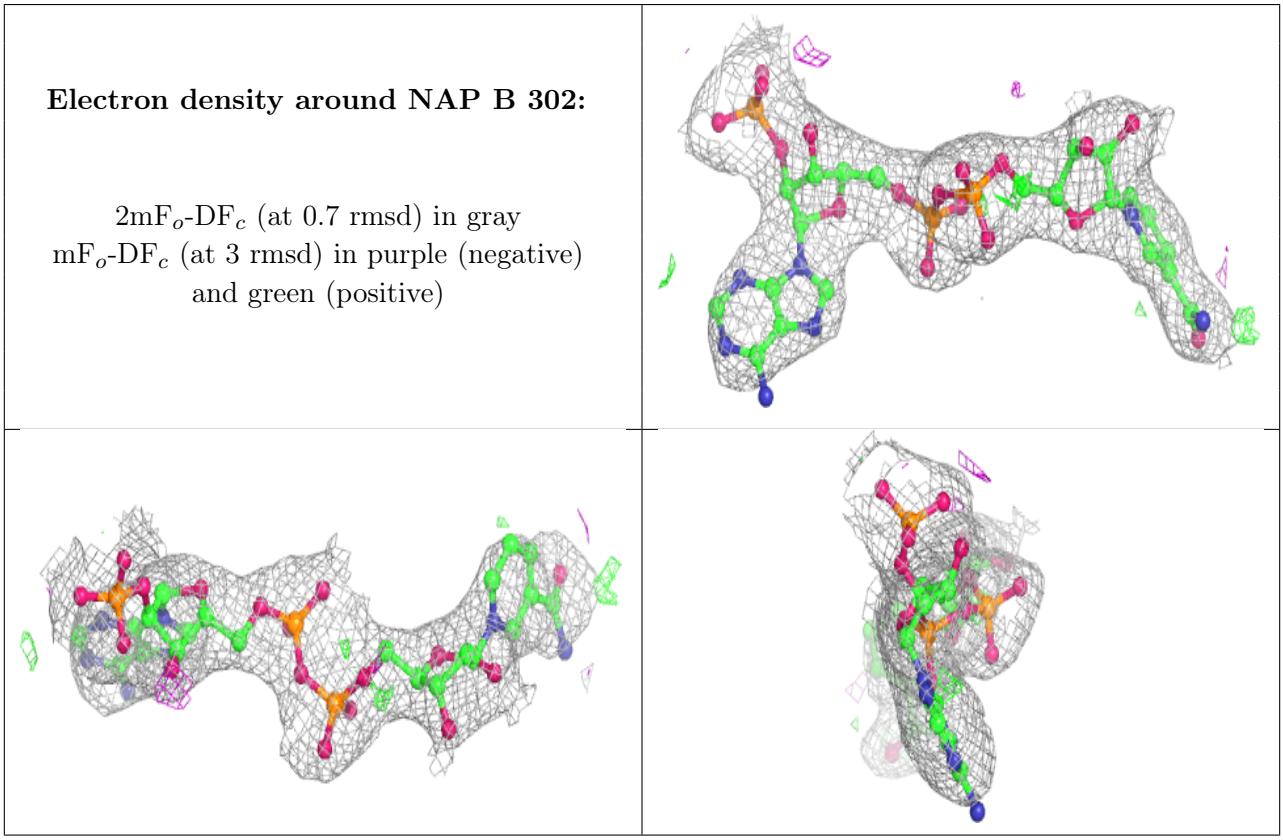
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAP	D	303	48/48	0.95	0.15	38,51,57,65	0
3	NAP	E	302	48/48	0.95	0.16	48,58,64,66	0
4	SO4	F	304	5/5	0.95	0.16	77,77,88,92	5
3	NAP	G	303	48/48	0.95	0.15	42,52,57,60	0
4	SO4	D	304	5/5	0.95	0.19	58,61,68,74	5
3	NAP	H	303	48/48	0.95	0.15	45,57,68,71	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.

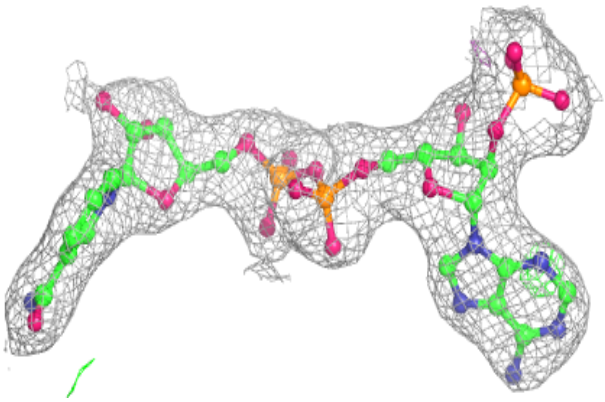
Electron density around NAP B 302:

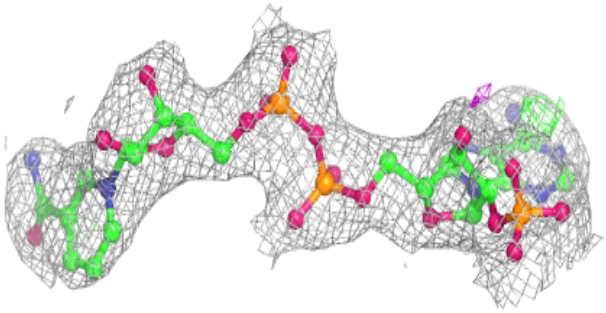
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

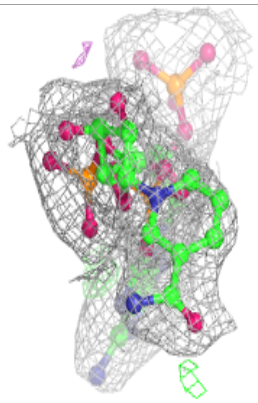


Electron density around NAP I 303:

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

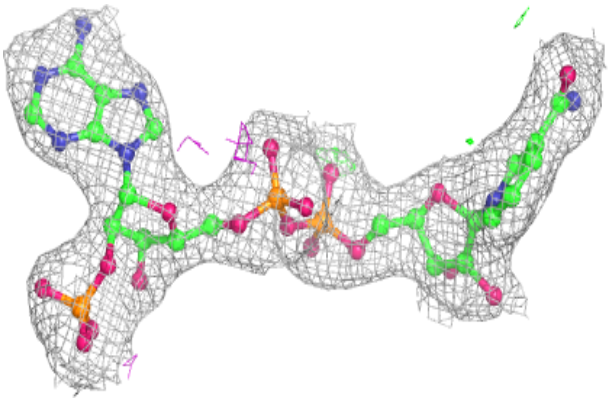


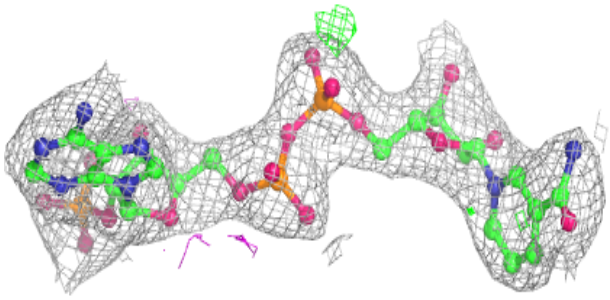


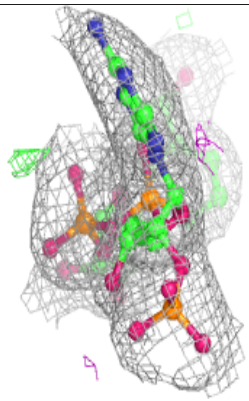


Electron density around NAP D 303:

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

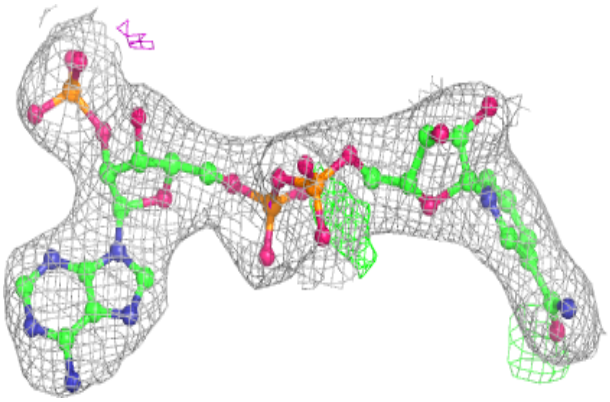


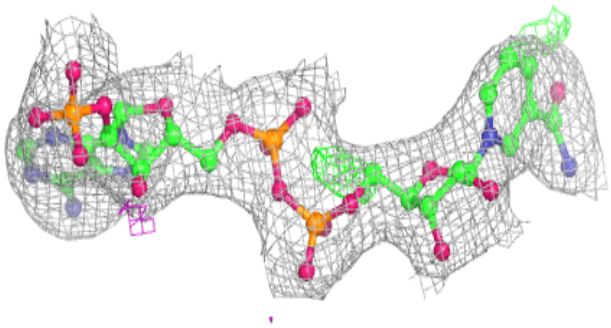


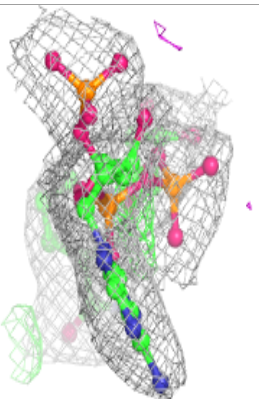


Electron density around NAP E 302:

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

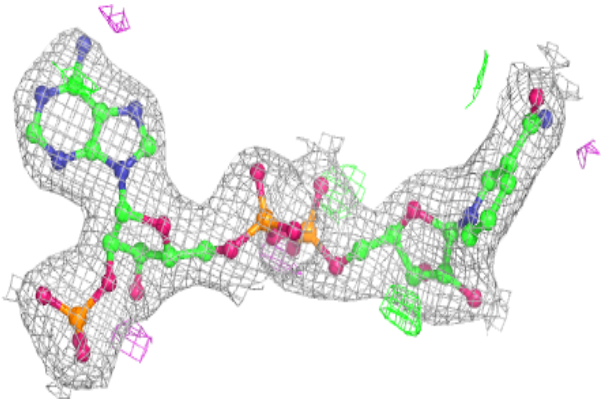


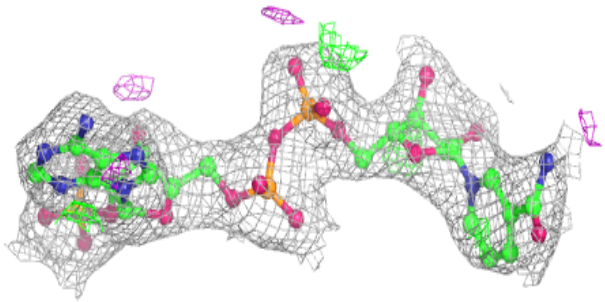


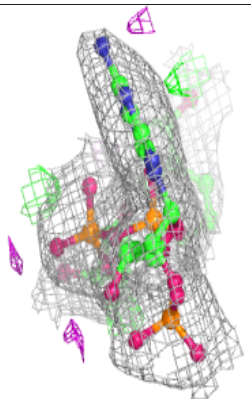


Electron density around NAP G 303:

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

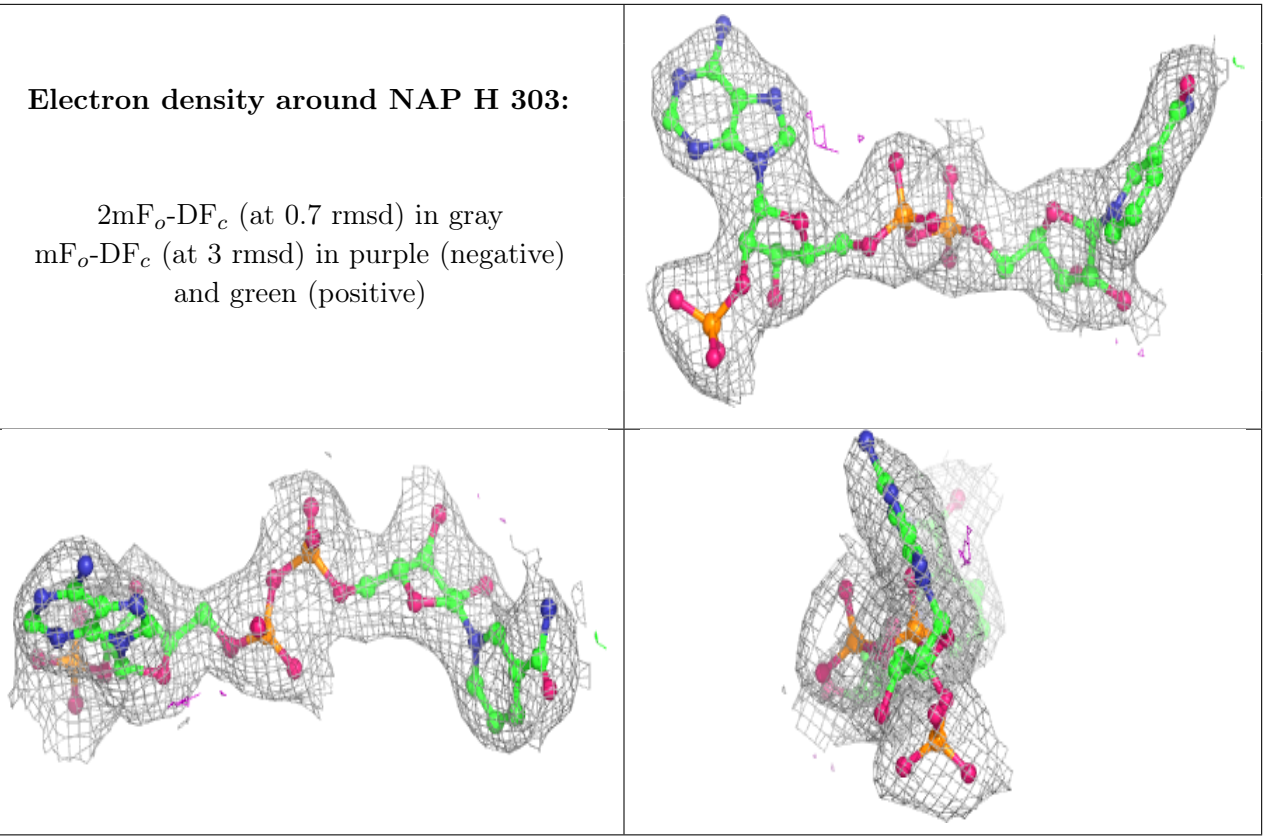






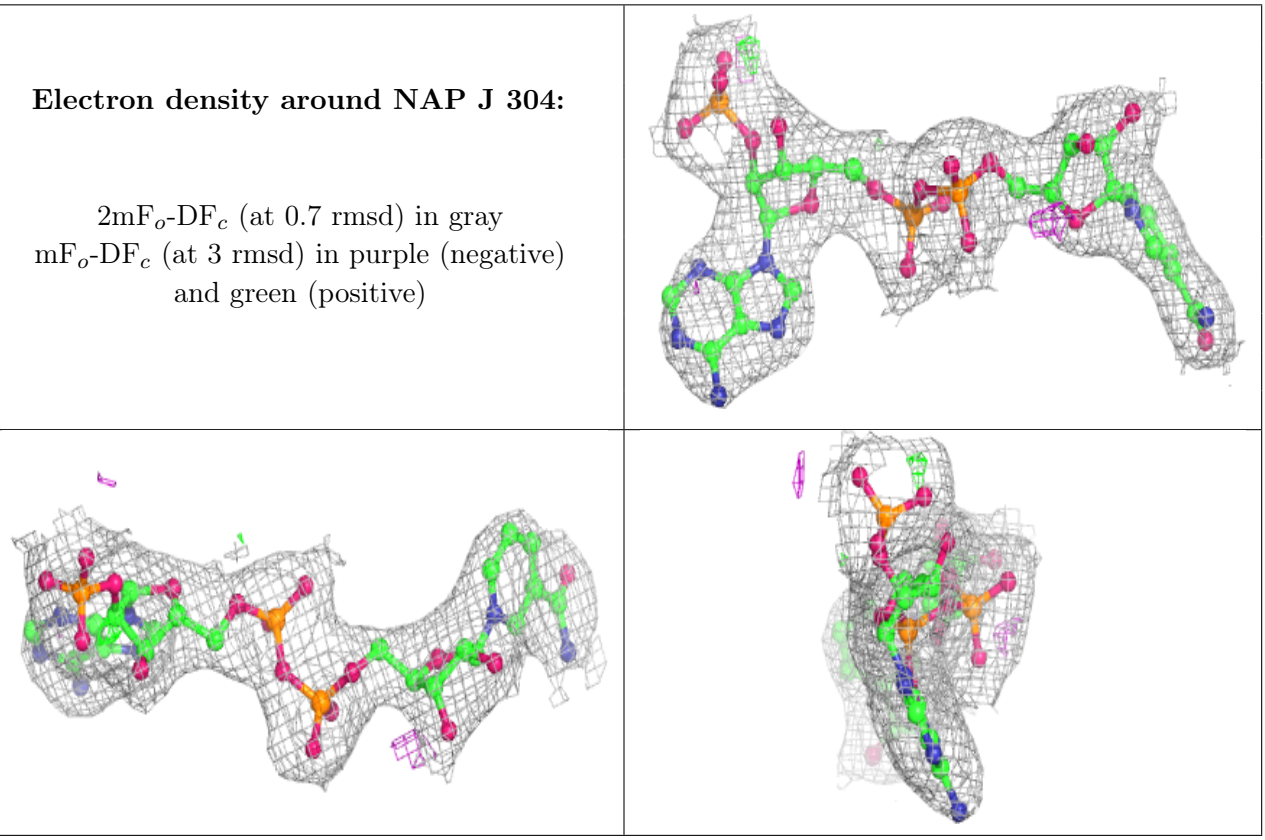
Electron density around NAP H 303:

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



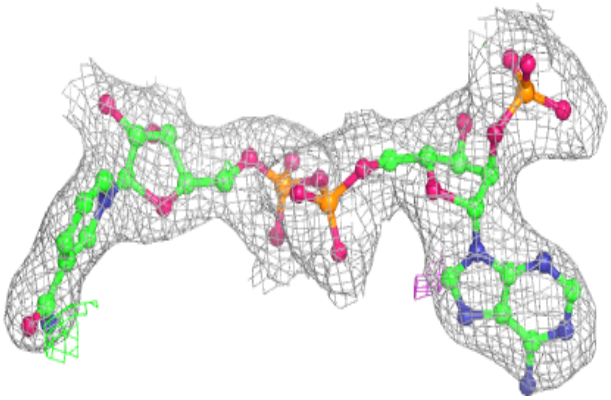
Electron density around NAP J 304:

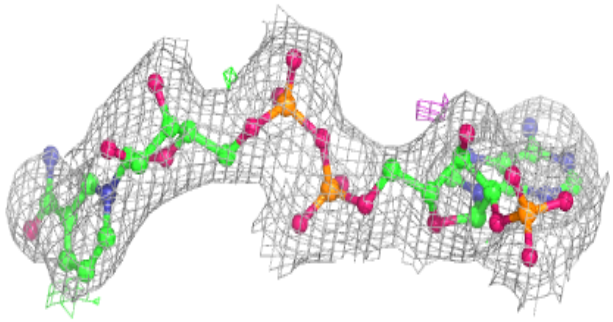
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

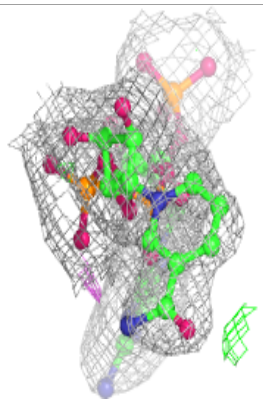


Electron density around NAP C 302:

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

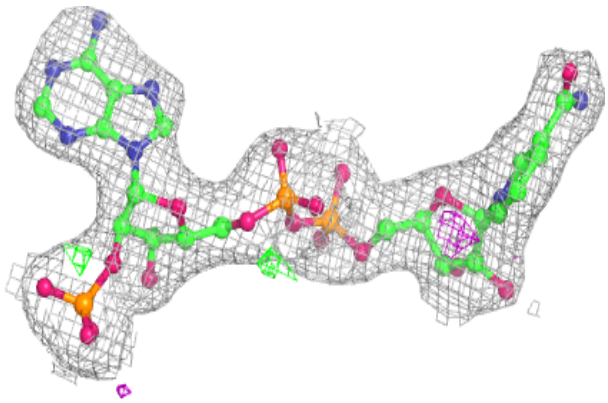


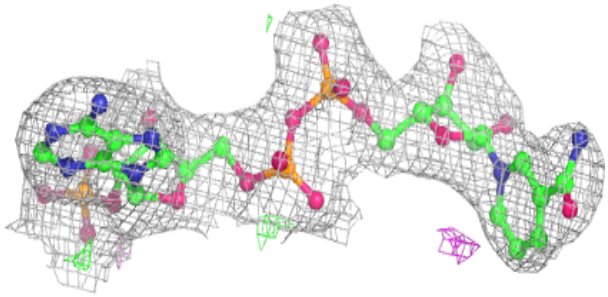


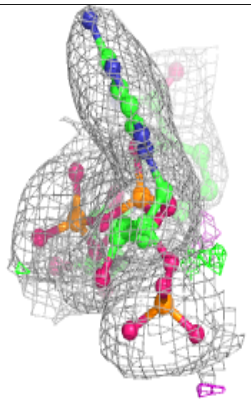


Electron density around NAP A 303:

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

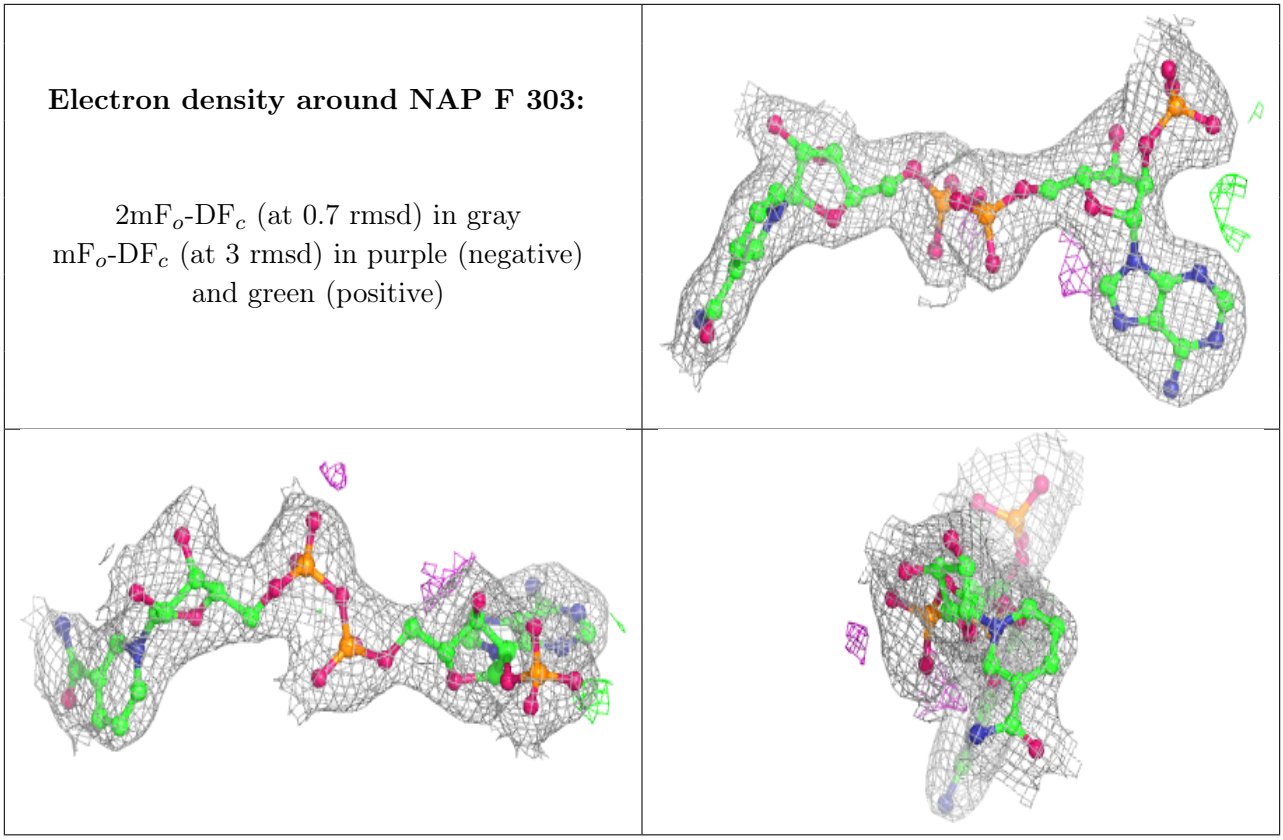






Electron density around NAP F 303:

$2mF_o$-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 (i)

There are no such residues in this entry.