



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:10 pm BST

PDB ID : 6CAV
Title : Aminoglycoside Phosphotransferase (2'')-Ia in complex with GMPPNP, Magnesium, and Dibekacin
Authors : Caldwell, S.J.; Berghuis, A.M.
Deposited on : 2018-02-01
Resolution : 2.60 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

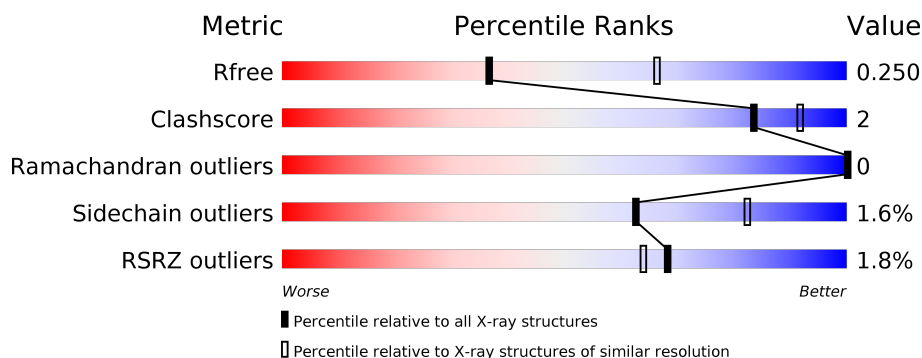
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	305	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	305	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>•</div> </div> </div>
1	C	305	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>•</div> <div>7%</div> </div> </div>
1	D	305	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>7%</div> </div> </div>

2 Entry composition [i](#)

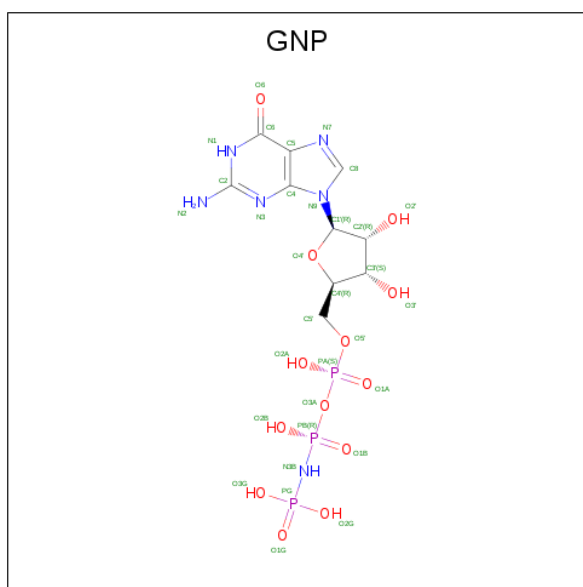
There are 6 unique types of molecules in this entry. The entry contains 10248 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	288	Total	C	N	O	S	0	0	0
			2383	1525	368	480	10			
1	B	292	Total	C	N	O	S	0	0	0
			2402	1536	372	484	10			
1	C	285	Total	C	N	O	S	0	0	0
			2363	1514	364	475	10			
1	D	284	Total	C	N	O	S	0	0	0
			2338	1497	361	470	10			

- 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
2	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
2	D	1	Total	C	N	O	P	0	0
			28	10	6	10	2		

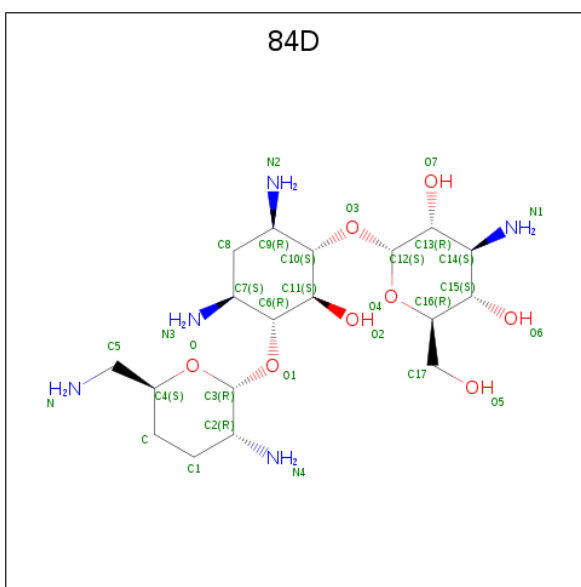
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 5 is Dibekacin (three-letter code: 84D) (formula: C₁₈H₃₇N₅O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 31	C 18	N 5	O 8	0	0
5	B	1	Total 31	C 18	N 5	O 8	0	0
5	C	1	Total 31	C 18	N 5	O 8	0	0
5	D	1	Total 31	C 18	N 5	O 8	0	0

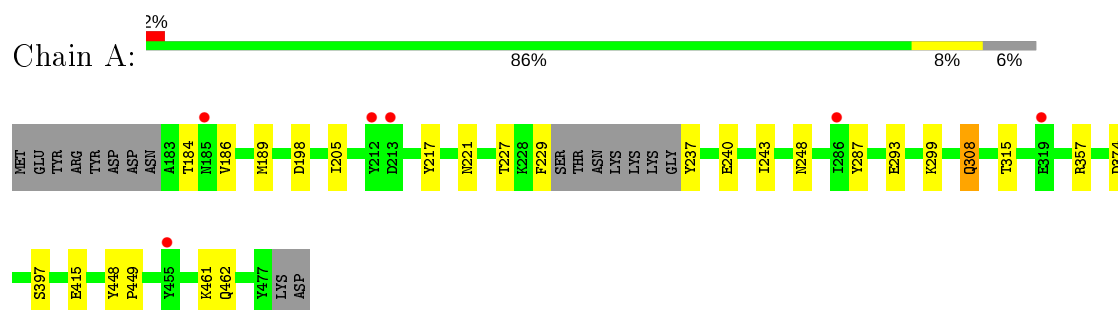
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	6	Total O 6 6	0	0
6	A	135	Total O 135 135	0	0
6	B	4	Total O 4 4	0	0
6	B	144	Total O 144 144	0	0
6	C	4	Total O 4 4	0	0
6	C	107	Total O 107 107	0	0
6	D	2	Total O 2 2	0	0
6	D	101	Total O 101 101	0	0

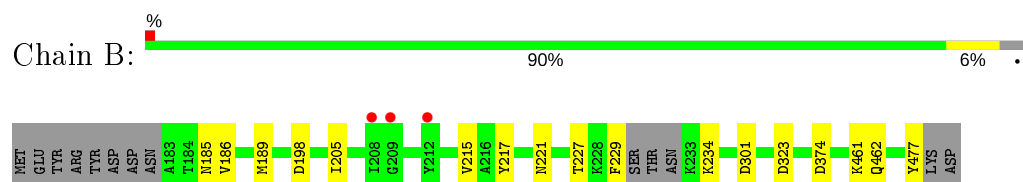
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

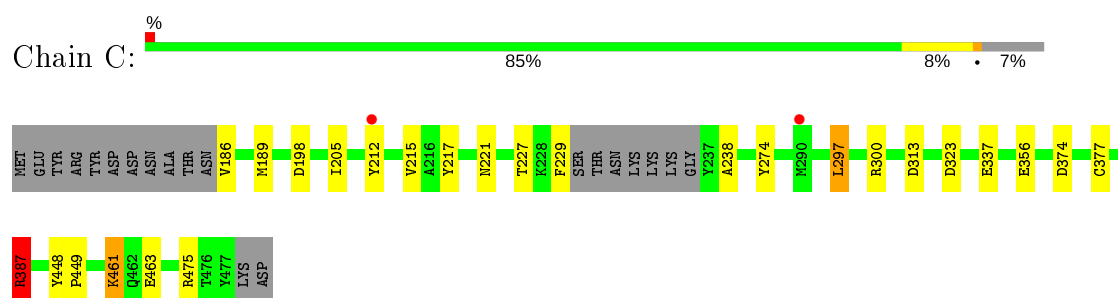
• Molecule 1: Bifunctional AAC/APH



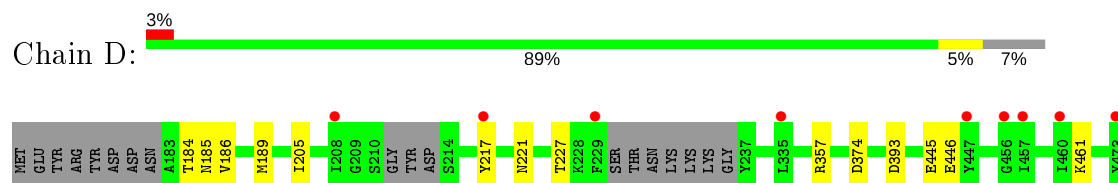
• Molecule 1: Bifunctional AAC/APH




• Molecule 1: Bifunctional AAC/APH



• Molecule 1: Bifunctional AAC/APH





K474	
R475	
T476	
TYR	
LYS	
ASP	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.99 Å 98.34 Å 93.22 Å 90.00° 105.24° 90.00°	Depositor
Resolution (Å)	89.94 – 2.60 86.83 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (89.94-2.60) 100.0 (86.83-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 2.58 Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.192 , 0.244 0.196 , 0.250	Depositor DCC
R_{free} test set	2438 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10248	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, 84D, MG, CL

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	0.91	1/2426 (0.0%)	0.92	2/3272 (0.1%)
1	B	0.91	1/2445 (0.0%)	0.91	2/3298 (0.1%)
1	C	0.92	3/2406 (0.1%)	0.93	6/3244 (0.2%)
1	D	0.86	0/2378	0.89	1/3206 (0.0%)
All	All	0.90	5/9655 (0.1%)	0.91	11/13020 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	356	GLU	CD-OE2	7.08	1.33	1.25
1	A	240	GLU	CD-OE1	6.41	1.32	1.25
1	C	229	PHE	C-O	-6.06	1.11	1.23
1	C	377	CYS	CB-SG	-5.48	1.72	1.81
1	B	229	PHE	C-O	-5.40	1.13	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	374	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	B	301	ASP	CB-CG-OD2	-8.14	110.97	118.30
1	C	475	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	387	ARG	NE-CZ-NH2	-6.32	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	297	LEU	CB-CG-CD1	6.26	121.64	111.00
1	C	374	ASP	CB-CG-OD1	5.71	123.44	118.30
1	C	323	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	357	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	323	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	C	337	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	374	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	234	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2383	0	2300	18	0
1	B	2402	0	2309	9	1
1	C	2363	0	2282	13	0
1	D	2338	0	2261	8	0
2	A	32	0	13	0	0
2	B	32	0	13	1	0
2	C	32	0	13	2	0
2	D	28	0	12	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	1	0
4	B	1	0	0	1	0
4	C	1	0	0	0	0
5	A	31	0	0	2	0
5	B	31	0	0	1	0
5	C	31	0	0	0	0
5	D	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	141	0	0	4	1
6	B	148	0	0	1	0
6	C	111	0	0	6	0
6	D	103	0	0	1	0
All	All	10248	0	9203	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:A:600:84D:O7	6:A:904:HOH:O	2.01	0.77
2:C:500:GNP:O2A	6:C:900:HOH:O	2.10	0.69
2:B:500:GNP:O3G	6:B:921:HOH:O	2.16	0.61
1:D:445:GLU:HG3	6:D:1160:HOH:O	2.01	0.60
1:D:186:VAL:HG13	1:D:205:ILE:HG23	1.85	0.58
1:A:184:THR:HB	1:B:185:ASN:OD1	2.05	0.57
1:A:315:THR:CG2	1:C:238:ALA:HB2	2.36	0.55
1:A:415:GLU:OE1	5:A:600:84D:N3	2.40	0.55
1:B:189:MET:HG2	1:B:217:TYR:CE1	2.41	0.55
1:A:189:MET:HG2	1:A:217:TYR:CE1	2.42	0.55
1:C:189:MET:HG2	1:C:217:TYR:CE1	2.42	0.55
1:A:229:PHE:C	6:A:1443:HOH:O	2.46	0.54
1:D:189:MET:HG2	1:D:217:TYR:CE1	2.43	0.53
1:A:237:TYR:HA	6:A:1103:HOH:O	2.10	0.52
1:A:462:GLN:NE2	4:A:802:CL:CL	2.77	0.52
1:A:184:THR:HG21	1:B:215:VAL:HG21	1.93	0.49
1:D:189:MET:SD	1:D:227:THR:HG21	2.54	0.48
1:A:186:VAL:HG13	1:A:205:ILE:HG23	1.96	0.47
1:C:212:TYR:HB2	6:C:1577:HOH:O	2.15	0.47
1:B:189:MET:SD	1:B:227:THR:HG21	2.56	0.46
1:D:186:VAL:CG1	1:D:205:ILE:HG23	2.44	0.46
1:A:248:ASN:OD1	6:A:1144:HOH:O	2.20	0.46
1:A:315:THR:HG23	1:C:238:ALA:HB2	1.98	0.45
1:C:387:ARG:HA	6:C:1268:HOH:O	2.16	0.45
1:A:243:ILE:HD13	1:A:397:SER:HB2	1.99	0.45
1:B:462:GLN:NE2	4:B:802:CL:CL	2.87	0.45
1:C:215:VAL:HG21	1:D:184:THR:HG21	1.98	0.44
1:A:184:THR:CG2	1:B:215:VAL:HG21	2.48	0.43
1:A:189:MET:SD	1:A:227:THR:HG21	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:VAL:HG13	1:B:205:ILE:HG23	2.01	0.43
1:C:463:GLU:HB3	6:C:1001:HOH:O	2.18	0.43
1:A:308:GLN:HB2	1:A:308:GLN:HE21	1.72	0.42
1:B:186:VAL:CG1	1:B:205:ILE:HG23	2.49	0.42
1:A:186:VAL:CG1	1:A:205:ILE:HG23	2.49	0.42
1:C:189:MET:SD	1:C:227:THR:HG21	2.60	0.42
1:C:461:LYS:HG3	6:C:1001:HOH:O	2.20	0.41
1:C:186:VAL:HG13	1:C:205:ILE:HG23	2.02	0.41
1:A:287:TYR:OH	1:A:299:LYS:HE3	2.19	0.41
1:D:393:ASP:OD2	2:D:500:GNP:N3B	2.53	0.41
1:C:448:TYR:HB3	1:C:449:PRO:HD3	2.03	0.41
1:C:274:TYR:OH	2:C:500:GNP:N7	2.41	0.41
1:C:313:ASP:HA	6:C:1401:HOH:O	2.21	0.41
1:A:448:TYR:HB3	1:A:449:PRO:HD3	2.03	0.40
1:B:374:ASP:OD2	5:B:600:84D:N1	2.54	0.40
1:D:357:ARG:NH1	1:D:446:GLU:OE2	2.45	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:B:477:TYR:O	6:A:1217:HOH:O[2_646]	1.94	0.26

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/305 (93%)	276 (97%)	8 (3%)	0	100	100
1	B	288/305 (94%)	277 (96%)	11 (4%)	0	100	100
1	C	281/305 (92%)	272 (97%)	9 (3%)	0	100	100
1	D	278/305 (91%)	267 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1131/1220 (93%)	1092 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/281 (94%)	260 (98%)	5 (2%)	57	79
1	B	265/281 (94%)	262 (99%)	3 (1%)	73	88
1	C	263/281 (94%)	257 (98%)	6 (2%)	50	75
1	D	260/281 (92%)	257 (99%)	3 (1%)	71	87
All	All	1053/1124 (94%)	1036 (98%)	17 (2%)	62	82

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	221	ASN
1	A	293	GLU
1	A	308	GLN
1	A	461	LYS
1	B	198	ASP
1	B	221	ASN
1	B	461	LYS
1	C	198	ASP
1	C	221	ASN
1	C	297	LEU
1	C	300	ARG
1	C	387	ARG
1	C	461	LYS
1	D	185	ASN
1	D	221	ASN
1	D	461	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	ASN
1	A	459	ASN
1	A	467	ASN
1	B	420	ASN
1	C	327	ASN
1	C	341	ASN
1	D	185	ASN
1	D	295	GLN
1	D	326	GLN
1	D	420	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 11 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	B	500	3	28,34,34	4.47	9 (32%)	30,54,54	2.87	12 (40%)
2	GNP	D	500	3	23,30,34	3.76	7 (30%)	24,47,54	2.27	6 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GNP	A	500	3	28,34,34	3.53	11 (39%)	30,54,54	1.85	5 (16%)
5	84D	D	600	-	32,33,33	0.82	1 (3%)	40,48,48	2.61	11 (27%)
5	84D	B	600	-	32,33,33	1.01	1 (3%)	40,48,48	2.18	9 (22%)
5	84D	C	600	-	32,33,33	0.44	0	40,48,48	1.38	8 (20%)
5	84D	A	600	-	32,33,33	0.53	0	40,48,48	1.77	10 (25%)
2	GNP	C	500	3	28,34,34	3.51	11 (39%)	30,54,54	2.02	5 (16%)

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	B	500	3	-	4/17/38/38	0/3/3/3
2	GNP	D	500	3	-	3/12/32/38	0/3/3/3
2	GNP	A	500	3	-	5/17/38/38	0/3/3/3
5	84D	D	600	-	-	3/12/65/65	0/3/3/3
5	84D	B	600	-	-	3/12/65/65	0/3/3/3
5	84D	C	600	-	-	2/12/65/65	0/3/3/3
5	84D	A	600	-	-	4/12/65/65	0/3/3/3
2	GNP	C	500	3	-	6/17/38/38	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	GNP	PG-O1G	17.01	1.73	1.46
2	D	500	GNP	PB-O1B	13.85	1.68	1.46
2	A	500	GNP	C5-C6	-10.17	1.35	1.52
2	A	500	GNP	C4-N9	-9.70	1.34	1.47
2	B	500	GNP	PB-O3A	8.93	1.70	1.59
2	C	500	GNP	C5-C6	-8.72	1.37	1.52
2	C	500	GNP	PG-O1G	8.65	1.59	1.46
2	B	500	GNP	C4-N9	-8.35	1.36	1.47
2	D	500	GNP	C4-N9	-8.06	1.37	1.47
2	C	500	GNP	PB-O1B	8.01	1.58	1.46
2	C	500	GNP	C4-N9	-7.89	1.37	1.47
2	B	500	GNP	C5-C6	-7.68	1.39	1.52
2	A	500	GNP	PG-O1G	6.72	1.56	1.46
2	A	500	GNP	PB-O1B	4.66	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	GNP	PB-O3A	4.64	1.64	1.59
2	D	500	GNP	PB-O2B	-4.43	1.44	1.56
2	A	500	GNP	PB-O2B	-4.39	1.44	1.56
2	A	500	GNP	C6-N1	4.08	1.39	1.33
2	C	500	GNP	PB-O2B	-3.83	1.46	1.56
5	B	600	84D	O7-C13	3.83	1.52	1.43
2	A	500	GNP	PG-O2G	-3.74	1.46	1.56
2	C	500	GNP	PG-O2G	-3.66	1.46	1.56
2	D	500	GNP	C6-N1	3.34	1.38	1.33
2	B	500	GNP	PG-O3G	-3.23	1.48	1.56
2	B	500	GNP	C5-C4	-3.07	1.34	1.53
2	B	500	GNP	C8-N9	-3.03	1.35	1.45
5	D	600	84D	O7-C13	2.98	1.50	1.43
2	C	500	GNP	C6-N1	2.93	1.38	1.33
2	B	500	GNP	PB-O1B	2.86	1.50	1.46
2	A	500	GNP	PG-O3G	2.84	1.64	1.56
2	C	500	GNP	PG-O3G	2.62	1.63	1.56
2	A	500	GNP	C5-C4	-2.44	1.38	1.53
2	A	500	GNP	C2-N1	-2.31	1.34	1.44
2	A	500	GNP	C8-N9	-2.29	1.37	1.45
2	D	500	GNP	C8-N9	-2.28	1.37	1.45
2	B	500	GNP	C2-N1	-2.25	1.35	1.44
2	D	500	GNP	C5-C4	-2.11	1.40	1.53
2	C	500	GNP	C5-C4	-2.11	1.40	1.53
2	C	500	GNP	C2-N1	-2.02	1.36	1.44
2	C	500	GNP	C8-N9	-2.01	1.38	1.45

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	600	84D	C3-O-C4	9.16	123.28	113.13
2	B	500	GNP	O1G-PG-N3B	-8.68	98.99	111.77
2	A	500	GNP	C4-C5-N7	6.98	111.71	102.46
2	C	500	GNP	C4-C5-N7	6.32	110.84	102.46
2	B	500	GNP	C4-C5-N7	5.87	110.23	102.46
5	D	600	84D	O7-C13-C12	5.83	124.20	110.05
2	D	500	GNP	C4-C5-N7	5.74	110.06	102.46
5	B	600	84D	C12-C13-C14	-5.66	102.79	110.40
5	B	600	84D	O7-C13-C14	5.64	120.35	110.22
2	D	500	GNP	C5-C6-N1	-5.52	111.39	118.19
2	C	500	GNP	C5-C6-N1	-5.29	111.67	118.19
5	B	600	84D	O3-C12-O4	-5.25	96.01	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	600	84D	O3-C10-C11	5.21	121.15	107.28
5	B	600	84D	O7-C13-C12	5.07	122.36	110.05
2	D	500	GNP	O6-C6-C5	4.97	130.01	119.86
5	D	600	84D	O3-C12-O4	-4.85	97.12	110.67
5	D	600	84D	C12-C13-C14	-4.84	103.90	110.40
2	B	500	GNP	O6-C6-C5	4.58	129.22	119.86
2	B	500	GNP	C5-C6-N1	-4.51	112.63	118.19
5	A	600	84D	C3-O-C4	4.30	117.89	113.13
5	D	600	84D	O1-C3-C2	4.21	115.27	108.23
2	B	500	GNP	O3A-PB-N3B	-4.03	95.42	106.59
2	C	500	GNP	O6-C6-C5	4.00	128.02	119.86
2	C	500	GNP	O1G-PG-N3B	-3.89	106.04	111.77
5	A	600	84D	O3-C12-O4	-3.86	99.89	110.67
5	A	600	84D	O6-C15-C14	3.71	116.89	110.22
2	B	500	GNP	O6-C6-N1	-3.54	117.93	122.69
5	D	600	84D	O7-C13-C14	3.54	116.57	110.22
2	B	500	GNP	O2B-PB-O1B	-3.53	102.52	109.92
5	A	600	84D	O7-C13-C14	3.43	116.38	110.22
5	A	600	84D	C12-C13-C14	-3.23	106.06	110.40
5	D	600	84D	O3-C12-C13	3.18	116.34	108.10
5	A	600	84D	C-C1-C2	3.17	119.21	111.29
2	D	500	GNP	O6-C6-N1	-3.05	118.60	122.69
2	A	500	GNP	C5-C6-N1	-3.02	114.47	118.19
5	B	600	84D	O3-C12-C13	3.02	115.92	108.10
2	B	500	GNP	O2B-PB-O3A	3.00	114.64	104.64
2	B	500	GNP	O3'-C3'-C4'	-2.97	102.46	111.05
2	B	500	GNP	O3G-PG-O1G	2.95	120.87	113.45
5	D	600	84D	O1-C6-C11	2.85	114.85	107.28
5	C	600	84D	C3-O1-C6	2.84	124.98	117.96
5	C	600	84D	O6-C15-C16	-2.82	102.29	109.30
2	A	500	GNP	O3G-PG-O2G	2.82	115.15	107.64
5	C	600	84D	O2-C11-C6	2.70	117.10	109.94
5	B	600	84D	C-C1-C2	-2.69	104.56	111.29
5	A	600	84D	C13-C14-N1	2.68	116.55	111.05
5	C	600	84D	C12-C13-C14	-2.67	106.82	110.40
5	C	600	84D	O7-C13-C14	2.53	114.76	110.22
2	A	500	GNP	O6-C6-C5	2.53	125.02	119.86
2	A	500	GNP	O5'-PA-O1A	2.50	118.82	109.07
2	D	500	GNP	O3'-C3'-C4'	2.42	118.04	111.05
5	B	600	84D	C-C4-C5	-2.40	108.25	112.83
5	B	600	84D	O1-C6-C7	-2.33	103.62	109.18
5	A	600	84D	O2-C11-C6	2.33	116.11	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	600	84D	C3-O-C4	2.30	115.68	113.13
5	D	600	84D	C9-C8-C7	-2.28	106.50	111.18
2	D	500	GNP	O2B-PB-O3A	-2.24	97.17	104.64
5	B	600	84D	O3-C10-C9	-2.21	103.91	109.18
5	A	600	84D	C12-O4-C16	2.16	117.93	113.69
5	C	600	84D	O6-C15-C14	2.13	114.05	110.22
5	A	600	84D	C3-O1-C6	2.12	123.21	117.96
5	C	600	84D	O-C4-C5	-2.11	101.05	108.89
5	D	600	84D	O1-C6-C7	-2.09	104.18	109.18
2	C	500	GNP	PA-O3A-PB	-2.08	125.28	132.62
2	B	500	GNP	O2A-PA-O1A	2.06	122.42	112.24
2	B	500	GNP	O3G-PG-O2G	2.02	113.03	107.64

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	GNP	PB-N3B-PG-O1G
2	B	500	GNP	C2'-C1'-N9-C8
2	B	500	GNP	C2'-C1'-N9-C4
2	D	500	GNP	C2'-C1'-N9-C8
2	D	500	GNP	C2'-C1'-N9-C4
2	A	500	GNP	PG-N3B-PB-O1B
2	A	500	GNP	O4'-C1'-N9-C4
2	A	500	GNP	C2'-C1'-N9-C8
2	A	500	GNP	C2'-C1'-N9-C4
2	C	500	GNP	PB-N3B-PG-O1G
2	C	500	GNP	PG-N3B-PB-O1B
2	C	500	GNP	C2'-C1'-N9-C8
5	A	600	84D	O4-C16-C17-O5
5	B	600	84D	C11-C6-O1-C3
5	A	600	84D	C15-C16-C17-O5
5	C	600	84D	O-C3-O1-C6
5	A	600	84D	C11-C6-O1-C3
5	D	600	84D	C11-C6-O1-C3
5	B	600	84D	O-C3-O1-C6
5	C	600	84D	C11-C6-O1-C3
5	B	600	84D	C7-C6-O1-C3
5	A	600	84D	C7-C6-O1-C3
2	C	500	GNP	PG-N3B-PB-O3A
5	D	600	84D	O-C3-O1-C6
2	A	500	GNP	PB-O3A-PA-O2A

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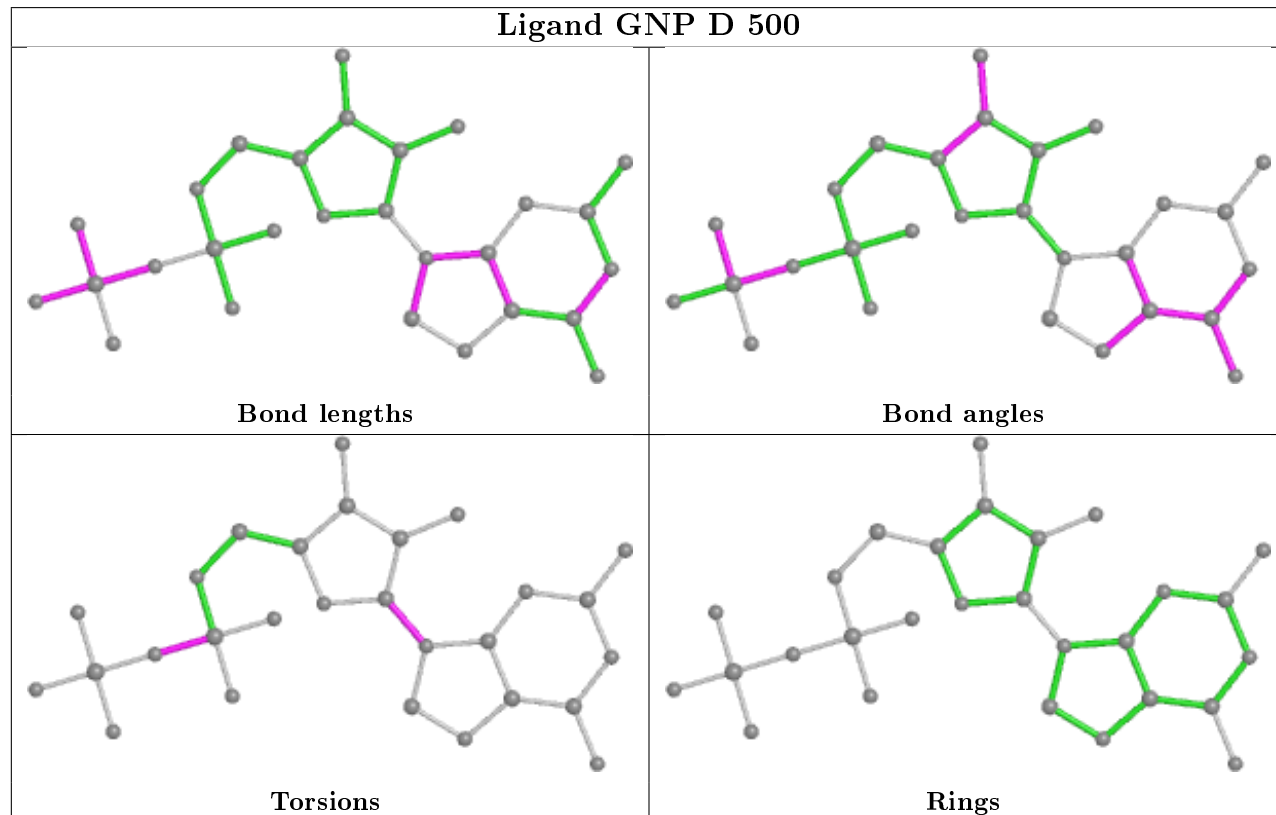
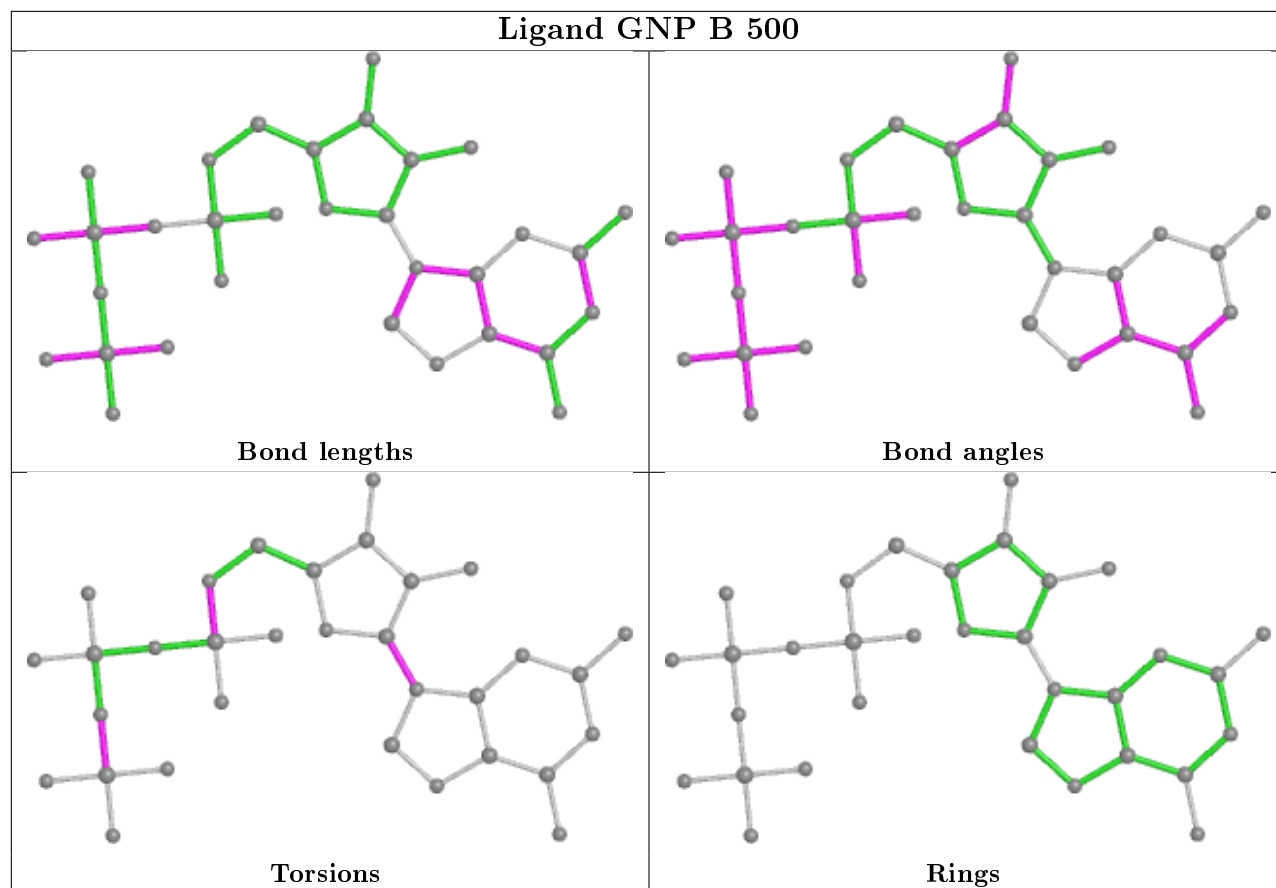
Mol	Chain	Res	Type	Atoms
2	C	500	GNP	PB-O3A-PA-O1A
2	D	500	GNP	PB-O3A-PA-O2A
5	D	600	84D	C7-C6-O1-C3
2	B	500	GNP	C5'-O5'-PA-O1A
2	C	500	GNP	C2'-C1'-N9-C4

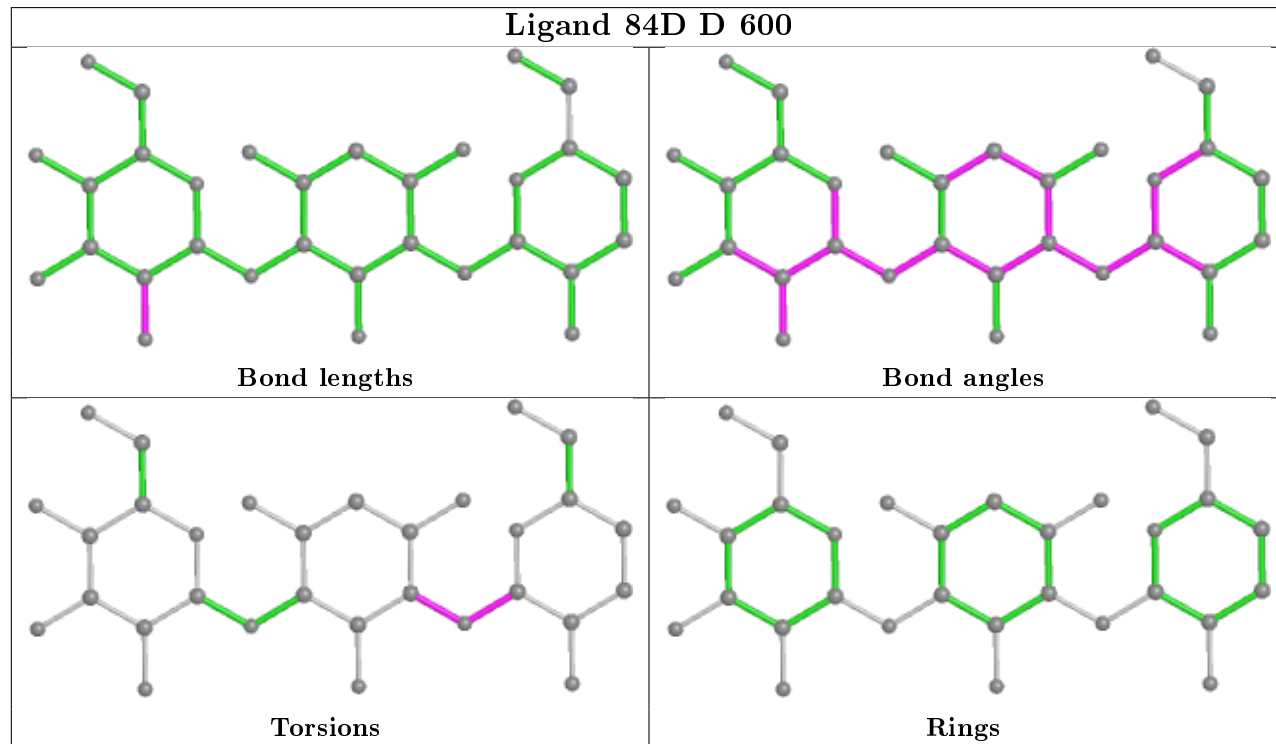
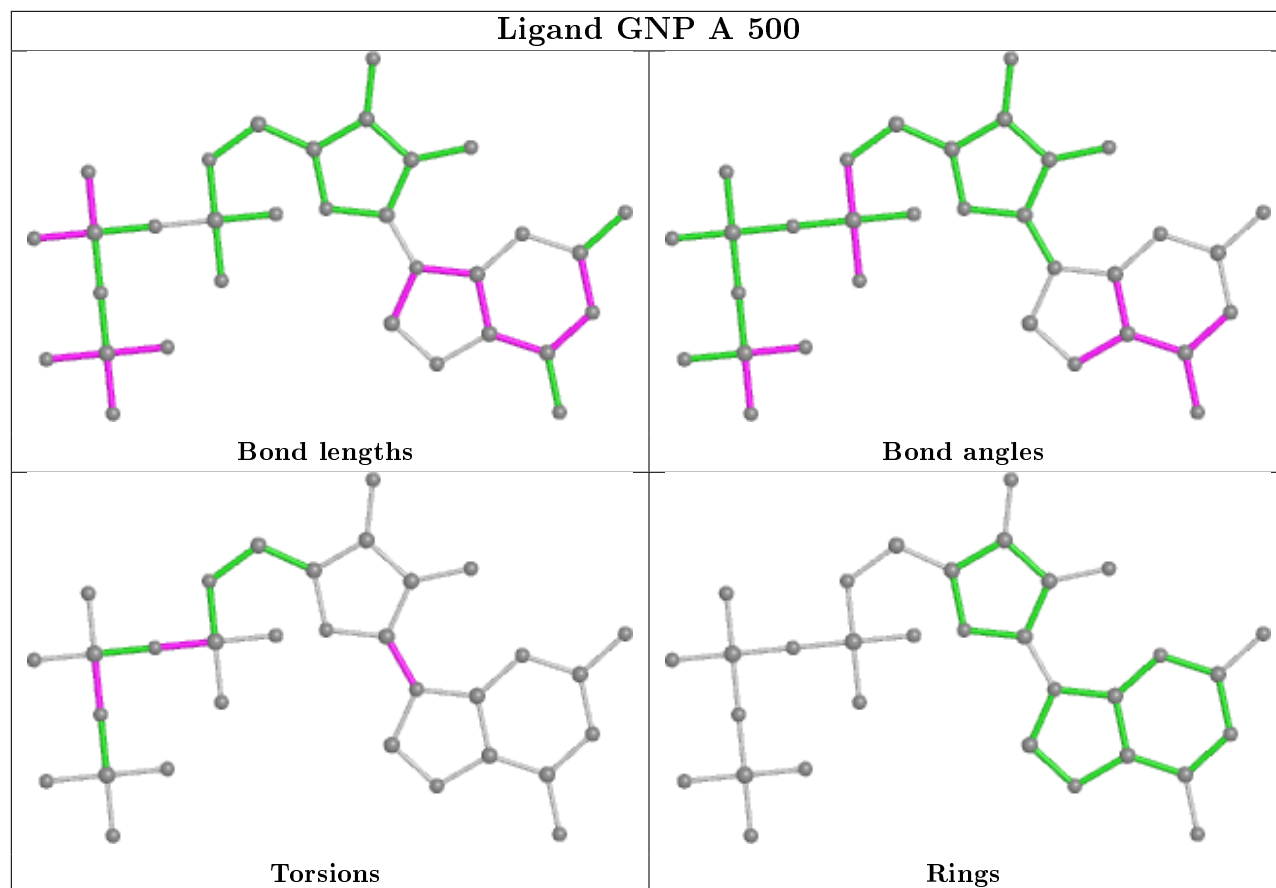
There are no ring outliers.

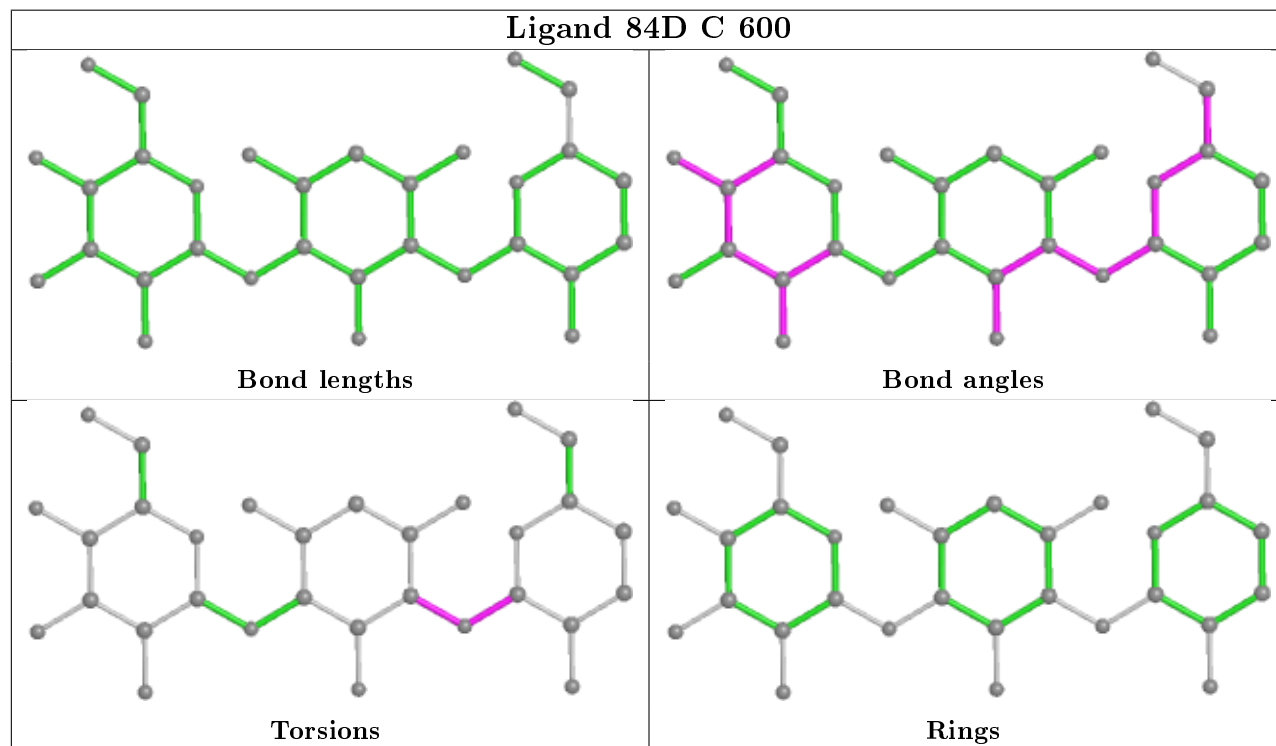
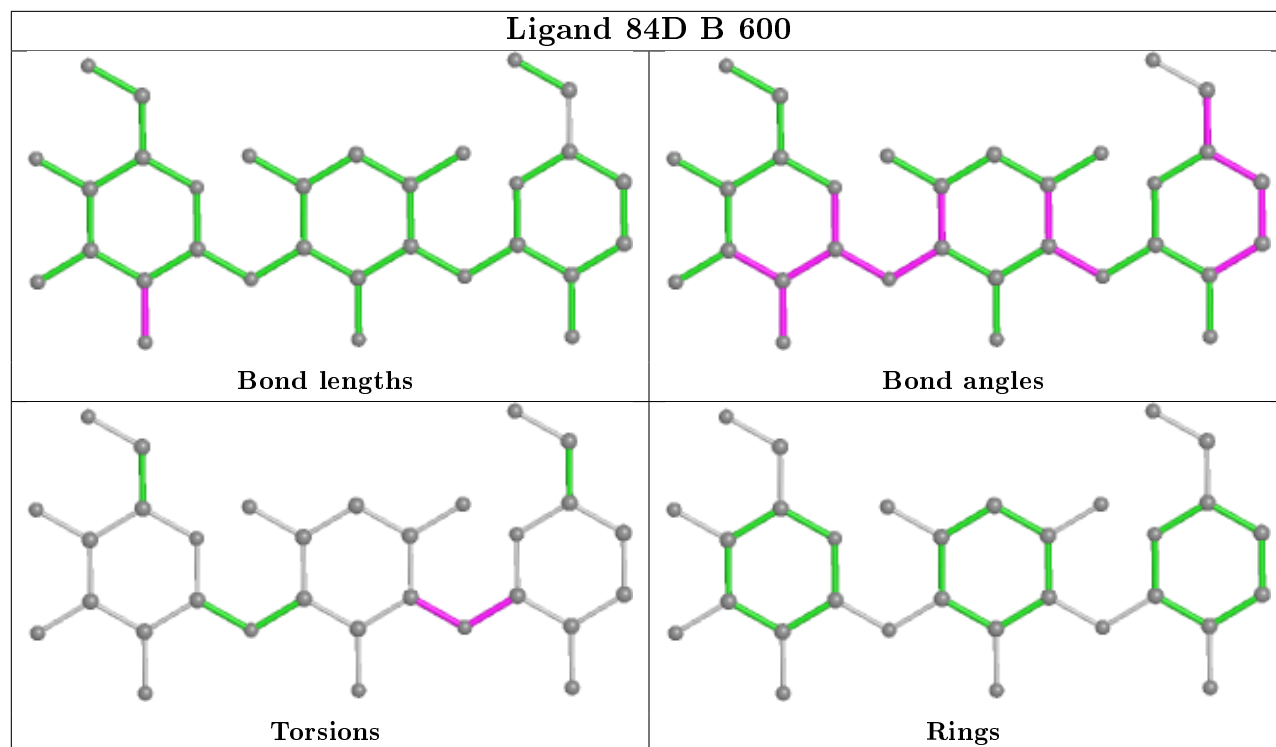
5 monomers are involved in 7 short contacts:

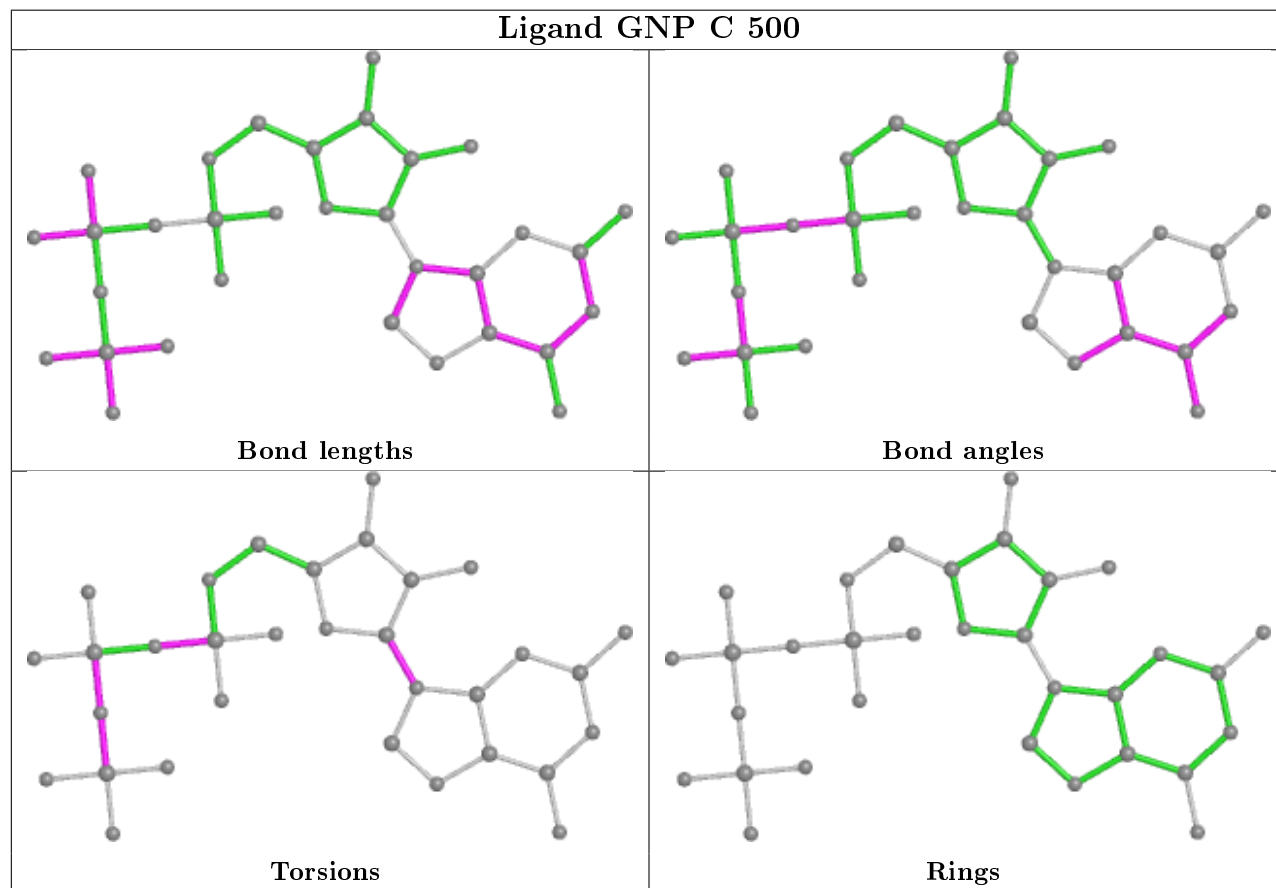
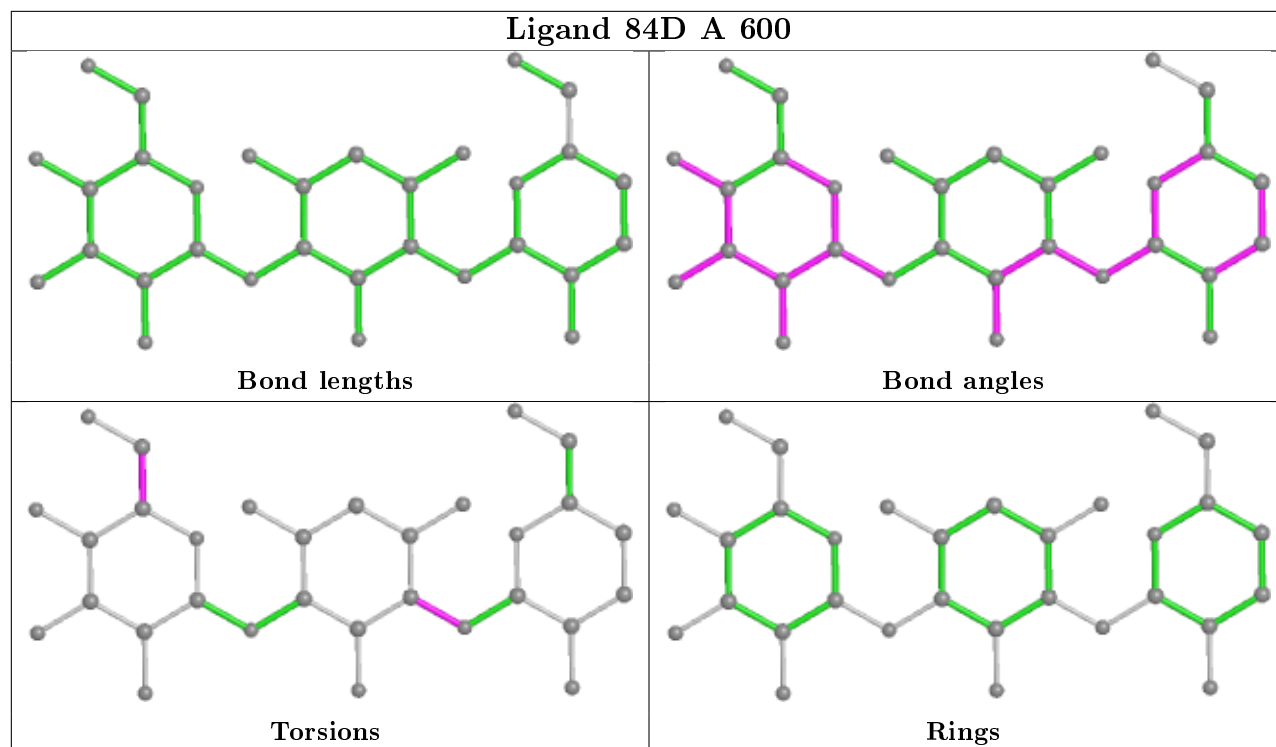
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	GNP	1	0
2	D	500	GNP	1	0
5	B	600	84D	1	0
5	A	600	84D	2	0
2	C	500	GNP	2	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	288/305 (94%)	0.02	6 (2%) 63 58	40, 60, 84, 114	0
1	B	292/305 (95%)	-0.02	3 (1%) 82 80	39, 57, 85, 106	0
1	C	285/305 (93%)	0.18	2 (0%) 87 86	37, 63, 98, 128	0
1	D	284/305 (93%)	0.17	10 (3%) 44 36	49, 68, 94, 115	0
All	All	1149/1220 (94%)	0.09	21 (1%) 68 64	37, 61, 92, 128	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	290	MET	3.7
1	B	212	TYR	3.6
1	B	209	GLY	2.9
1	A	455	TYR	2.9
1	D	473	TYR	2.9
1	D	474	LYS	2.8
1	D	460	ILE	2.7
1	D	217	TYR	2.7
1	C	212	TYR	2.5
1	B	208	ILE	2.5
1	D	456	GLY	2.5
1	A	212	TYR	2.4
1	D	457	ILE	2.3
1	D	335	LEU	2.3
1	A	185	ASN	2.3
1	D	229	PHE	2.3
1	D	208	ILE	2.2
1	A	213	ASP	2.1
1	D	447	TYR	2.1
1	A	319	GLU	2.1
1	A	286	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

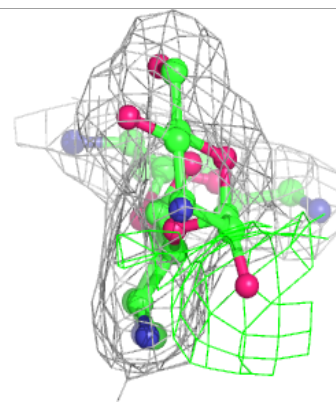
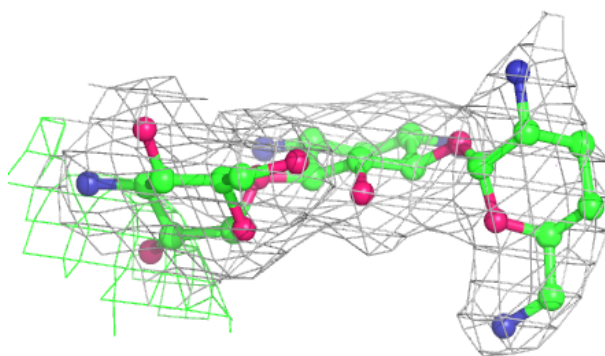
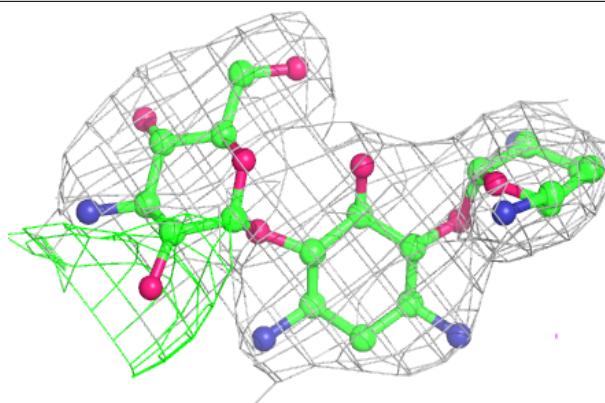
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	D	700	1/1	0.77	0.25	64,64,64,64	0
4	CL	C	802	1/1	0.87	0.10	69,69,69,69	0
4	CL	B	802	1/1	0.89	0.11	85,85,85,85	0
5	84D	D	600	31/31	0.90	0.16	47,55,62,62	0
5	84D	C	600	31/31	0.92	0.16	60,64,74,76	0
2	GNP	D	500	28/32	0.92	0.15	57,61,70,72	0
3	MG	B	700	1/1	0.92	0.26	52,52,52,52	0
5	84D	B	600	31/31	0.93	0.18	49,54,56,58	0
5	84D	A	600	31/31	0.94	0.14	52,57,65,66	0
3	MG	B	702	1/1	0.95	0.12	69,69,69,69	0
2	GNP	A	500	32/32	0.96	0.16	45,51,58,59	0
3	MG	A	700	1/1	0.96	0.10	48,48,48,48	0
2	GNP	B	500	32/32	0.96	0.17	51,56,67,71	0
2	GNP	C	500	32/32	0.97	0.15	49,54,58,62	0
3	MG	C	702	1/1	0.97	0.17	56,56,56,56	0
3	MG	D	702	1/1	0.97	0.26	59,59,59,59	0
3	MG	A	702	1/1	0.98	0.12	53,53,53,53	0
4	CL	A	802	1/1	0.98	0.23	72,72,72,72	0
3	MG	C	700	1/1	0.98	0.13	46,46,46,46	0

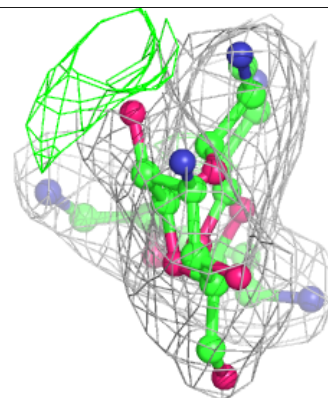
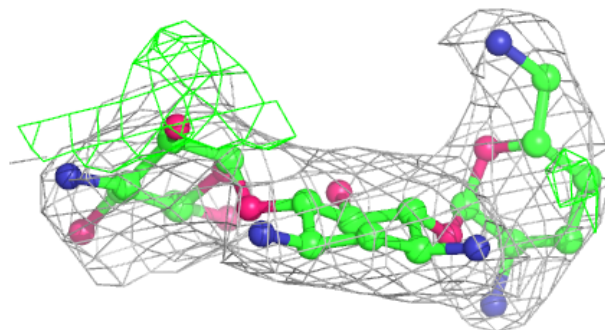
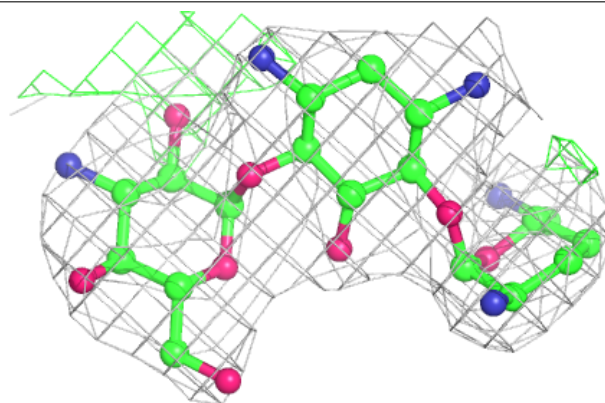
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 84D D 600:

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

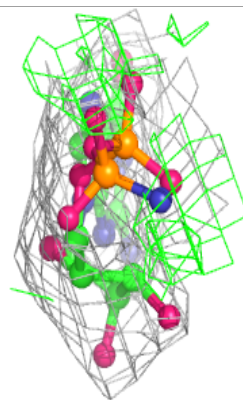
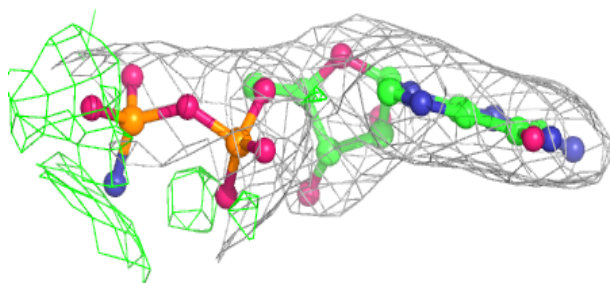
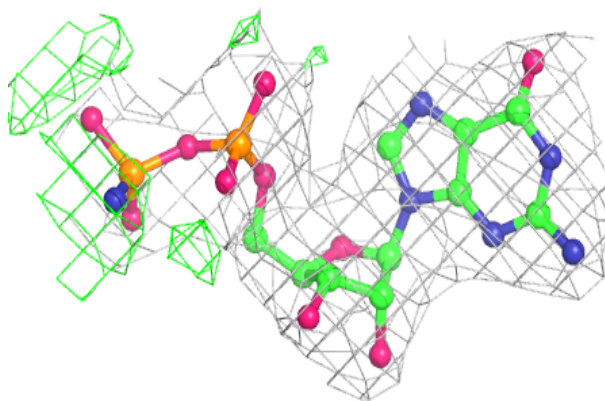
**Electron density around 84D C 600:**

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

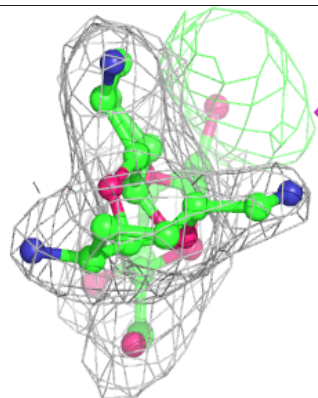
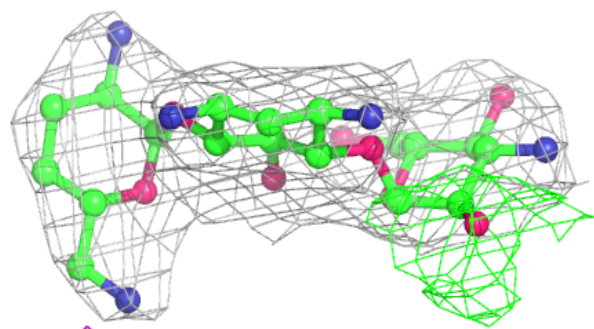
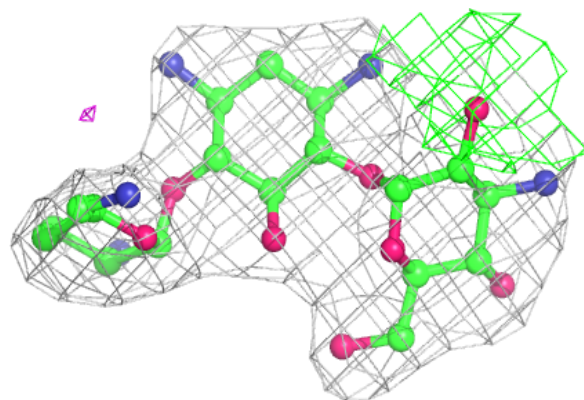


Electron density around GNP D 500:

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

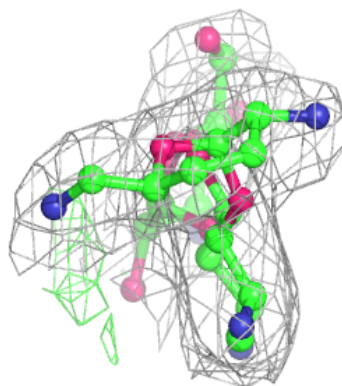
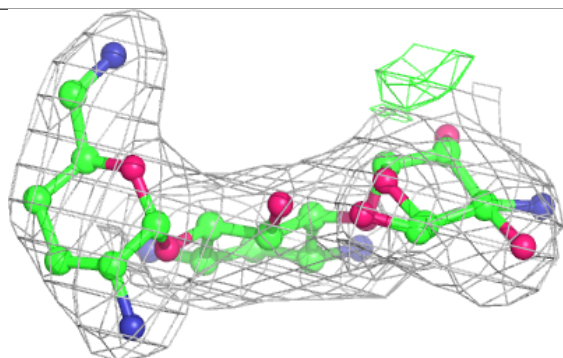
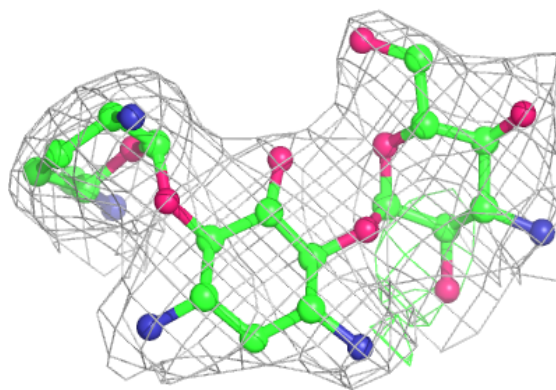
**Electron density around 84D B 600:**

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

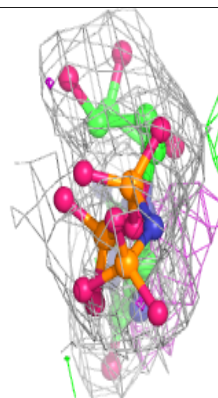
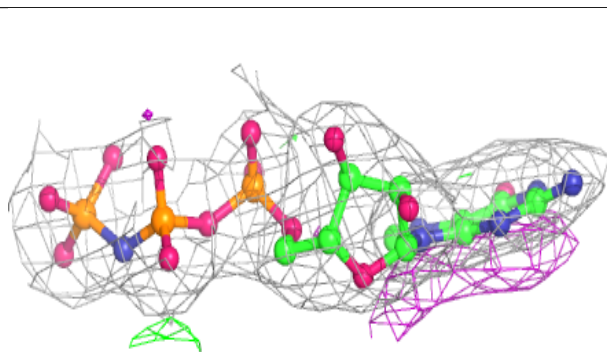
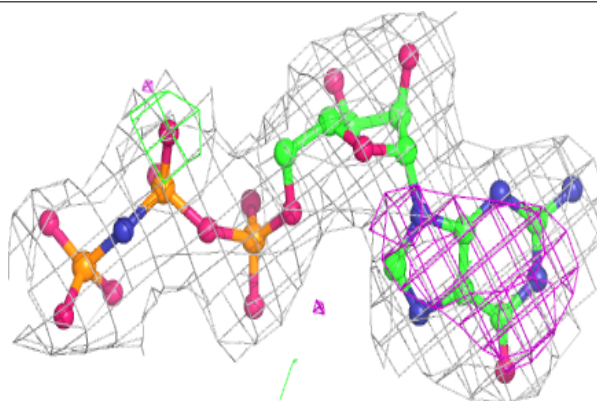


Electron density around 84D A 600:

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

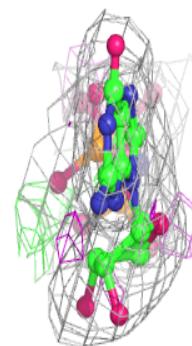
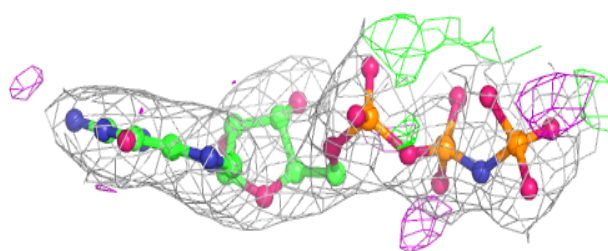
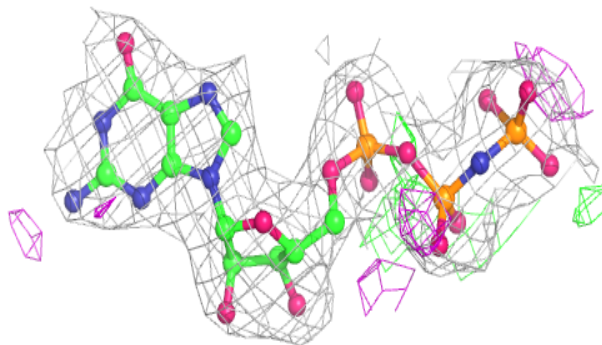
**Electron density around GNP A 500:**

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

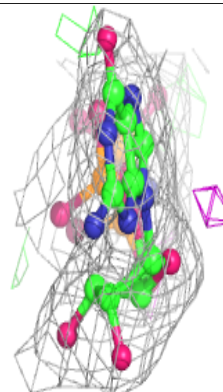
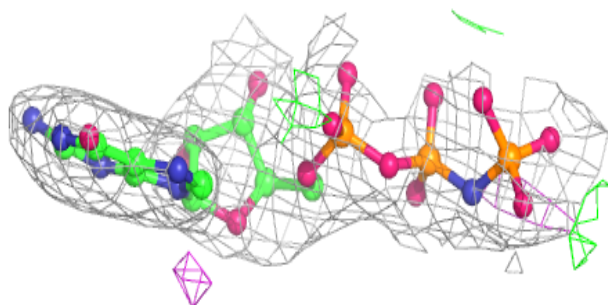
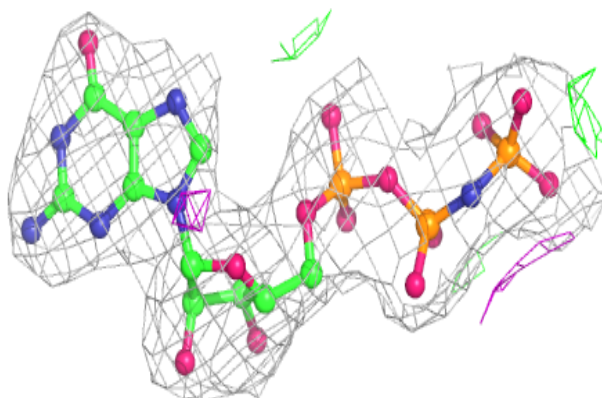


Electron density around GNP B 500:

$2mF_o-DF_c$ (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:**

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



6.5 Other polymers

There are no such residues in this entry.