Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 10:49 PM EDT

PDB ID	:	6CEY
Title	:	Aminoglycoside Phosphotransferase (2")-Ia in complex with GMPPNP, Magnesium, and Lividomycin moieties
Authors	:	Caldwell, S.J.; Berghuis, A.M.
Deposited on	:	2018-02-13
Resolution	:	2.40 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:

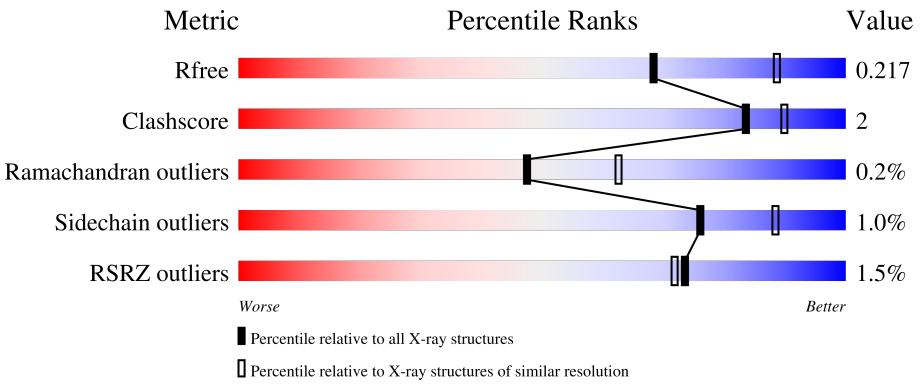
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	305	85% 9% • 6%
1	B	305	% 90% 7% •
1	C	305	84% 10% • 5%
1	D	305	4% 87% 8% • •

2 Entry composition (i)

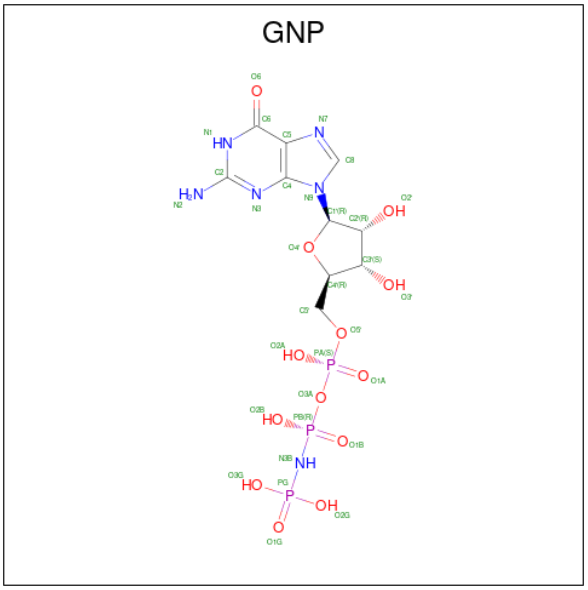
There are 6 unique types of molecules in this entry. The entry contains 10349 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional AAC/APH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2377	1522	367	478	10	0	0	0
1	B	295	2427	1551	376	490	10	0	0	0
1	C	289	2385	1526	369	480	10	0	0	0
1	D	293	2399	1530	373	486	10	0	0	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	41	10	7	19	5	0	1
2	B	1	32	10	6	13	3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	41	10	7	19	5	0	1
			Total	C	N	O	P		
2	D	1	32	10	6	13	3	0	0

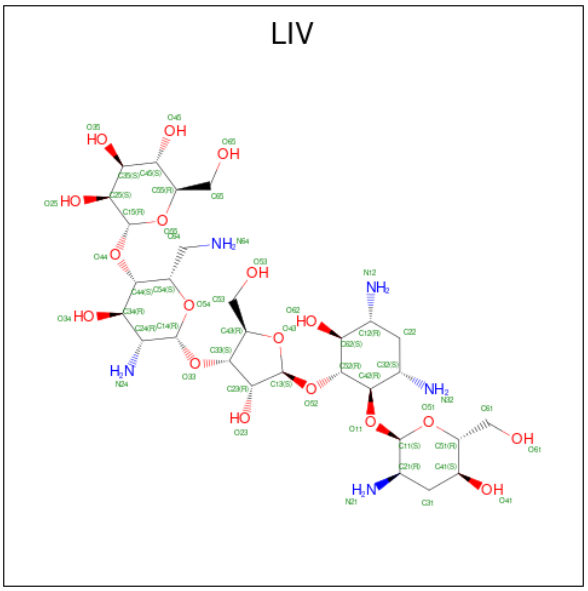
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0
			Total	Mg		
3	B	2	2	2	0	0
			Total	Mg		
3	C	3	3	3	0	0
			Total	Mg		
3	D	2	2	2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0
			Total	Cl		
4	B	1	1	1	0	0
			Total	Cl		
4	C	1	1	1	0	0

- Molecule 5 is (2R,3S,4S,5S,6R)-2-((2S,3S,4R,5R,6R)-5-AMINO-2-(AMINOMETHYL)-6-((2R,3S,4R,5S)-5-((1R,2R,3S,5R,6S)-3,5-DIAMINO-2-((2S,3R ,5S,6R)-3-AMINO-5-HYDROXY-6-(HYDROXYMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-6-HYDROXYCYCLOHEXYLOXY)-4-HYDROXY-2-(HYDROXYMET HYL)-TETRAHYDROFURAN-3-YLOXY)-4-HYDROXY-TETRAHYDRO-2H-PYRAN-3-YLOXY)-6-(HYDROXYMETHYL)-TETRAHYDRO-2H-PYRAN-3,4,5-TRIOL (three-letter code: LIV) (formula: $C_{29}H_{55}N_5O_{18}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	D	1	62	34	5	23	0	1

- Molecule 6 is water.

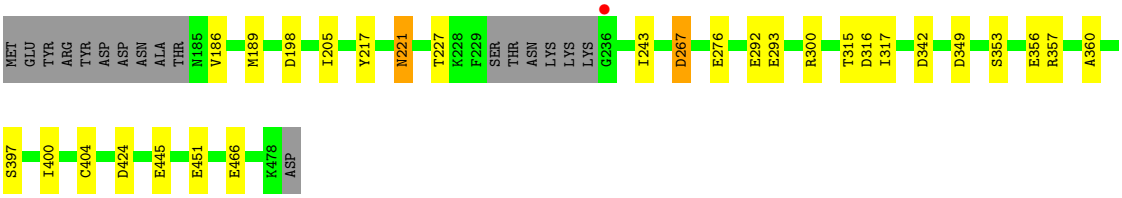
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	138	138	138	0	0
6	B	174	174	174	0	0
6	C	137	137	137	0	0
6	C	3	3	3	0	0
6	D	89	89	89	0	0

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.

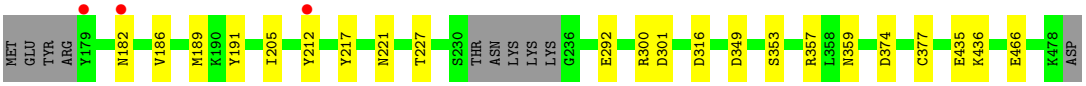
• Molecule 1: Bifunctional AAC/APH

Chain A:



• Molecule 1: Bifunctional AAC/APH

Chain B:

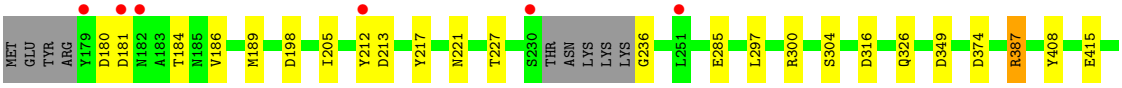


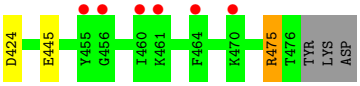
• Molecule 1: Bifunctional AAC/APH

Chain C:

• Molecule 1: Bifunctional AAC/APH

Chain D:




D424
E445
Y455
G456
I460
K461
F464
K470
R475
T476
TYR
LYS
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.25Å 100.24Å 94.01Å 90.00° 105.17° 90.00°	Depositor
Resolution (Å)	90.73 – 2.40 55.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (90.73-2.40) 100.0 (55.95-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.171 , 0.216 0.177 , 0.217	Depositor DCC
R_{free} test set	3190 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	52.1	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10349	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, LIV, CL, MG

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	1.11	5/2420 (0.2%)	1.02	9/3263 (0.3%)
1	B	1.16	9/2471 (0.4%)	1.02	8/3334 (0.2%)
1	C	1.19	13/2428 (0.5%)	1.02	8/3275 (0.2%)
1	D	1.03	6/2441 (0.2%)	0.98	8/3294 (0.2%)
All	All	1.12	33/9760 (0.3%)	1.01	33/13166 (0.3%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	445	GLU	CD-OE1	8.64	1.35	1.25
1	B	466	GLU	CD-OE1	8.40	1.34	1.25
1	C	356	GLU	CD-OE1	7.91	1.34	1.25
1	C	304	SER	CB-OG	-7.82	1.32	1.42
1	C	356	GLU	CD-OE2	7.50	1.33	1.25
1	A	445	GLU	CD-OE1	7.48	1.33	1.25
1	C	439	GLU	CD-OE2	7.20	1.33	1.25
1	B	377	CYS	CB-SG	-7.15	1.70	1.82
1	C	478	LYS	N-CA	6.66	1.59	1.46
1	C	471	GLU	CD-OE2	6.49	1.32	1.25
1	A	292	GLU	CD-OE2	6.25	1.32	1.25
1	B	466	GLU	CD-OE2	6.19	1.32	1.25
1	B	301	ASP	CB-CG	6.11	1.64	1.51
1	C	356	GLU	CG-CD	5.97	1.60	1.51
1	C	466	GLU	CG-CD	5.91	1.60	1.51
1	B	292	GLU	CG-CD	5.84	1.60	1.51
1	D	415	GLU	CG-CD	5.81	1.60	1.51
1	C	365	GLU	CD-OE2	5.78	1.32	1.25
1	C	337	GLU	CD-OE1	5.77	1.31	1.25
1	D	285	GLU	CD-OE1	5.77	1.31	1.25
1	D	236	GLY	C-O	5.76	1.32	1.23
1	A	353	SER	CB-OG	-5.62	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	304	SER	CB-OG	-5.54	1.35	1.42
1	C	240	GLU	CD-OE1	5.43	1.31	1.25
1	A	356	GLU	CD-OE1	5.36	1.31	1.25
1	C	477	TYR	CG-CD1	-5.28	1.32	1.39
1	D	181	ASP	CB-CG	5.27	1.62	1.51
1	B	191	TYR	CG-CD1	-5.21	1.32	1.39
1	D	212	TYR	CE1-CZ	5.17	1.45	1.38
1	B	353	SER	CB-OG	-5.16	1.35	1.42
1	A	360	ALA	C-O	-5.16	1.13	1.23
1	B	435	GLU	CD-OE2	5.07	1.31	1.25
1	B	212	TYR	CE1-CZ	5.01	1.45	1.38

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	475	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	A	300	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	349	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	D	424	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	D	387	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	B	301	ASP	CB-CG-OD1	7.04	124.63	118.30
1	A	451	GLU	OE1-CD-OE2	-6.92	115.00	123.30
1	B	301	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	A	404	CYS	CA-CB-SG	-6.49	102.32	114.00
1	C	404	CYS	CA-CB-SG	-6.35	102.57	114.00
1	C	475	ARG	NH1-CZ-NH2	-6.24	112.54	119.40
1	C	478	LYS	N-CA-CB	6.02	121.43	110.60
1	A	316	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	316	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	D	374	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	D	475	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	357	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	B	349	ASP	CB-CG-OD1	5.72	123.44	118.30
1	D	316	ASP	CB-CG-OD1	5.66	123.39	118.30
1	D	300	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	300	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	424	ASP	CB-CG-OD1	5.36	123.12	118.30
1	C	323	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	374	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	342	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	357	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	349	ASP	CB-CG-OD1	5.16	122.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	301	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	D	297	LEU	CB-CG-CD2	5.14	119.74	111.00
1	A	276	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	C	292	GLU	OE1-CD-OE2	5.08	129.39	123.30
1	B	300	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	C	387	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2377	0	2289	9	1
1	B	2427	0	2327	6	0
1	C	2385	0	2298	12	0
1	D	2399	0	2298	11	0
2	A	41	0	2	4	0
2	B	32	0	13	0	0
2	C	41	0	2	0	0
2	D	32	0	13	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	D	62	0	63	7	0
6	A	138	0	0	4	0
6	B	174	0	0	2	0
6	C	140	0	0	1	1
6	D	89	0	0	2	0
All	All	10349	0	9305	45	1

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 2.

All (45) 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)
5:D:600[A]:LIV:N64	5:D:600[A]:LIV:O23	1.78	1.15
2:A:500[B]:GNP:O2G	6:A:909:HOH:O	1.71	1.06
2:A:500[B]:GNP:PG	6:A:909:HOH:O	2.27	0.89
2:A:500[B]:GNP:O1B	6:A:901:HOH:O	2.03	0.76
1:D:180:ASP:O	1:D:184:THR:HG22	1.95	0.67
1:D:186:VAL:HG13	1:D:205:ILE:HG23	1.76	0.66
1:B:359:ASN:OD1	6:B:1050:HOH:O	2.15	0.64
2:A:500[B]:GNP:O2B	6:A:1221:HOH:O	2.14	0.64
1:D:213:ASP:O	6:D:1015:HOH:O	2.15	0.63
1:C:186:VAL:HG13	1:C:205:ILE:HG23	1.81	0.61
5:D:600[A]:LIV:C15	5:D:600[A]:LIV:H11A	2.34	0.57
1:C:243:ILE:HD13	1:C:397:SER:HB3	1.89	0.54
1:B:436:LYS:NZ	6:B:1113:HOH:O	2.40	0.54
1:B:189:MET:SD	1:B:227:THR:HG21	2.48	0.54
1:B:186:VAL:HG13	1:B:205:ILE:HG23	1.90	0.53
1:C:445:GLU:HG2	1:C:475:ARG:HH21	1.74	0.53
1:C:189:MET:HG2	1:C:217:TYR:CE1	2.44	0.53
1:D:408:TYR:CE1	5:D:600[A]:LIV:H44	2.44	0.53
1:D:189:MET:HG2	1:D:217:TYR:CE1	2.44	0.52
5:D:600[A]:LIV:H11A	5:D:600[A]:LIV:H15	1.91	0.52
1:B:189:MET:HG2	1:B:217:TYR:CE1	2.45	0.51
1:A:189:MET:SD	1:A:227:THR:HG21	2.51	0.50
1:D:186:VAL:CG1	1:D:205:ILE:HG23	2.41	0.50
1:C:189:MET:SD	1:C:227:THR:HG21	2.52	0.49
5:D:600[A]:LIV:H15	5:D:600[A]:LIV:C64	2.42	0.49
1:A:186:VAL:HG13	1:A:205:ILE:HG23	1.95	0.48
1:D:189:MET:SD	1:D:227:THR:HG21	2.53	0.48
1:C:186:VAL:CG1	1:C:205:ILE:HG23	2.44	0.47
1:A:189:MET:HG2	1:A:217:TYR:CE1	2.50	0.47
1:A:315:THR:HG22	1:C:265:ILE:HG21	1.97	0.47
1:D:326:GLN:NE2	6:D:1013:HOH:O	2.47	0.47
1:A:315:THR:HG21	1:C:238:ALA:HB2	1.97	0.46
1:D:445:GLU:HG2	1:D:475:ARG:NH2	2.30	0.45
1:D:408:TYR:HE1	5:D:600[A]:LIV:H44	1.81	0.44
1:B:186:VAL:CG1	1:B:205:ILE:HG23	2.47	0.44
1:C:328:VAL:HG11	1:C:358:LEU:HD22	1.99	0.44
1:A:243:ILE:HD13	1:A:397:SER:HB2	2.00	0.44
1:C:325:LYS:NZ	6:C:1258:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:LEU:HD23	1:C:387:ARG:NE	2.35	0.41
1:C:445:GLU:HG2	1:C:475:ARG:NH2	2.34	0.41
1:A:186:VAL:CG1	1:A:205:ILE:HG23	2.50	0.41
1:D:186:VAL:HG13	1:D:205:ILE:CG2	2.46	0.41
1:A:267:ASP:OD1	1:A:267:ASP:N	2.55	0.40
1:A:317:ILE:HD12	1:A:317:ILE:HA	1.87	0.40
5:D:600[A]:LIV:O23	5:D:600[A]:LIV:C64	2.62	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLU:OE1	6:C:1080:HOH:O[2_747]	2.19	0.01

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	284/305 (93%)	274 (96%)	8 (3%)	2 (1%)	22 32
1	B	291/305 (95%)	280 (96%)	11 (4%)	0	100 100
1	C	285/305 (93%)	273 (96%)	12 (4%)	0	100 100
1	D	289/305 (95%)	276 (96%)	13 (4%)	0	100 100
All	All	1149/1220 (94%)	1103 (96%)	44 (4%)	2 (0%)	47 62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	400	ILE

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	263/281 (94%)	259 (98%)	4 (2%)	65	80
1	B	268/281 (95%)	266 (99%)	2 (1%)	84	92
1	C	265/281 (94%)	263 (99%)	2 (1%)	81	91
1	D	265/281 (94%)	262 (99%)	3 (1%)	73	87
All	All	1061/1124 (94%)	1050 (99%)	11 (1%)	76	88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	221	ASN
1	A	267	ASP
1	A	466	GLU
1	B	182	ASN
1	B	221	ASN
1	C	221	ASN
1	C	285	GLU
1	D	198	ASP
1	D	221	ASN
1	D	387	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	359	ASN
1	A	467	ASN
1	B	467	ASN
1	C	296	ASN
1	C	341	ASN
1	D	295	GLN
1	D	296	ASN
1	D	326	GLN

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Mol	Chain	Res	Type
1	D	420	ASN

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)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GNP	A	500[B]	3	29,34,34	1.04	3 (10%)	33,54,54	2.34	9 (27%)
2	GNP	A	500[A]	3	29,34,34	1.18	4 (13%)	33,54,54	2.16	8 (24%)
2	GNP	B	500	3	29,34,34	2.55	9 (31%)	33,54,54	3.55	12 (36%)
2	GNP	C	500[B]	3	29,34,34	1.73	6 (20%)	33,54,54	2.65	9 (27%)
2	GNP	C	500[A]	3	29,34,34	1.80	5 (17%)	33,54,54	2.24	7 (21%)
2	GNP	D	500	3	29,34,34	1.34	3 (10%)	33,54,54	2.40	10 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GNP	A	500[B]	3	-	4/14/38/38	0/3/3/3
2	GNP	A	500[A]	3	-	3/14/38/38	0/3/3/3
2	GNP	B	500	3	-	2/14/38/38	0/3/3/3
2	GNP	C	500[B]	3	-	3/14/38/38	0/3/3/3
2	GNP	C	500[A]	3	-	2/14/38/38	0/3/3/3
2	GNP	D	500	3	-	2/14/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	GNP	PG-O3G	6.59	1.74	1.56
2	C	500[A]	GNP	C5-C6	6.30	1.52	1.41
2	C	500[B]	GNP	C5-C6	6.30	1.52	1.41
2	B	500	GNP	PB-O3A	5.91	1.66	1.59
2	C	500[A]	GNP	PB-O3A	4.75	1.65	1.59
2	B	500	GNP	PB-O2B	4.68	1.69	1.56
2	B	500	GNP	C5-C6	4.22	1.48	1.41
2	B	500	GNP	C8-N7	-4.05	1.27	1.34
2	B	500	GNP	PG-O2G	3.80	1.67	1.56
2	D	500	GNP	PB-O3A	3.78	1.63	1.59
2	B	500	GNP	C6-N1	3.77	1.39	1.33
2	D	500	GNP	PG-O2G	3.50	1.66	1.56
2	C	500[B]	GNP	PB-O3A	3.31	1.63	1.59
2	D	500	GNP	C6-N1	3.26	1.38	1.33
2	A	500[A]	GNP	PB-O3A	-2.83	1.55	1.59
2	A	500[A]	GNP	C4-N3	-2.70	1.31	1.35
2	A	500[B]	GNP	C4-N3	-2.70	1.31	1.35
2	B	500	GNP	C5-C4	-2.51	1.34	1.40
2	A	500[A]	GNP	PG-O2G	2.32	1.63	1.56
2	C	500[B]	GNP	PG-O3G	2.27	1.62	1.56
2	A	500[A]	GNP	C6-N1	2.24	1.36	1.33
2	A	500[B]	GNP	C6-N1	2.24	1.36	1.33
2	A	500[B]	GNP	PG-O2G	2.23	1.62	1.56
2	C	500[A]	GNP	C5-C4	-2.19	1.35	1.40
2	C	500[B]	GNP	C5-C4	-2.19	1.35	1.40
2	C	500[A]	GNP	C6-N1	2.19	1.36	1.33
2	C	500[B]	GNP	C6-N1	2.19	1.36	1.33
2	C	500[A]	GNP	C8-N7	-2.13	1.30	1.34
2	C	500[B]	GNP	C8-N7	-2.13	1.30	1.34
2	B	500	GNP	C4-N3	2.12	1.39	1.35

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	GNP	O2B-PB-O1B	-10.82	87.25	109.92
2	B	500	GNP	O1G-PG-N3B	-9.10	98.38	111.77
2	C	500[A]	GNP	C5-C6-N1	-8.78	111.42	123.43
2	C	500[B]	GNP	C5-C6-N1	-8.78	111.42	123.43
2	D	500	GNP	C5-C6-N1	-8.38	111.97	123.43
2	A	500[A]	GNP	C5-C6-N1	-8.27	112.12	123.43
2	A	500[B]	GNP	C5-C6-N1	-8.27	112.12	123.43
2	B	500	GNP	O2G-PG-O1G	7.39	132.04	113.45
2	B	500	GNP	C5-C6-N1	-6.79	114.15	123.43
2	C	500[B]	GNP	O1G-PG-N3B	6.31	121.06	111.77
2	D	500	GNP	C2-N1-C6	5.74	125.06	115.93
2	A	500[B]	GNP	O2G-PG-O3G	-5.49	93.03	107.64
2	C	500[A]	GNP	C2-N1-C6	5.46	124.61	115.93
2	C	500[B]	GNP	C2-N1-C6	5.46	124.61	115.93
2	B	500	GNP	C4-C5-C6	-5.33	115.71	120.80
2	A	500[A]	GNP	C2-N1-C6	5.25	124.28	115.93
2	A	500[B]	GNP	C2-N1-C6	5.25	124.28	115.93
2	B	500	GNP	C2-N1-C6	4.98	123.84	115.93
2	C	500[B]	GNP	O2B-PB-O1B	-4.55	100.39	109.92
2	D	500	GNP	O3G-PG-O1G	-4.30	102.64	113.45
2	C	500[B]	GNP	O3G-PG-O1G	-4.21	102.86	113.45
2	B	500	GNP	O3A-PB-N3B	3.69	116.81	106.59
2	D	500	GNP	O2B-PB-O1B	-3.64	102.28	109.92
2	A	500[A]	GNP	O1G-PG-N3B	-3.54	106.56	111.77
2	A	500[A]	GNP	O2B-PB-O1B	-3.11	103.40	109.92
2	A	500[B]	GNP	O1G-PG-N3B	3.02	116.21	111.77
2	D	500	GNP	O3A-PB-N3B	3.00	114.92	106.59
2	B	500	GNP	N3-C2-N1	-2.98	123.25	127.22
2	C	500[A]	GNP	C4-C5-C6	-2.86	118.06	120.80
2	C	500[B]	GNP	C4-C5-C6	-2.86	118.06	120.80
2	A	500[B]	GNP	O2B-PB-O3A	2.78	113.92	104.64
2	B	500	GNP	O3G-PG-O1G	-2.70	106.66	113.45
2	B	500	GNP	O5'-PA-O1A	2.61	119.25	109.07
2	D	500	GNP	C4-C5-C6	-2.59	118.32	120.80
2	C	500[A]	GNP	O3A-PB-N3B	2.57	113.71	106.59
2	D	500	GNP	C2-N3-C4	-2.52	112.48	115.36
2	B	500	GNP	O1B-PB-N3B	2.48	115.42	111.77
2	D	500	GNP	N3-C2-N1	-2.43	123.98	127.22
2	A	500[A]	GNP	N3-C2-N1	-2.41	124.00	127.22
2	A	500[B]	GNP	N3-C2-N1	-2.41	124.00	127.22
2	A	500[A]	GNP	C2-N3-C4	-2.38	112.63	115.36
2	A	500[B]	GNP	C2-N3-C4	-2.38	112.63	115.36
2	A	500[B]	GNP	PB-O3A-PA	2.26	140.58	132.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500[A]	GNP	O2B-PB-O3A	2.24	112.12	104.64
2	D	500	GNP	O2'-C2'-C3'	-2.22	104.65	111.82
2	C	500[B]	GNP	O3A-PB-N3B	2.21	112.73	106.59
2	D	500	GNP	O5'-PA-O1A	2.19	117.64	109.07
2	B	500	GNP	C2-N3-C4	-2.14	112.91	115.36
2	C	500[A]	GNP	O5'-PA-O1A	2.13	117.40	109.07
2	C	500[B]	GNP	O5'-PA-O1A	2.13	117.40	109.07
2	C	500[A]	GNP	N3-C2-N1	-2.12	124.39	127.22
2	C	500[B]	GNP	N3-C2-N1	-2.12	124.39	127.22
2	A	500[A]	GNP	O2G-PG-O1G	2.10	118.72	113.45
2	A	500[A]	GNP	C4-C5-C6	-2.08	118.81	120.80
2	A	500[B]	GNP	C4-C5-C6	-2.08	118.81	120.80

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500[A]	GNP	PG-N3B-PB-O1B
2	A	500[A]	GNP	PA-O3A-PB-O1B
2	A	500[B]	GNP	PB-N3B-PG-O1G
2	B	500	GNP	PB-N3B-PG-O1G
2	B	500	GNP	PG-N3B-PB-O1B
2	C	500[A]	GNP	PB-N3B-PG-O1G
2	C	500[A]	GNP	PG-N3B-PB-O1B
2	C	500[B]	GNP	PB-N3B-PG-O1G
2	C	500[B]	GNP	PA-O3A-PB-O1B
2	D	500	GNP	PB-N3B-PG-O1G
2	D	500	GNP	PG-N3B-PB-O1B
2	A	500[B]	GNP	PB-O3A-PA-O1A
2	A	500[B]	GNP	PB-O3A-PA-O2A
2	C	500[B]	GNP	PB-O3A-PA-O2A
2	A	500[A]	GNP	C5'-O5'-PA-O1A
2	A	500[B]	GNP	C5'-O5'-PA-O1A

There are no ring outliers.

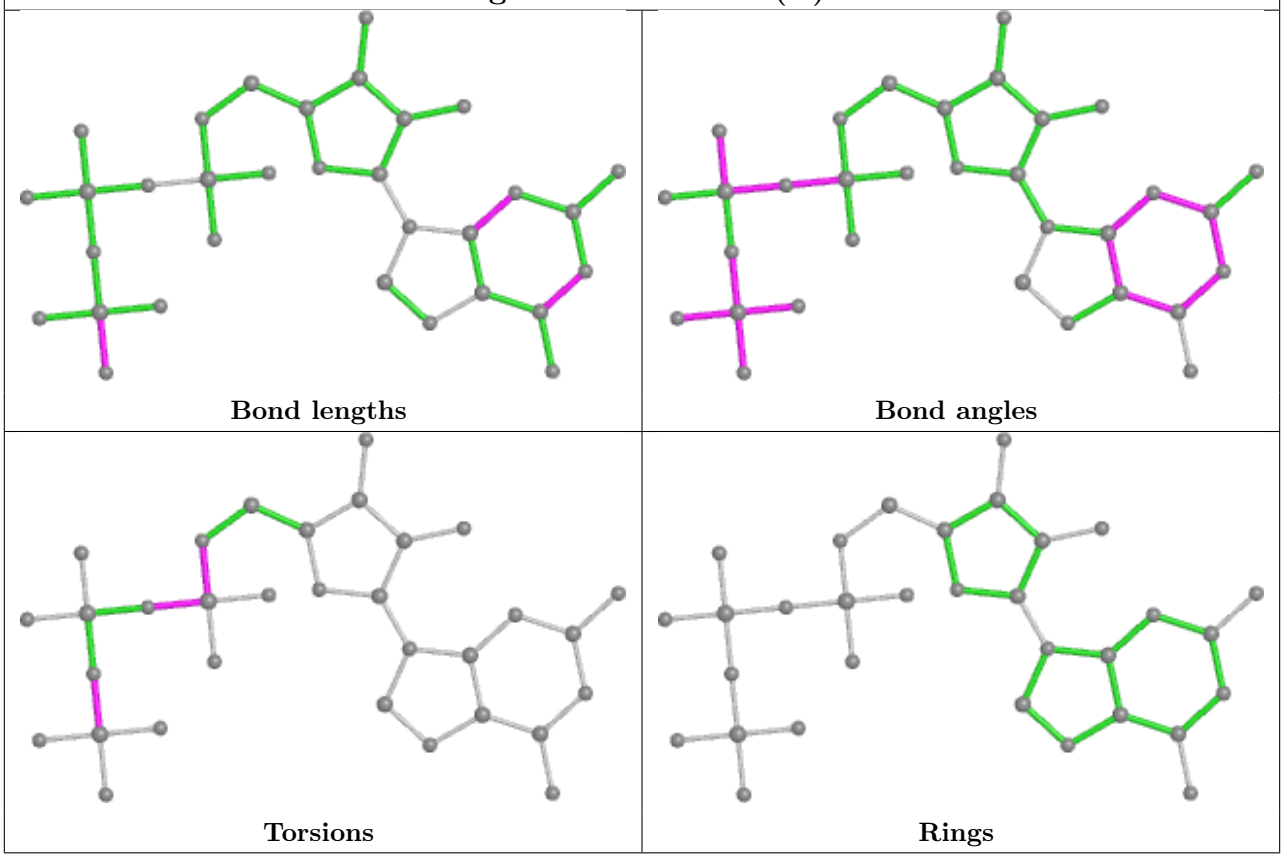
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500[B]	GNP	4	0

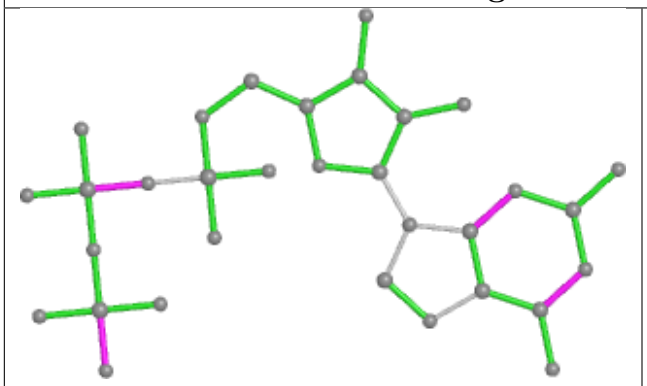
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

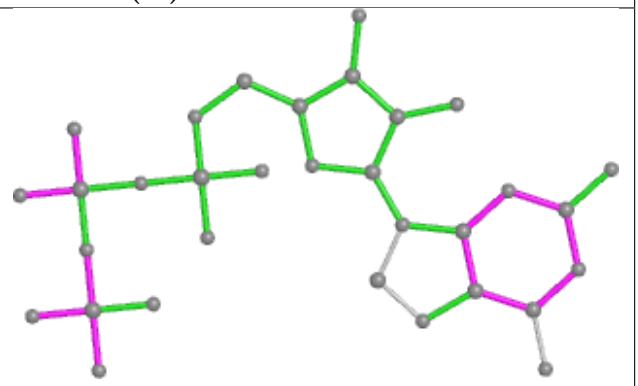
Ligand GNP A 500 (B)



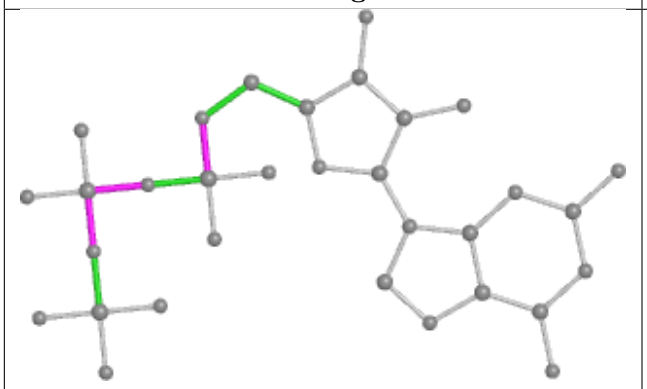
Ligand GNP A 500 (A)



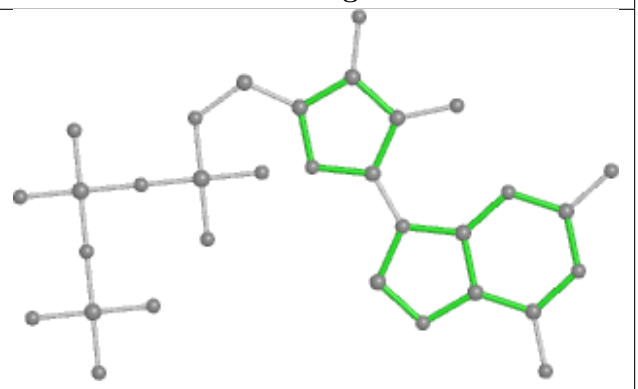
Bond lengths



Bond angles

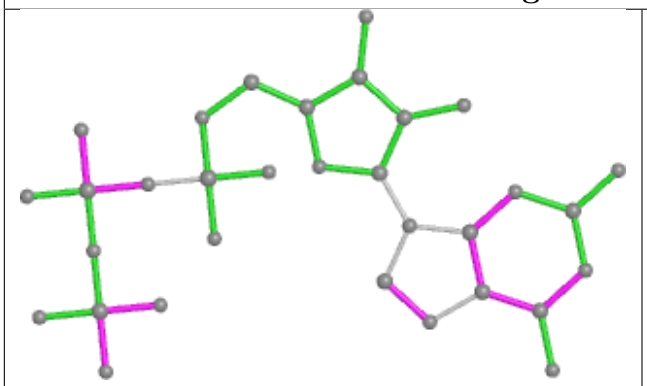


Torsions

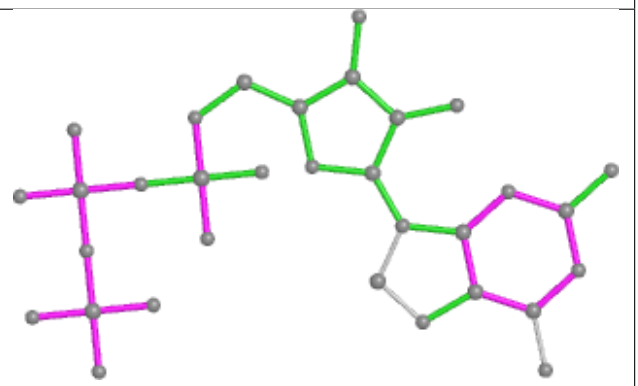


Rings

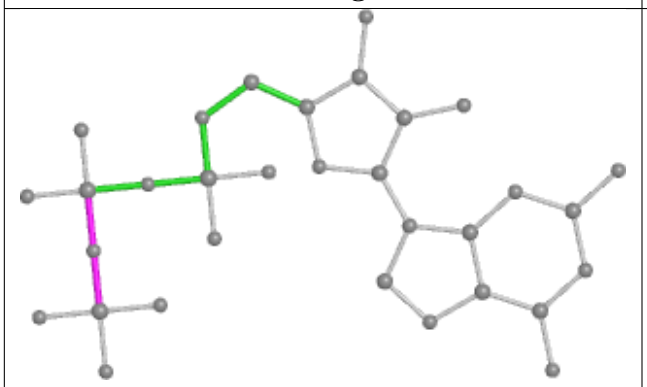
Ligand GNP B 500



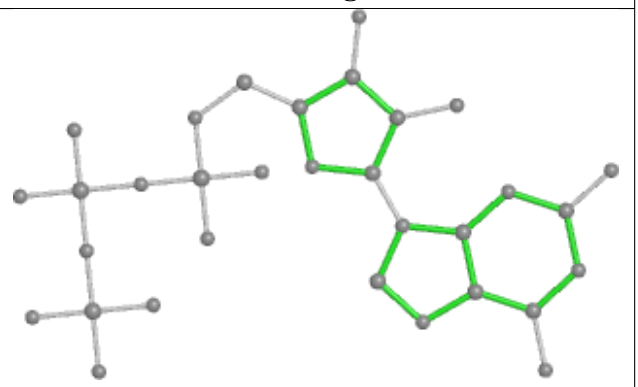
Bond lengths



Bond angles

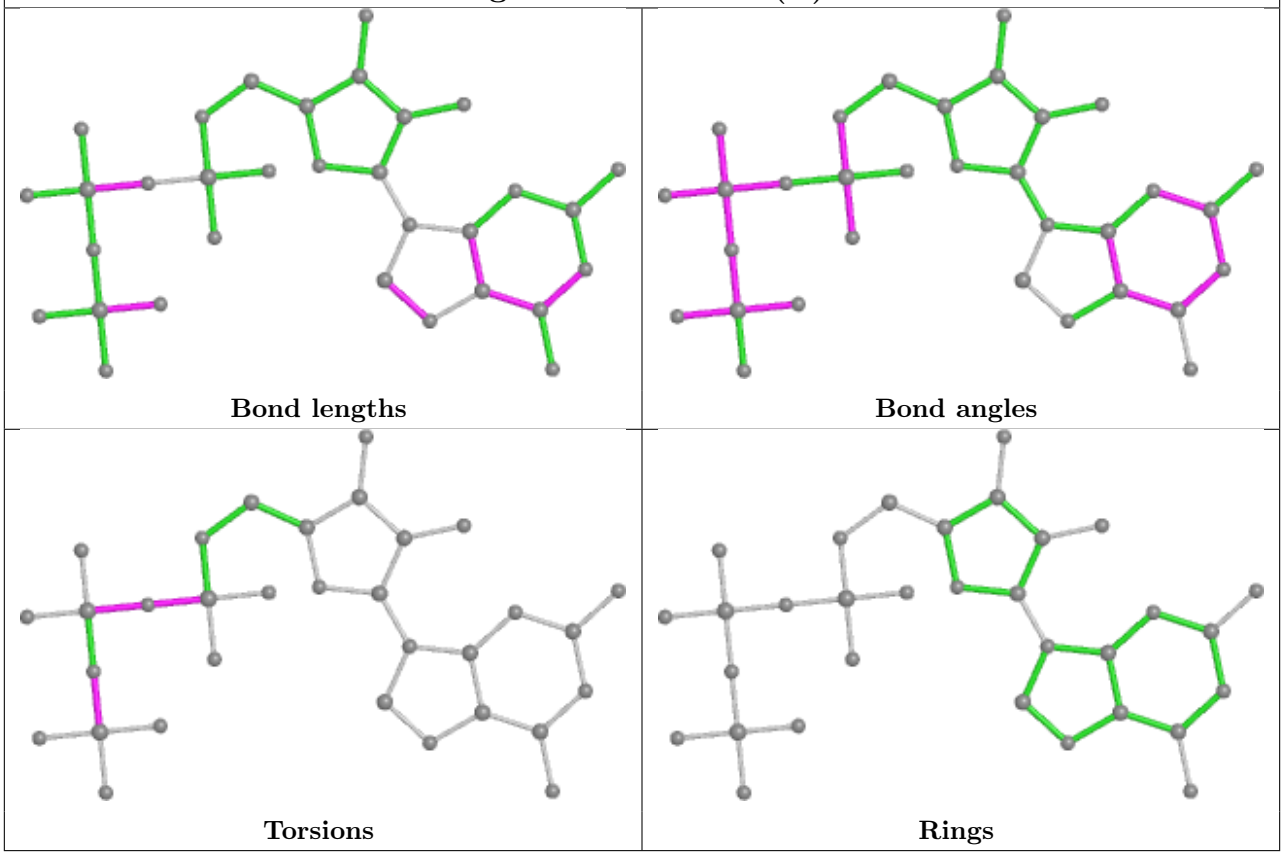


Torsions

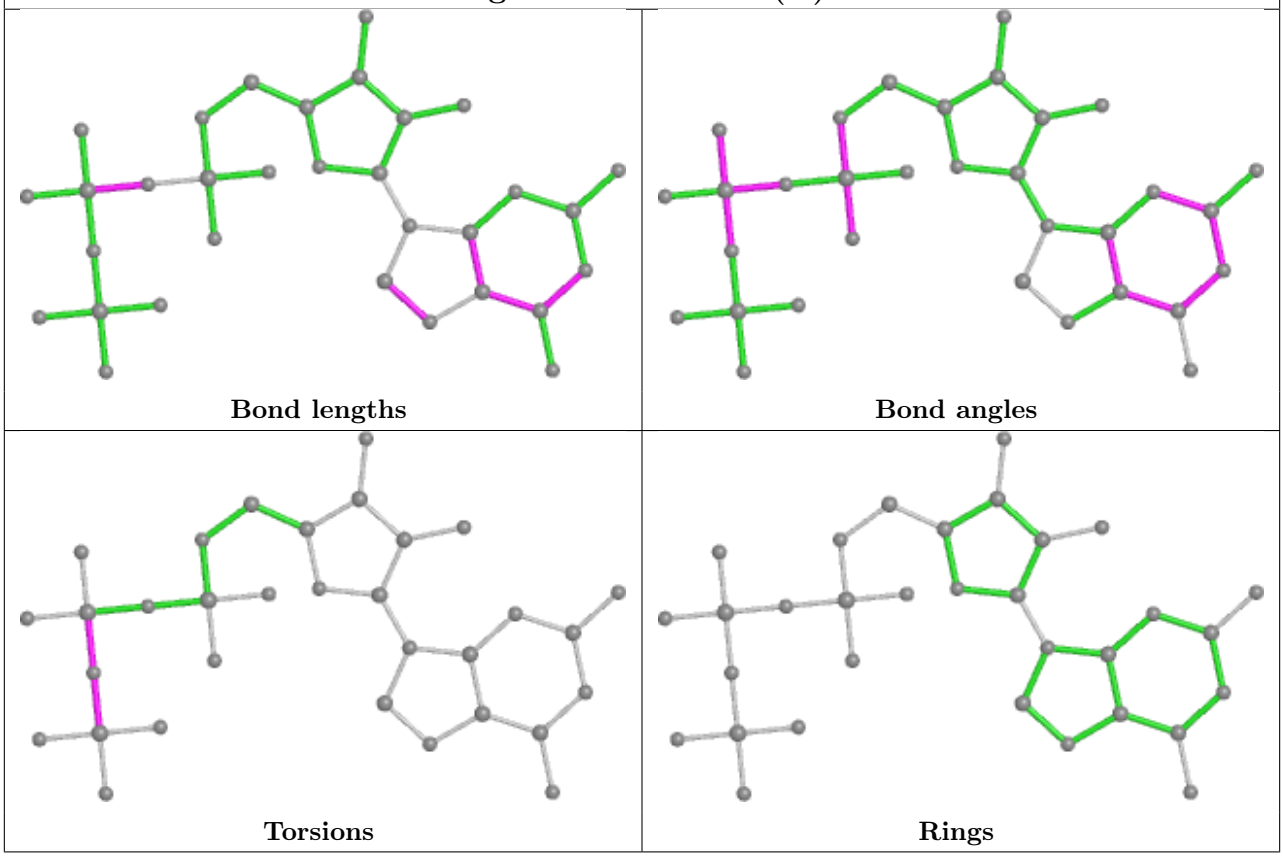


Rings

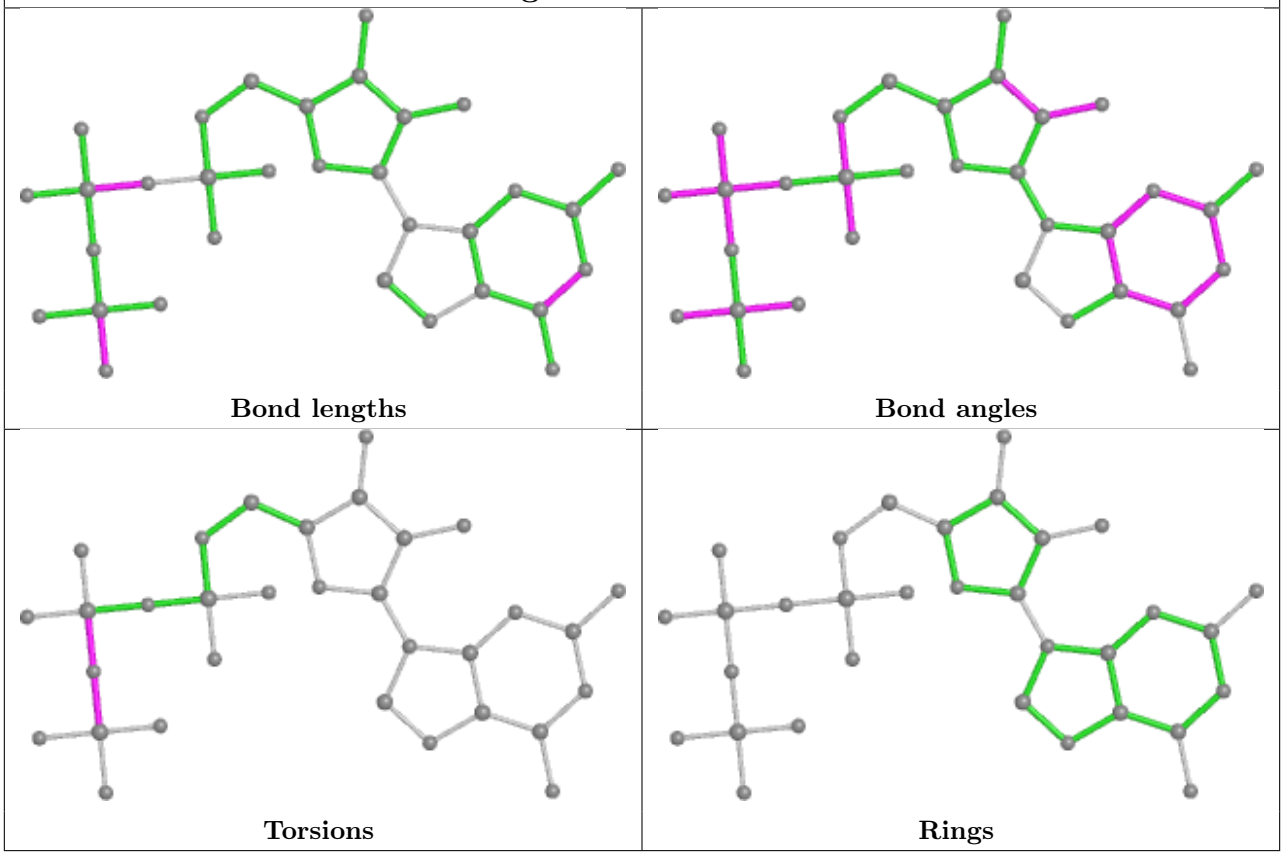
Ligand GNP C 500 (B)



Ligand GNP C 500 (A)



Ligand GNP D 500



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	288/305 (94%)	-0.05	1 (0%)	94	93	39, 57, 78, 177	0
1	B	295/305 (96%)	-0.04	3 (1%)	82	80	38, 54, 82, 101	0
1	C	289/305 (94%)	-0.06	1 (0%)	94	93	35, 57, 85, 110	0
1	D	293/305 (96%)	0.14	12 (4%)	37	36	49, 68, 98, 111	0
All	All	1165/1220 (95%)	-0.00	17 (1%)	73	72	35, 59, 89, 177	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	464	PHE	4.8
1	B	179	TYR	4.7
1	D	212	TYR	4.7
1	D	179	TYR	4.5
1	A	236	GLY	4.0
1	D	455	TYR	3.4
1	D	460	ILE	3.4
1	D	251	LEU	3.1
1	D	230	SER	2.8
1	B	182	ASN	2.7
1	D	181	ASP	2.6
1	B	212	TYR	2.4
1	D	461	LYS	2.2
1	D	182	ASN	2.1
1	D	470	LYS	2.1
1	D	456	GLY	2.1
1	C	212	TYR	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

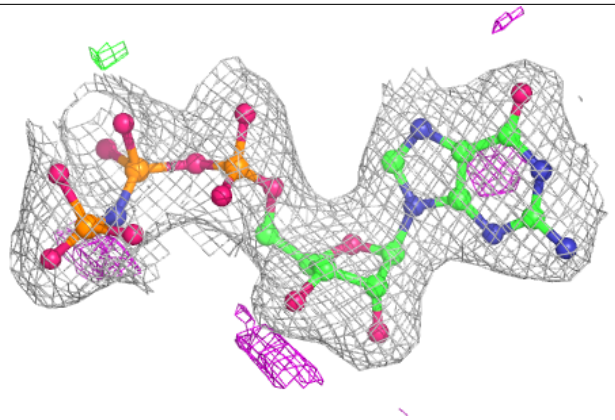
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

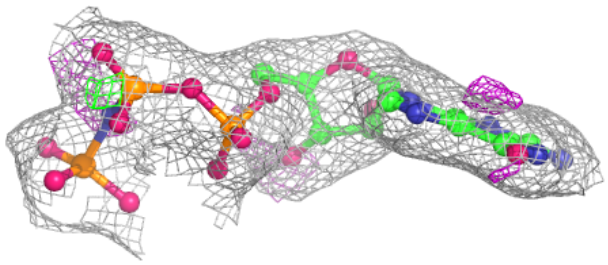
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	800	1/1	0.71	0.12	73,73,73,73	0
5	LIV	D	600[B]	30/52	0.80	0.30	88,96,110,115	30
5	LIV	D	600[A]	32/52	0.80	0.30	85,99,119,122	32
4	CL	C	802	1/1	0.85	0.10	77,77,77,77	0
4	CL	B	802	1/1	0.88	0.46	82,82,82,82	0
3	MG	C	702	1/1	0.95	0.10	51,51,51,51	0
3	MG	B	702	1/1	0.97	0.07	50,50,50,50	0
4	CL	A	802	1/1	0.97	0.38	77,77,77,77	0
2	GNP	B	500	32/32	0.98	0.13	39,49,58,59	0
2	GNP	C	500[A]	32/32	0.98	0.13	40,48,52,56	9
2	GNP	C	500[B]	32/32	0.98	0.13	40,49,52,56	9
3	MG	A	700	1/1	0.98	0.19	37,37,37,37	0
2	GNP	A	500[A]	32/32	0.98	0.16	41,44,49,52	9
2	GNP	A	500[B]	32/32	0.98	0.16	41,44,49,52	9
3	MG	D	702	1/1	0.99	0.06	58,58,58,58	0
3	MG	A	702	1/1	0.99	0.10	55,55,55,55	0
2	GNP	D	500	32/32	0.99	0.13	43,55,61,63	0
3	MG	B	700	1/1	1.00	0.20	26,26,26,26	0
3	MG	C	700	1/1	1.00	0.19	33,33,33,33	0
3	MG	D	700	1/1	1.00	0.17	29,29,29,29	0

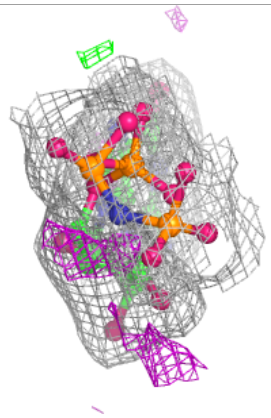
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GNP B 500:

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

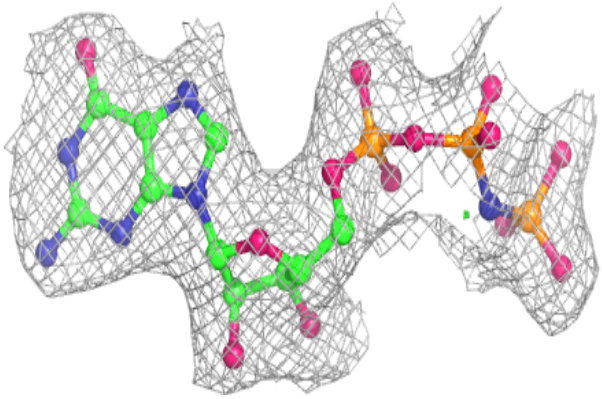


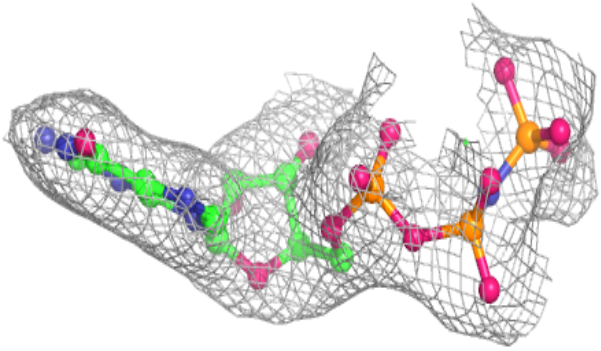


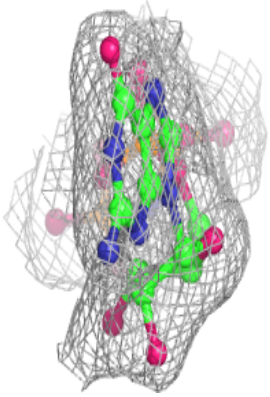


Electron density around GNP C 500 (A):

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

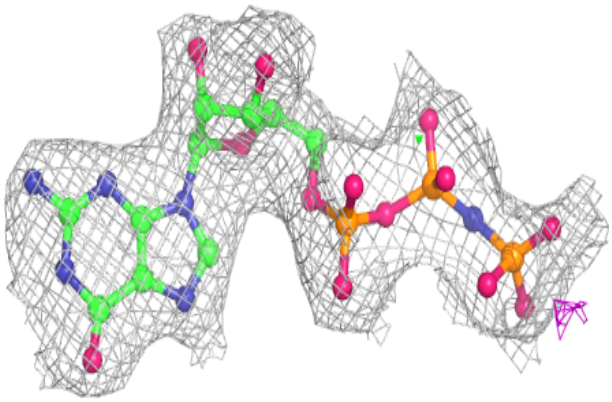


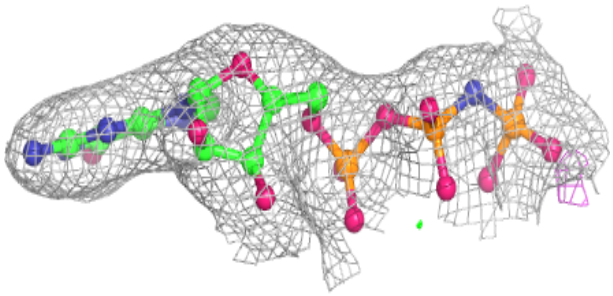


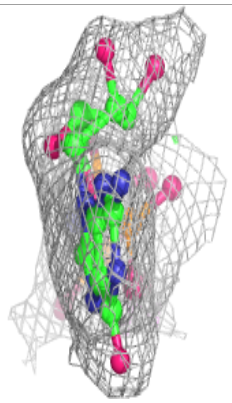


Electron density around GNP C 500 (B):

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

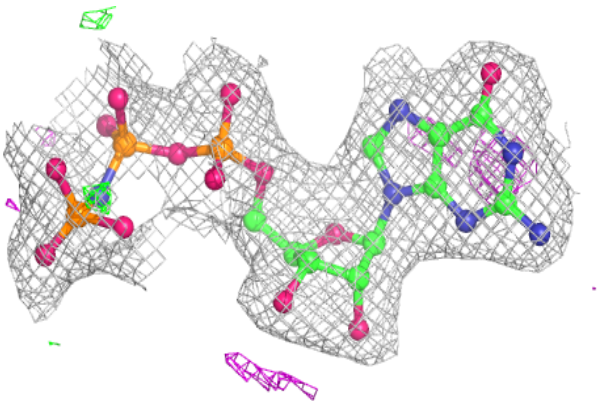


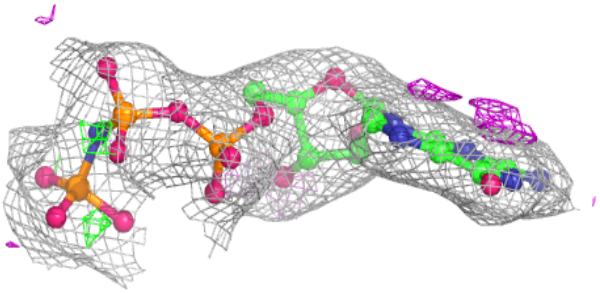


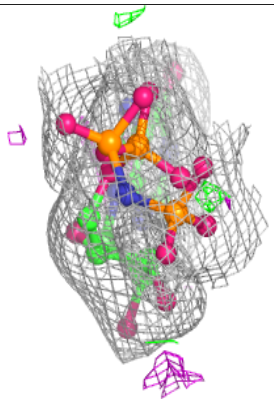


Electron density around GNP A 500 (A):

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

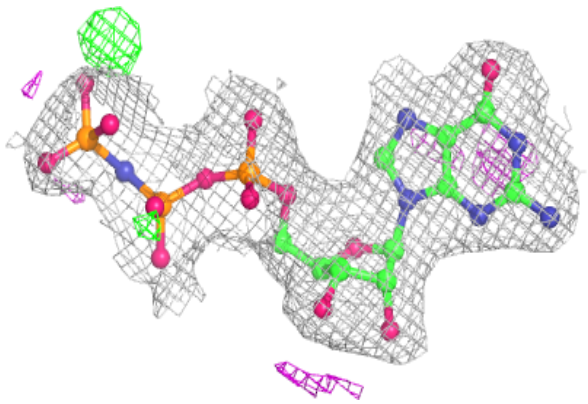


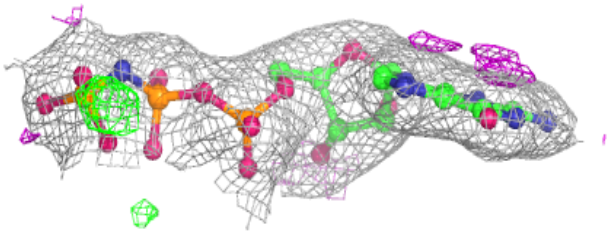


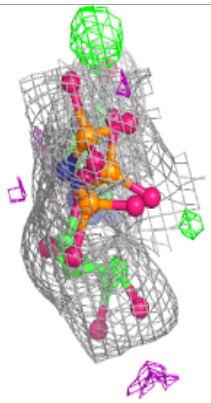


Electron density around GNP A 500 (B):

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

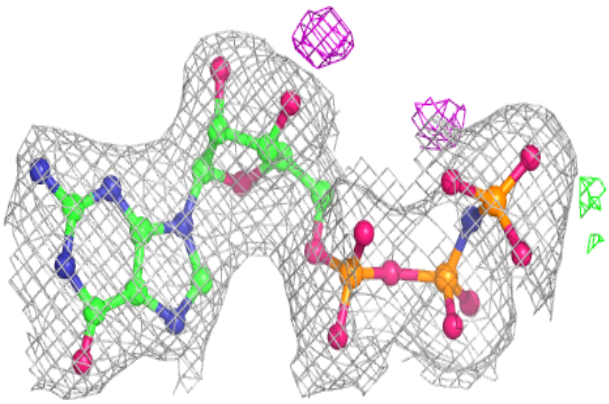


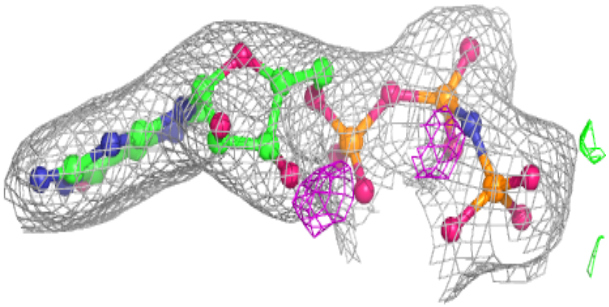


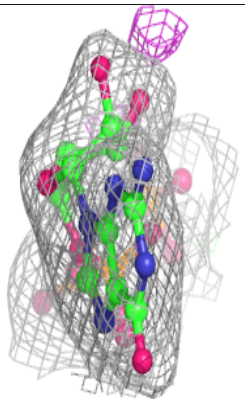


Electron density around GNP D 500:

$2mF_o$-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.