



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:01 AM UTC

PDB ID : 5IQE / pdb_00005iqe
Title : Aminoglycoside Phosphotransferase (2'')-Ia (CTD of AAC(6')-Ie/APH(2'')-Ia)
in complex with GMPPNP, Magnesium, and Neomycin B
Authors : Caldwell, S.J.; Berghuis, A.M.
Deposited on : 2016-03-10
Resolution : 2.50 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 types of validation reports are described at

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

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

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

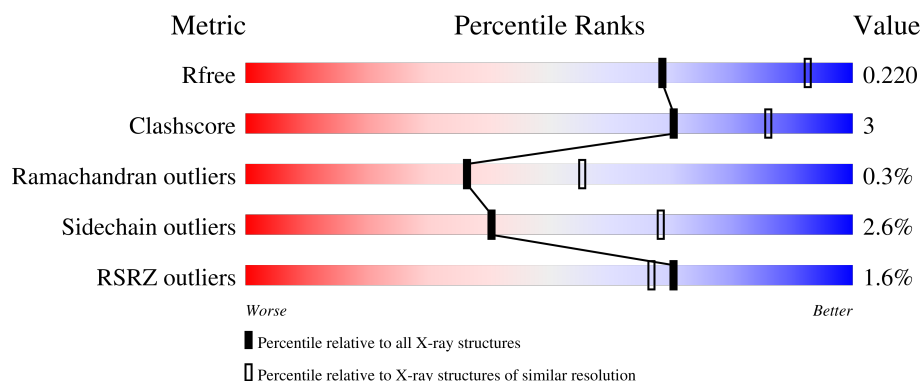
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	 2% 90% 6% . .
1	B	305	 2% 88% 7% . .
1	C	305	 2% 88% 7% . .
1	D	305	 % 91% . . .

2 Entry composition [i](#)

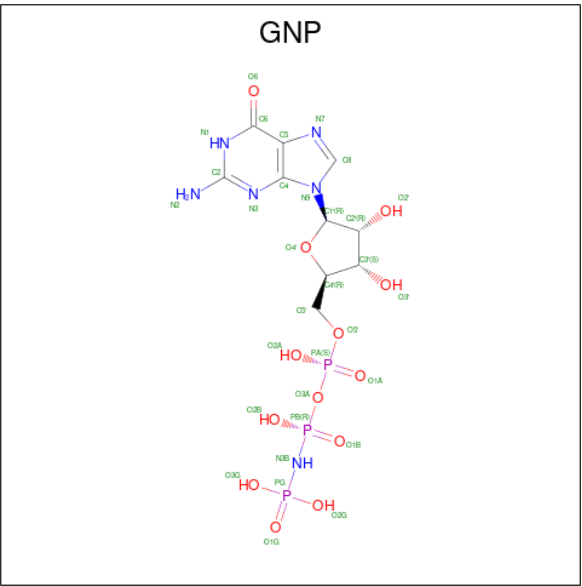
There are 6 unique types of molecules in this entry. The entry contains 10539 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	295	Total	C	N	O	S	0	0	0
			2423	1547	376	490	10			
1	B	295	Total	C	N	O	S	0	0	0
			2425	1551	374	490	10			
1	C	292	Total	C	N	O	S	0	0	0
			2410	1540	373	487	10			
1	D	292	Total	C	N	O	S	0	0	0
			2411	1540	372	489	10			

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



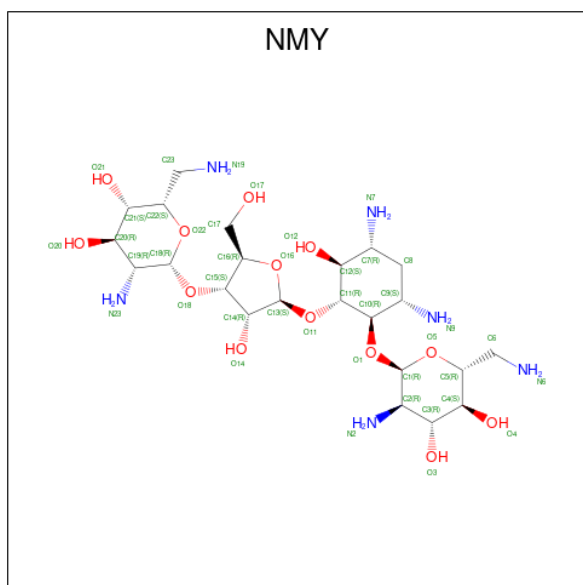
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
2	B	1	Total	C	N	O	P	0	1
			41	10	7	19	5		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is NEOMYCIN (CCD ID: NMY) (formula: $\text{C}_{23}\text{H}_{46}\text{N}_6\text{O}_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 42	C 23	N 6	O 13	0	0
3	B	1	Total 42	C 23	N 6	O 13	0	0
3	C	1	Total 42	C 23	N 6	O 13	0	0
3	D	1	Total 42	C 23	N 6	O 13	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

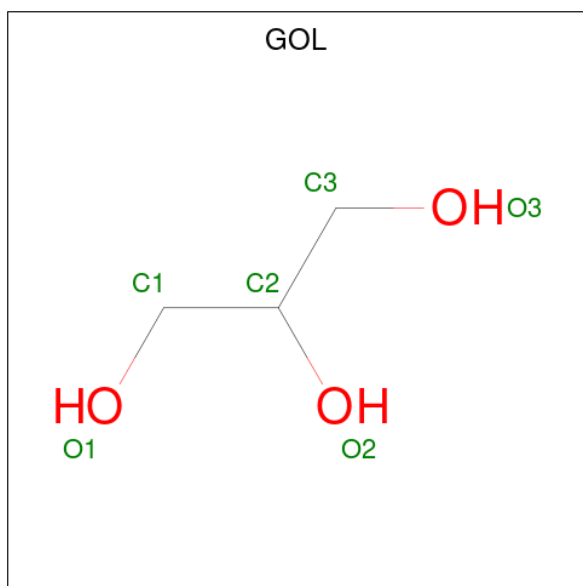
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Mg 2 2	0	0
4	B	2	Total Mg 2 2	0	0
4	C	2	Total Mg 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Mg	0	0
			2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

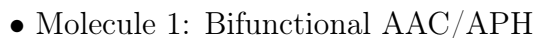


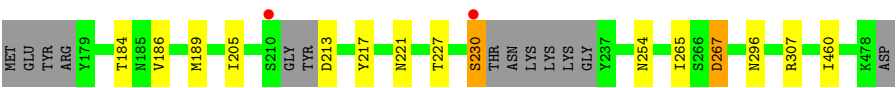
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	147	Total	O	0	0
			147	147		
6	B	167	Total	O	0	0
			167	167		
6	C	138	Total	O	0	0
			138	138		
6	D	99	Total	O	0	0
			99	99		

- Molecule 1: Bifunctional AAC/APH





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.18Å 100.36Å 93.94Å 90.00° 105.30° 90.00°	Depositor
Resolution (Å)	90.61 – 2.50 90.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (90.61-2.50) 99.9 (90.61-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.169 , 0.214 (Not available) , 0.220	Depositor DCC
R_{free} test set	2804 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.2	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	0.97	EDS
Total number of atoms	10539	wwPDB-VP
Average B, all atoms (Å ²)	70.0	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, GOL, NMY, 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	0.87	0/2466	0.90	1/3327 (0.0%)
1	B	0.88	0/2469	0.89	2/3331 (0.1%)
1	C	0.90	0/2453	0.91	3/3306 (0.1%)
1	D	0.79	0/2453	0.86	0/3308
All	All	0.86	0/9841	0.89	6/13272 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	CYS	CB-CA-C	-7.13	98.91	110.74
1	A	339	ILE	N-CA-C	6.20	118.97	112.83
1	C	407	ILE	N-CA-CB	5.72	118.33	110.54
1	C	339	ILE	N-CA-C	5.64	118.41	112.83
1	B	339	ILE	N-CA-C	5.54	118.32	112.83
1	C	394	PHE	N-CA-C	-5.20	107.11	112.93

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	2423	0	2327	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2425	0	2323	16	0
1	C	2410	0	2322	13	0
1	D	2411	0	2313	9	0
2	A	32	0	13	1	0
2	B	41	0	2	0	0
2	C	32	0	13	1	0
2	D	32	0	13	1	0
3	A	42	0	46	7	0
3	B	42	0	46	6	0
3	C	42	0	46	3	0
3	D	42	0	46	3	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	B	6	0	8	0	0
6	A	147	0	0	8	0
6	B	167	0	0	4	0
6	C	138	0	0	9	0
6	D	99	0	0	4	0
All	All	10539	0	9518	66	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 3.

All (66) 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:A:230:SER:HB2	1:A:267:ASP:O	1.54	1.05
1:D:230:SER:HB2	1:D:267:ASP:O	1.65	0.94
1:B:230:SER:HB2	1:B:267:ASP:O	1.66	0.93
1:A:319:GLU:OE2	6:A:1274:HOH:O	2.01	0.78
1:B:374:ASP:OD1	3:B:600:NMY:N7	2.17	0.78
1:D:254:ASN:HB2	6:D:1500:HOH:O	1.87	0.73
2:A:500:GNP:O1B	6:A:901:HOH:O	2.08	0.72
6:A:1274:HOH:O	1:C:265:ILE:O	2.10	0.68
1:A:230:SER:CB	1:A:267:ASP:O	2.35	0.68
1:A:267:ASP:HB2	6:D:1123:HOH:O	1.96	0.65
1:D:307:ARG:NH2	6:D:1005:HOH:O	2.30	0.64
1:C:185:ASN:ND2	1:D:184:THR:OG1	2.31	0.64
1:B:237:TYR:OH	6:B:909:HOH:O	2.14	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:ASN:ND2	6:D:1097:HOH:O	2.31	0.62
1:C:325:LYS:NZ	6:C:1258:HOH:O	2.31	0.61
1:C:298:LEU:HA	6:C:1268:HOH:O	2.03	0.58
1:A:451:GLU:OE2	3:A:600:NMY:N23	2.38	0.57
1:B:267:ASP:HB2	6:B:1058:HOH:O	2.04	0.57
3:A:600:NMY:N2	6:A:1151:HOH:O	2.31	0.57
1:B:298:LEU:HA	6:B:1268:HOH:O	2.05	0.56
1:A:319:GLU:HB3	6:A:1317:HOH:O	2.08	0.54
1:C:228:LYS:HE3	6:C:1038:HOH:O	2.07	0.54
1:A:230:SER:HB3	1:A:268:GLU:HA	1.91	0.53
3:A:600:NMY:H1	3:A:600:NMY:C13	2.39	0.53
1:B:211:GLY:HA3	6:B:1091:HOH:O	2.09	0.53
6:C:1220:HOH:O	1:D:184:THR:HG22	2.09	0.52
3:D:600:NMY:H1	3:D:600:NMY:H13	1.90	0.52
1:B:189:MET:SD	1:B:227:THR:HG21	2.50	0.52
3:B:600:NMY:H13	3:B:600:NMY:H1	1.92	0.52
1:C:413:SER:HB2	3:C:600:NMY:N6	2.25	0.52
1:A:185:ASN:OD1	1:B:179:TYR:OH	2.26	0.51
3:C:600:NMY:H13	3:C:600:NMY:H2	1.92	0.51
1:C:427:ARG:NH2	6:C:1292:HOH:O	2.43	0.51
6:A:1018:HOH:O	1:B:191:TYR:OH	2.18	0.51
1:B:189:MET:HG2	1:B:217:TYR:CE1	2.46	0.51
1:B:451:GLU:OE2	3:B:600:NMY:N23	2.43	0.50
1:C:189:MET:HG2	1:C:217:TYR:CE1	2.47	0.50
1:A:374:ASP:OD1	3:A:600:NMY:N7	2.44	0.50
1:A:189:MET:SD	1:A:227:THR:HG21	2.52	0.50
3:A:600:NMY:H1	3:A:600:NMY:H13	1.94	0.49
1:B:286:ILE:O	1:B:289:THR:HB	2.13	0.49
1:C:395:GLY:HA3	6:C:902:HOH:O	2.13	0.48
1:D:189:MET:SD	1:D:227:THR:HG21	2.53	0.48
2:C:500:GNP:O2B	6:C:1221:HOH:O	2.20	0.47
1:C:189:MET:SD	1:C:227:THR:HG21	2.55	0.47
3:B:600:NMY:H231	3:B:600:NMY:O18	2.15	0.46
1:A:324:ASN:OD1	6:A:980:HOH:O	2.20	0.46
1:A:415:GLU:OE2	3:A:600:NMY:H62	2.16	0.46
1:C:228:LYS:CE	6:C:1038:HOH:O	2.63	0.46
1:D:186:VAL:HG13	1:D:205:ILE:HG23	1.98	0.46
1:B:198:ASP:OD1	1:B:199:ASN:N	2.42	0.45
3:B:600:NMY:H1	3:B:600:NMY:C13	2.46	0.45
3:C:600:NMY:O21	6:C:1019:HOH:O	2.20	0.45
1:A:189:MET:HG2	1:A:217:TYR:CE1	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:GLU:OE2	3:B:600:NMV:H62	2.17	0.45
1:A:186:VAL:HG13	1:A:205:ILE:HG23	1.99	0.44
1:D:189:MET:HG2	1:D:217:TYR:CE2	2.52	0.44
3:D:600:NMV:H1	3:D:600:NMV:C13	2.47	0.44
3:A:600:NMV:H232	3:A:600:NMV:O18	2.17	0.44
2:D:500:GNP:O1G	3:D:600:NMV:N19	2.47	0.44
1:A:319:GLU:CB	6:A:1317:HOH:O	2.65	0.43
1:B:186:VAL:HG13	1:B:205:ILE:HG23	2.00	0.43
1:C:186:VAL:HG13	1:C:205:ILE:HG23	2.00	0.43
1:C:252:GLU:O	1:C:308:GLN:NE2	2.46	0.43
1:B:237:TYR:HB2	1:B:270:SER:HB3	2.02	0.41
1:A:229:PHE:O	1:A:230:SER:C	2.64	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	291/305 (95%)	278 (96%)	11 (4%)	2 (1%)	18	34
1	B	291/305 (95%)	279 (96%)	11 (4%)	1 (0%)	36	55
1	C	288/305 (94%)	276 (96%)	11 (4%)	1 (0%)	36	55
1	D	286/305 (94%)	276 (96%)	10 (4%)	0	100	100
All	All	1156/1220 (95%)	1109 (96%)	43 (4%)	4 (0%)	36	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	SER
1	A	198	ASP
1	B	198	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	198	ASP

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	268/281 (95%)	260 (97%)	8 (3%)	36	64
1	B	267/281 (95%)	260 (97%)	7 (3%)	40	68
1	C	267/281 (95%)	260 (97%)	7 (3%)	40	68
1	D	268/281 (95%)	262 (98%)	6 (2%)	45	73
All	All	1070/1124 (95%)	1042 (97%)	28 (3%)	40	68

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	221	ASN
1	A	230	SER
1	A	265	ILE
1	A	267	ASP
1	A	308	GLN
1	A	317	ILE
1	A	460	ILE
1	B	221	ASN
1	B	230	SER
1	B	265	ILE
1	B	267	ASP
1	B	285	GLU
1	B	289	THR
1	B	460	ILE
1	C	198	ASP
1	C	221	ASN
1	C	265	ILE
1	C	387	ARG
1	C	460	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	463	GLU
1	C	479	ASP
1	D	213	ASP
1	D	221	ASN
1	D	230	SER
1	D	265	ILE
1	D	267	ASP
1	D	460	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	467	ASN
1	B	221	ASN
1	C	221	ASN
1	C	327	ASN
1	C	386	ASN
1	D	221	ASN
1	D	295	GLN
1	D	296	ASN
1	D	326	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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[B]	4	34,34,34	0.66	1 (2%)	47,54,54	0.74	1 (2%)
3	NMY	B	600	-	43,45,45	0.29	0	62,67,67	1.54	6 (9%)
2	GNP	C	500	4	34,34,34	0.58	1 (2%)	47,54,54	0.79	2 (4%)
2	GNP	B	500[A]	4	34,34,34	0.68	1 (2%)	47,54,54	0.96	4 (8%)
3	NMY	A	600	-	43,45,45	0.26	0	62,67,67	1.54	4 (6%)
3	NMY	C	600	-	43,45,45	0.28	0	62,67,67	1.52	7 (11%)
3	NMY	D	600	-	43,45,45	0.33	0	62,67,67	1.36	8 (12%)
2	GNP	A	500	4	34,34,34	1.47	4 (11%)	47,54,54	0.98	4 (8%)
2	GNP	D	500	4	34,34,34	1.08	3 (8%)	47,54,54	1.11	4 (8%)
5	GOL	B	804	-	5,5,5	0.88	0	5,5,5	1.01	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
2	GNP	B	500[B]	4	-	2/18/38/38	0/3/3/3
3	NMY	B	600	-	-	7/18/94/94	0/4/4/4
2	GNP	C	500	4	-	5/18/38/38	0/3/3/3
2	GNP	B	500[A]	4	-	2/18/38/38	0/3/3/3
3	NMY	A	600	-	-	9/18/94/94	0/4/4/4
3	NMY	C	600	-	-	4/18/94/94	0/4/4/4
3	NMY	D	600	-	-	9/18/94/94	0/4/4/4
2	GNP	A	500	4	-	1/18/38/38	0/3/3/3
2	GNP	D	500	4	-	1/18/38/38	0/3/3/3
5	GOL	B	804	-	-	1/4/4/4	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	GNP	PG-O2G	4.53	1.68	1.56
2	A	500	GNP	PG-O3G	4.52	1.68	1.56
2	D	500	GNP	PG-O3G	4.31	1.68	1.56
2	A	500	GNP	PB-O3A	-4.24	1.53	1.59
2	D	500	GNP	PB-O2B	2.67	1.63	1.56
2	B	500[B]	GNP	PG-O2G	2.45	1.63	1.56
2	B	500[A]	GNP	PB-O2B	2.28	1.62	1.56
2	A	500	GNP	PA-O5'	2.20	1.68	1.59
2	C	500	GNP	PG-O2G	2.08	1.62	1.56
2	D	500	GNP	PB-O3A	-2.02	1.56	1.59

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	600	NMY	O12-C12-C7	7.69	124.28	109.90
3	A	600	NMY	O12-C12-C7	7.60	124.11	109.90
3	C	600	NMY	O11-C13-O16	-7.09	104.13	111.37
3	A	600	NMY	O11-C13-O16	-6.51	104.71	111.37
2	D	500	GNP	O2B-PB-O1B	-5.75	97.53	109.87
3	B	600	NMY	O11-C13-O16	-5.34	105.91	111.37
3	C	600	NMY	O12-C12-C7	4.16	117.67	109.90
3	D	600	NMY	O12-C12-C11	3.91	119.97	109.94
3	C	600	NMY	C11-C12-C7	3.84	119.20	109.93
3	D	600	NMY	O12-C12-C7	3.45	116.36	109.90
3	C	600	NMY	O12-C12-C11	3.35	118.53	109.94
3	D	600	NMY	C11-C12-C7	3.33	117.98	109.93
3	D	600	NMY	O11-C13-O16	-3.33	107.96	111.37
3	B	600	NMY	O1-C1-C2	3.28	113.44	108.08
2	D	500	GNP	O2G-PG-O1G	-3.04	105.82	113.45
2	B	500[A]	GNP	O2G-PG-O1G	-3.01	105.90	113.45
3	D	600	NMY	O1-C1-C2	2.96	112.92	108.08
3	C	600	NMY	O5-C1-C2	2.95	116.61	110.08
3	B	600	NMY	C9-C8-C7	-2.89	106.06	111.02
2	B	500[B]	GNP	O2B-PB-O1B	-2.89	103.67	109.87
3	A	600	NMY	C9-C8-C7	-2.83	106.17	111.02
3	D	600	NMY	O18-C18-O22	-2.81	103.30	110.69
2	A	500	GNP	O2B-PB-O1B	-2.54	104.42	109.87
2	A	500	GNP	O2'-C2'-C1'	-2.44	101.70	110.10
3	C	600	NMY	C9-C8-C7	-2.44	106.84	111.02
2	C	500	GNP	O1G-PG-N3B	2.41	115.32	111.77
2	A	500	GNP	O3'-C3'-C2'	-2.41	104.11	111.82
2	D	500	GNP	O1G-PG-N3B	-2.40	108.23	111.77
2	B	500[A]	GNP	O2B-PB-O1B	-2.36	104.81	109.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	GNP	O2B-PB-O1B	-2.29	104.94	109.87
3	B	600	NMY	O1-C10-C11	2.24	113.12	107.42
2	B	500[A]	GNP	O3G-PG-O1G	-2.24	107.83	113.45
3	B	600	NMY	O1-C10-C9	-2.22	103.88	109.18
3	D	600	NMY	O22-C22-C21	2.20	113.67	109.70
2	B	500[A]	GNP	O1G-PG-N3B	2.15	114.93	111.77
3	D	600	NMY	O1-C10-C9	-2.13	104.11	109.18
3	A	600	NMY	O22-C22-C23	2.06	110.03	106.07
2	D	500	GNP	O3A-PA-O1A	2.04	116.83	110.70
3	C	600	NMY	O18-C18-C19	-2.01	104.79	108.08
2	A	500	GNP	O3A-PA-O1A	-2.01	104.67	110.70

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500[A]	GNP	PB-N3B-PG-O1G
2	B	500[A]	GNP	PG-N3B-PB-O1B
2	C	500	GNP	PB-N3B-PG-O1G
2	C	500	GNP	PG-N3B-PB-O1B
2	D	500	GNP	PG-N3B-PB-O1B
3	A	600	NMY	O5-C5-C6-N6
3	A	600	NMY	C14-C13-O11-C11
3	A	600	NMY	O16-C13-O11-C11
3	B	600	NMY	C14-C13-O11-C11
3	B	600	NMY	O16-C13-O11-C11
3	B	600	NMY	O22-C22-C23-N19
3	C	600	NMY	C14-C13-O11-C11
3	C	600	NMY	O16-C13-O11-C11
3	C	600	NMY	C14-C15-O18-C18
3	D	600	NMY	C14-C13-O11-C11
3	D	600	NMY	O16-C13-O11-C11
3	D	600	NMY	C21-C22-C23-N19
3	D	600	NMY	O22-C22-C23-N19
3	D	600	NMY	O16-C16-C17-O17
3	D	600	NMY	C15-C16-C17-O17
3	B	600	NMY	O16-C16-C17-O17
3	B	600	NMY	C15-C16-C17-O17
3	C	600	NMY	O22-C18-O18-C15
3	A	600	NMY	O16-C16-C17-O17
3	A	600	NMY	C15-C16-C17-O17
2	A	500	GNP	PB-O3A-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	600	NMY	O5-C1-O1-C10
3	B	600	NMY	C11-C10-O1-C1
3	A	600	NMY	C4-C5-C6-N6
3	A	600	NMY	C21-C22-C23-N19
3	B	600	NMY	O5-C1-O1-C10
3	D	600	NMY	C11-C10-O1-C1
5	B	804	GOL	O1-C1-C2-O2
3	A	600	NMY	O5-C1-O1-C10
3	A	600	NMY	C11-C10-O1-C1
2	C	500	GNP	PG-N3B-PB-O3A
2	B	500[B]	GNP	PB-O3A-PA-O2A
2	C	500	GNP	PB-O3A-PA-O2A
3	D	600	NMY	O22-C18-O18-C15
2	B	500[B]	GNP	PB-O3A-PA-O1A
2	C	500	GNP	PB-O3A-PA-O1A

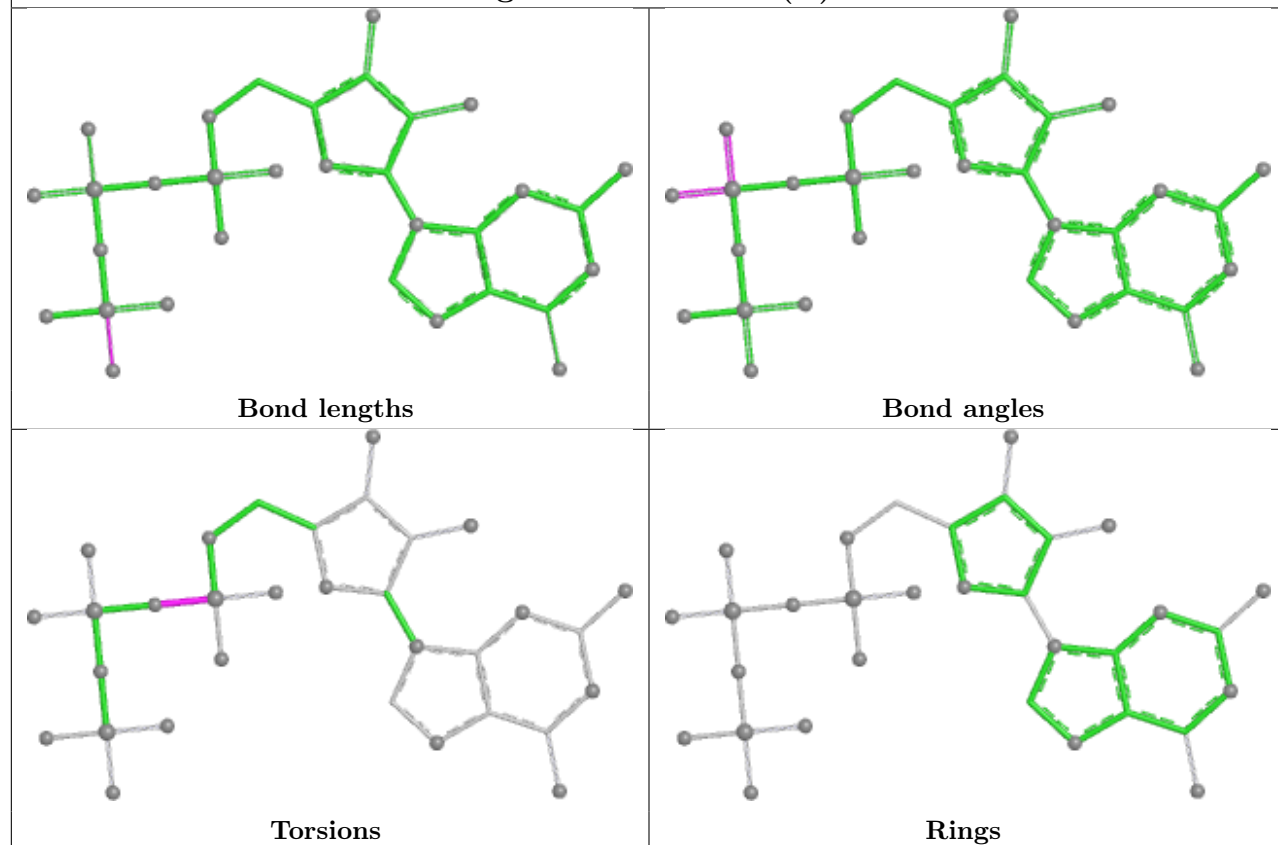
There are no ring outliers.

7 monomers are involved in 21 short contacts:

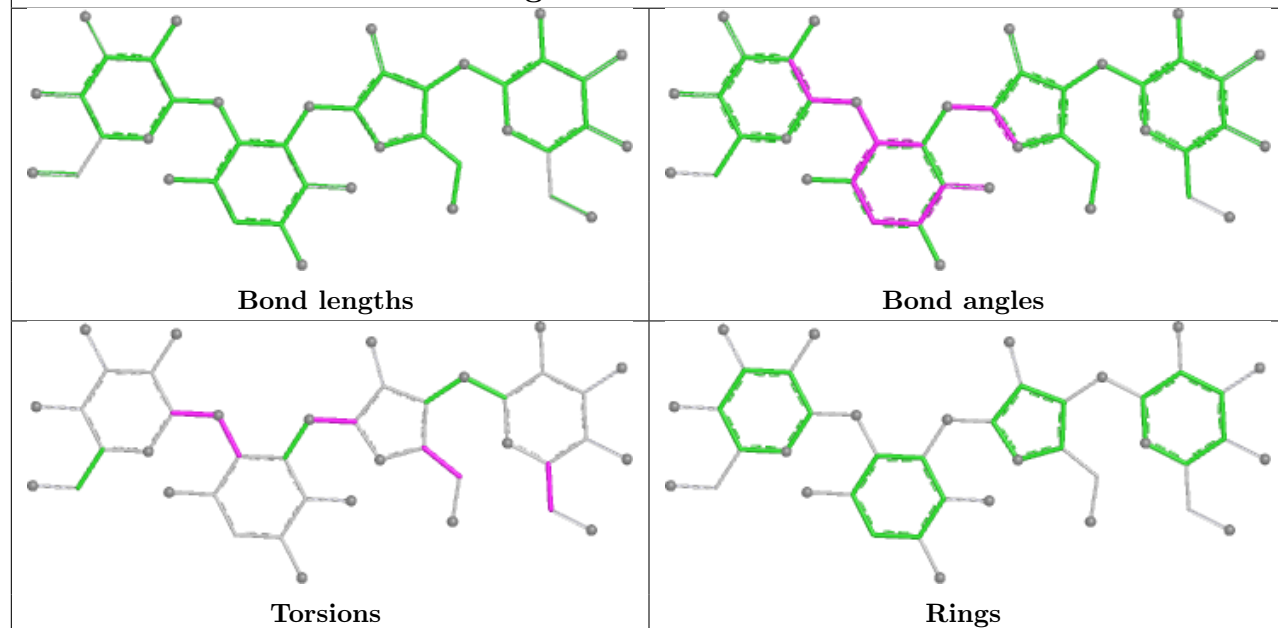
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	600	NMY	6	0
2	C	500	GNP	1	0
3	A	600	NMY	7	0
3	C	600	NMY	3	0
3	D	600	NMY	3	0
2	A	500	GNP	1	0
2	D	500	GNP	1	0

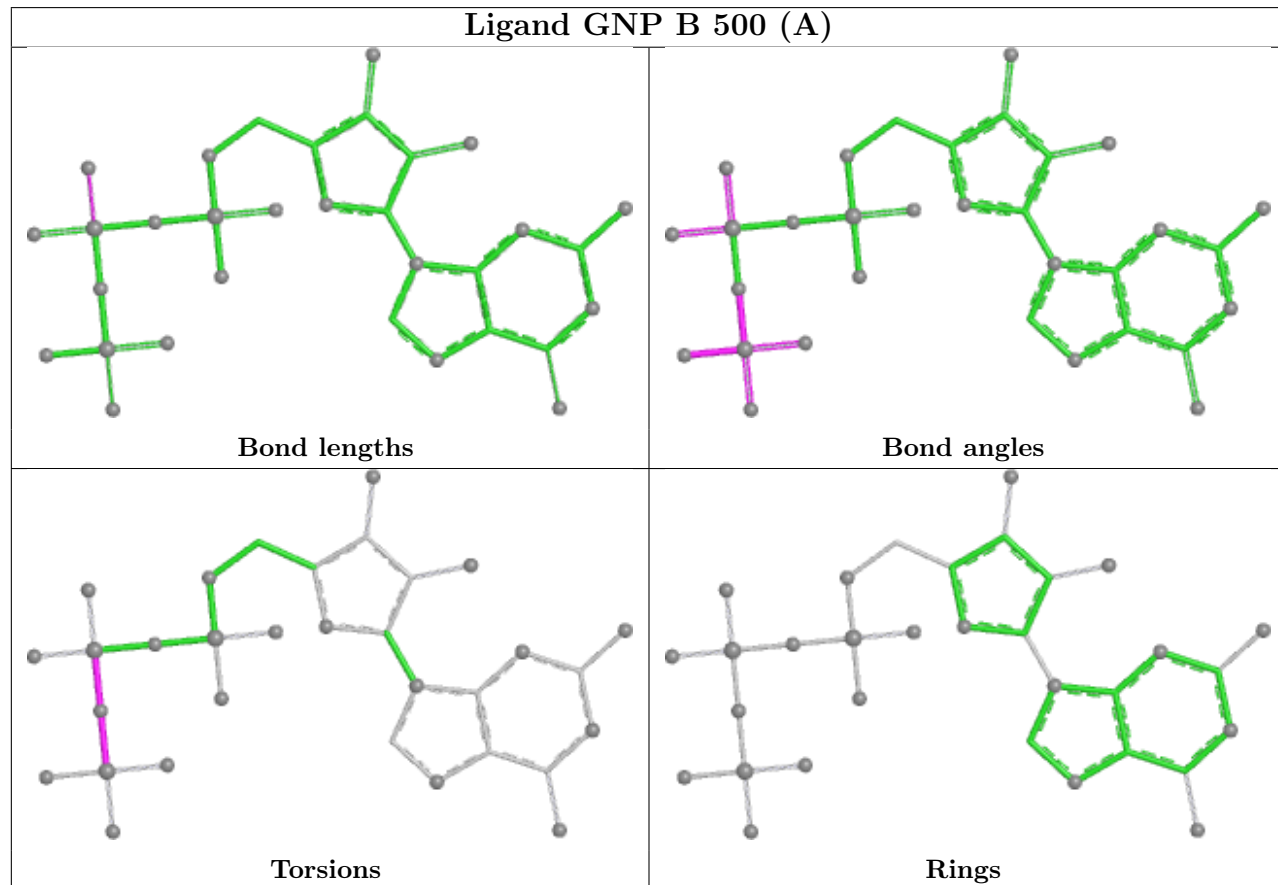
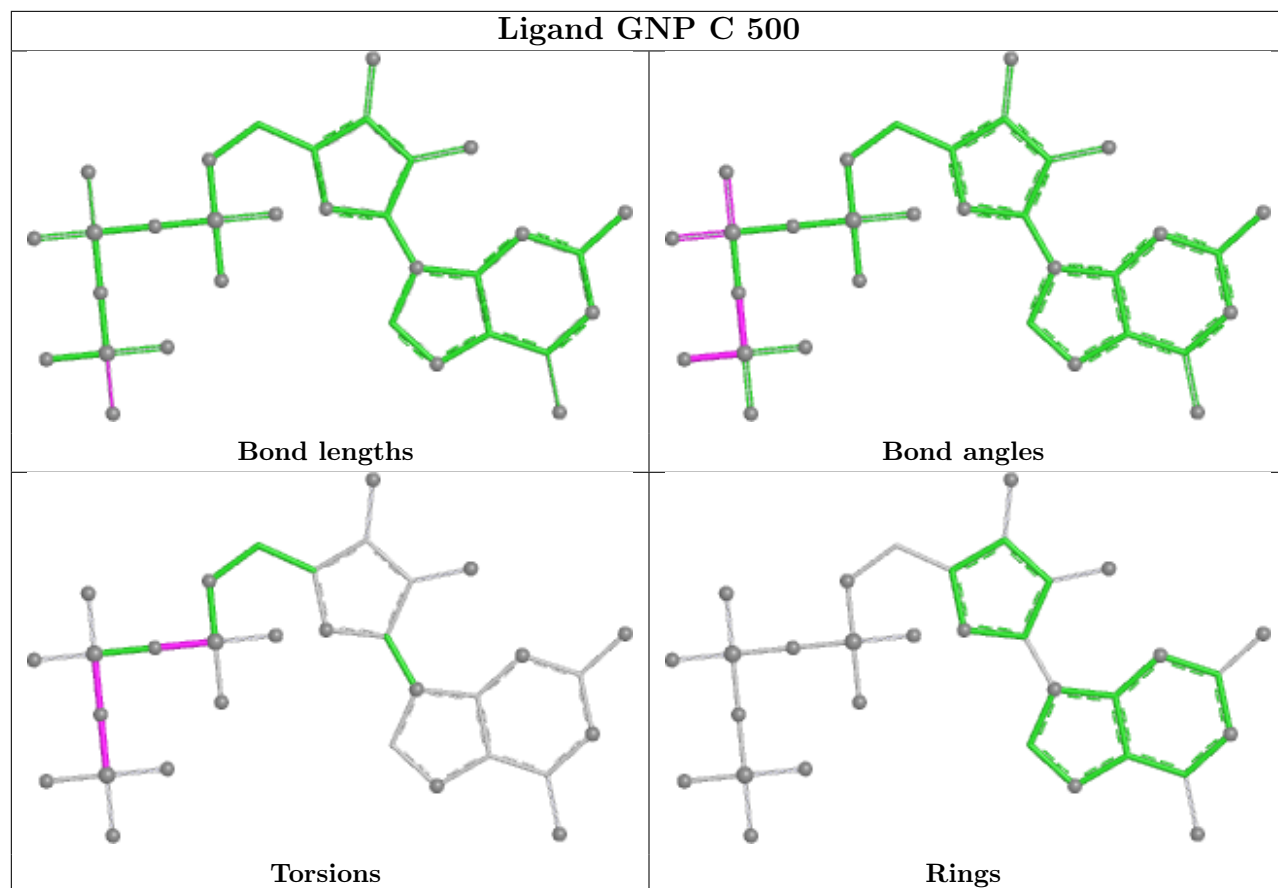
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

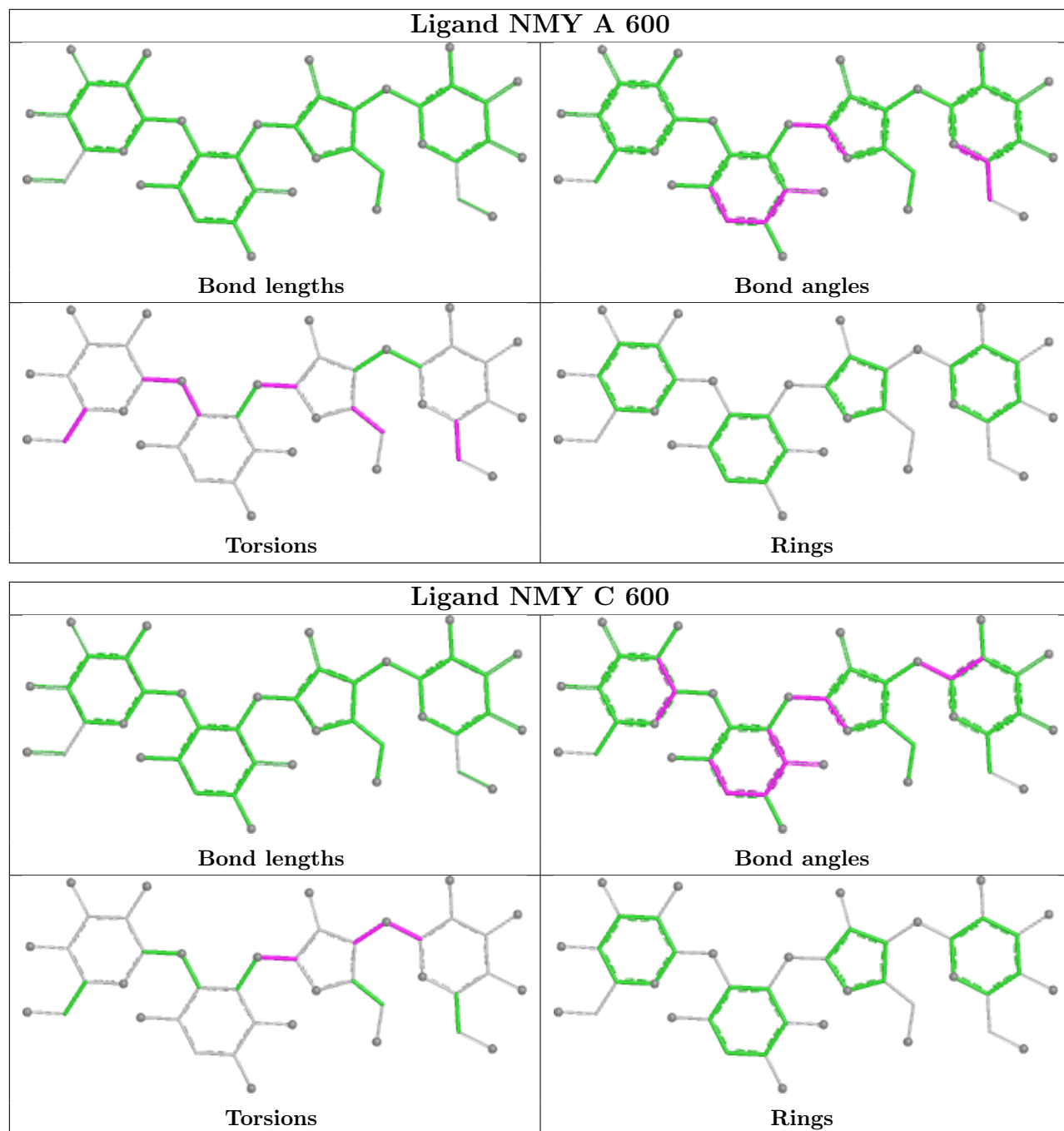
Ligand GNP B 500 (B)

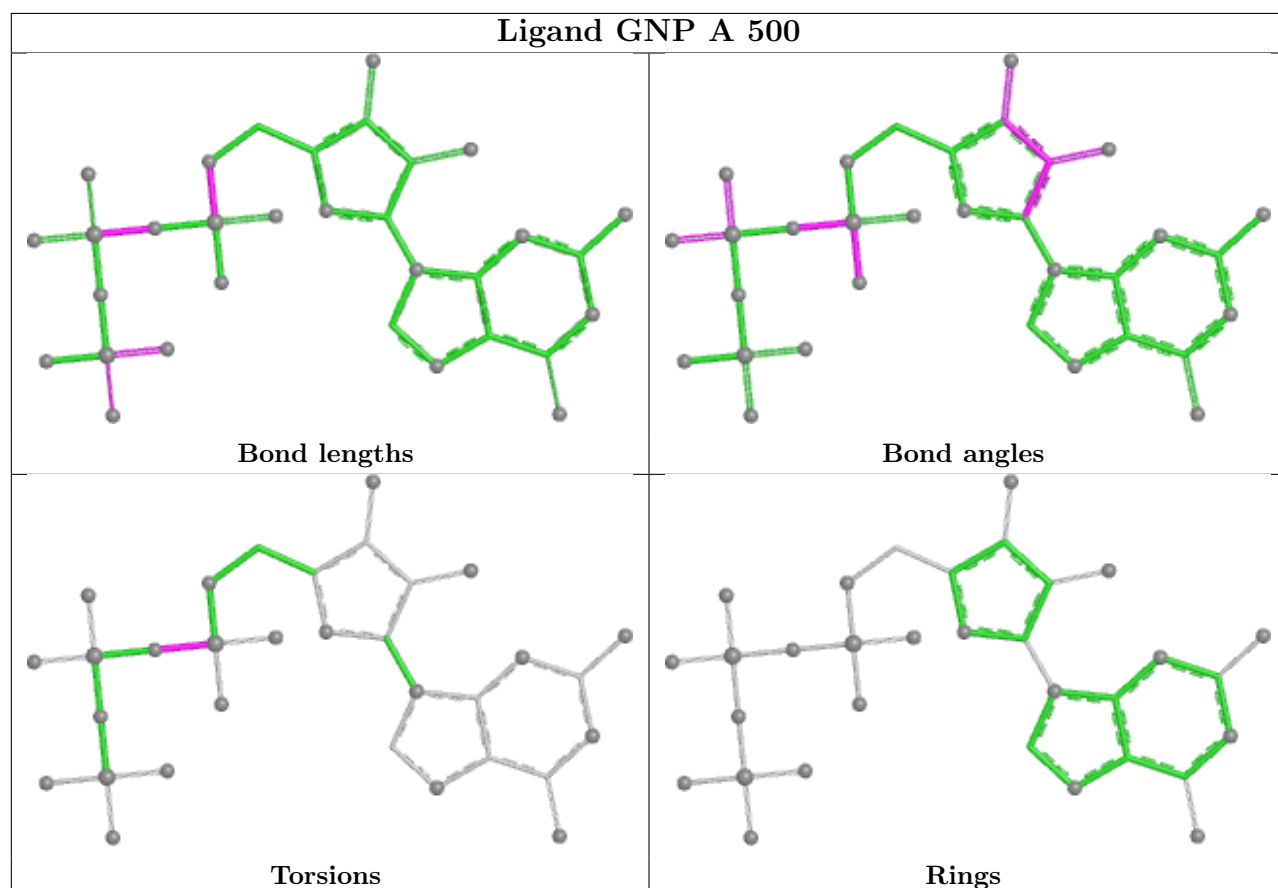
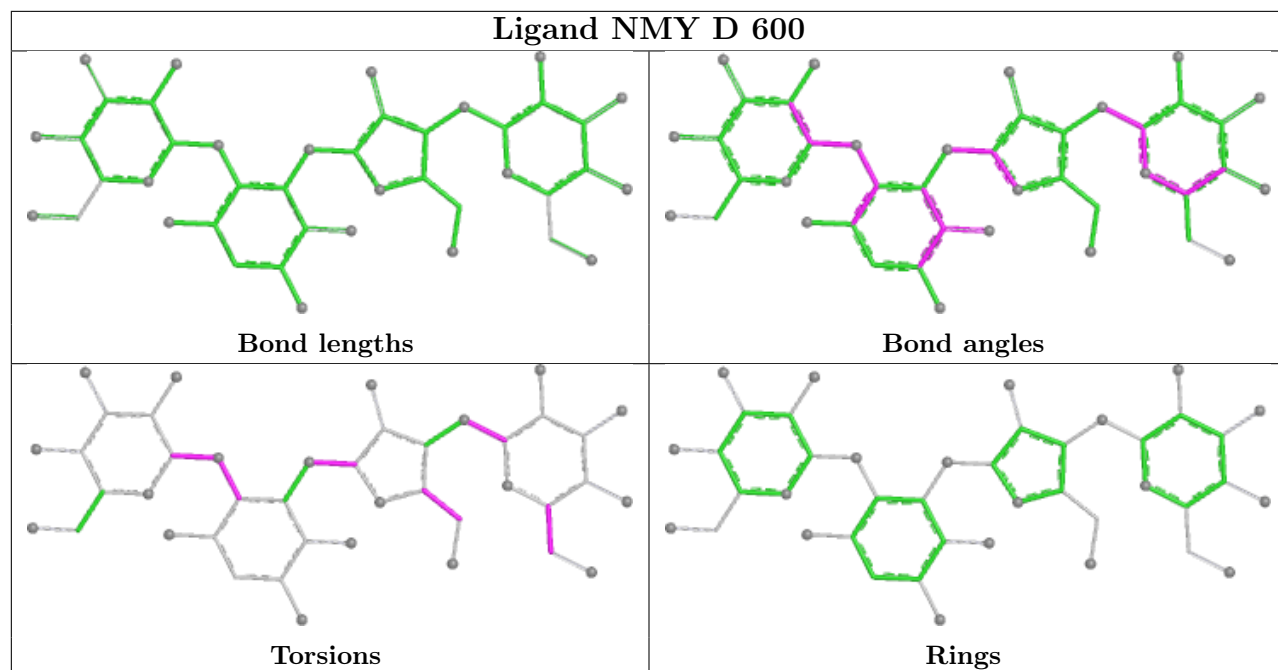


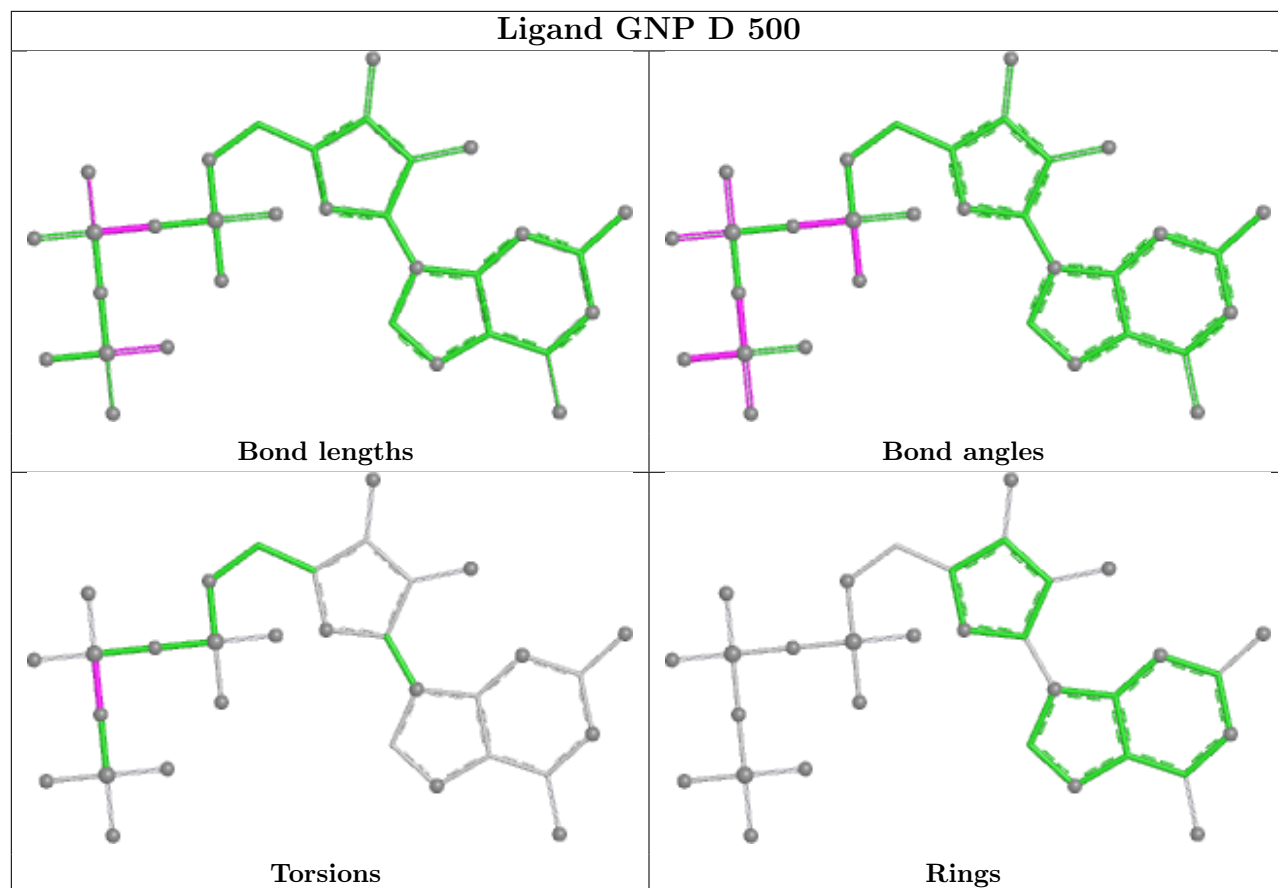
Ligand NMY B 600











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, 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	295/305 (96%)	-0.21	7 (2%) 59 55	40, 64, 97, 133	0
1	B	295/305 (96%)	-0.27	5 (1%) 69 65	40, 62, 97, 126	0
1	C	292/305 (95%)	-0.24	5 (1%) 69 65	36, 62, 100, 166	0
1	D	292/305 (95%)	-0.04	2 (0%) 84 81	54, 77, 114, 147	0
All	All	1174/1220 (96%)	-0.19	19 (1%) 70 67	36, 67, 104, 166	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	183	ALA	4.4
1	B	236	GLY	3.9
1	A	182	ASN	3.6
1	B	182	ASN	3.4
1	D	230	SER	3.0
1	B	230	SER	2.9
1	B	208	ILE	2.8
1	C	184	THR	2.8
1	A	236	GLY	2.6
1	A	233	LYS	2.5
1	C	235	LYS	2.5
1	C	186	VAL	2.5
1	A	183	ALA	2.4
1	C	187	LYS	2.4
1	A	208	ILE	2.2
1	A	478	LYS	2.2
1	A	212	TYR	2.1
1	D	210	SER	2.1
1	B	478	LYS	2.1

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

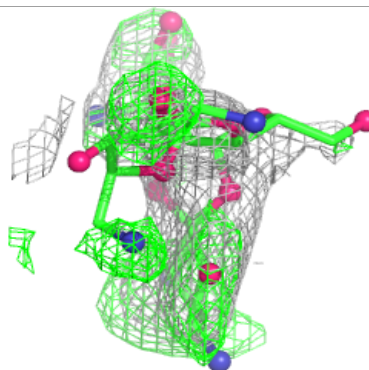
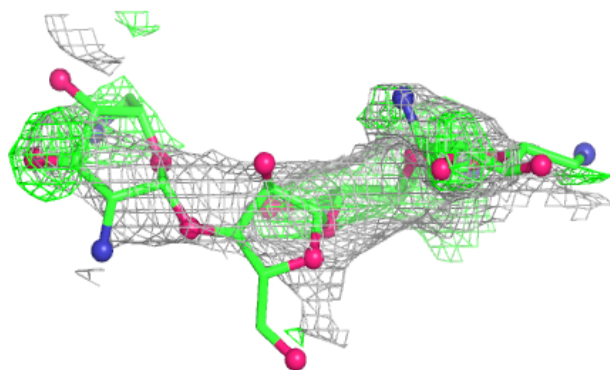
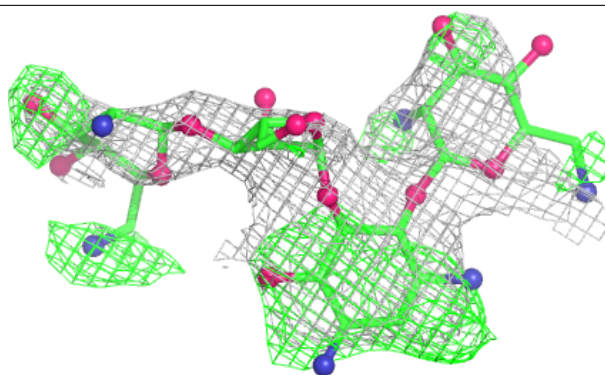
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NMY	C	600	42/42	0.74	0.22	193,217,282,324	0
3	NMY	A	600	42/42	0.75	0.18	153,177,217,242	0
3	NMY	B	600	42/42	0.85	0.13	114,121,154,169	0
5	GOL	B	804	6/6	0.88	0.11	72,87,96,99	0
3	NMY	D	600	42/42	0.95	0.07	68,78,89,93	0
2	GNP	A	500	32/32	0.97	0.06	39,46,57,63	0
2	GNP	B	500[B]	32/32	0.98	0.05	45,47,50,50	9
2	GNP	C	500	32/32	0.98	0.05	50,55,61,63	0
2	GNP	D	500	32/32	0.98	0.05	54,61,67,70	0
2	GNP	B	500[A]	32/32	0.98	0.05	45,47,52,53	9
4	MG	A	702	1/1	0.99	0.06	52,52,52,52	0
4	MG	B	702	1/1	0.99	0.03	59,59,59,59	0
4	MG	D	700	1/1	0.99	0.03	48,48,48,48	0
4	MG	D	702	1/1	0.99	0.04	59,59,59,59	0
4	MG	A	700	1/1	0.99	0.02	51,51,51,51	0
4	MG	B	700	1/1	1.00	0.02	43,43,43,43	0
4	MG	C	700	1/1	1.00	0.02	61,61,61,61	0
4	MG	C	702	1/1	1.00	0.04	58,58,58,58	0

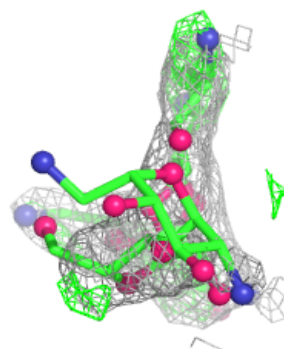
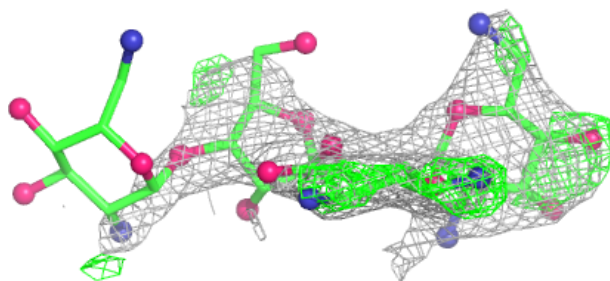
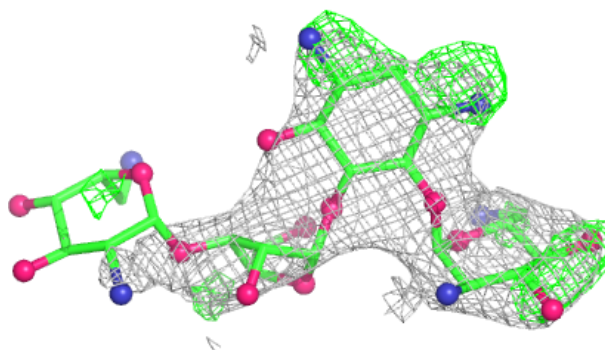
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NMY 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)

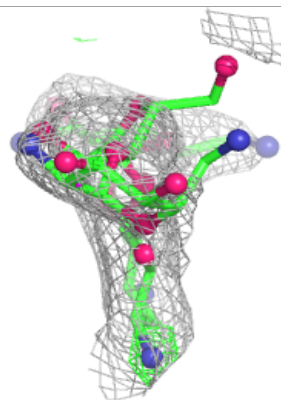
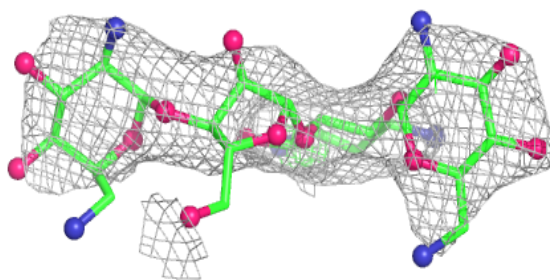
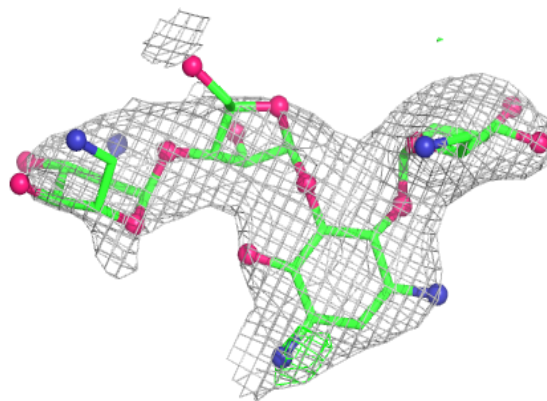
**Electron density around NMY A 600:**

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

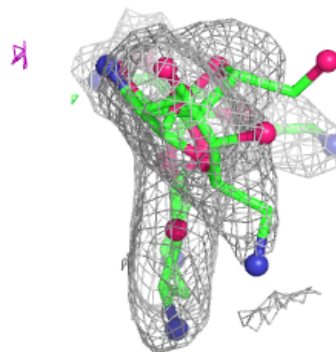
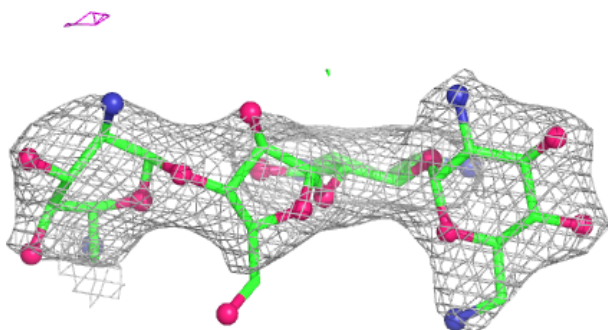
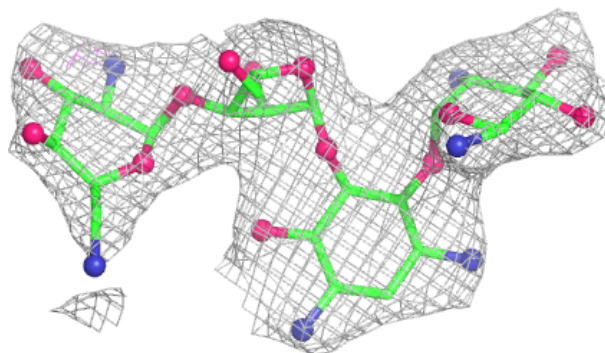


Electron density around NMY B 600:

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

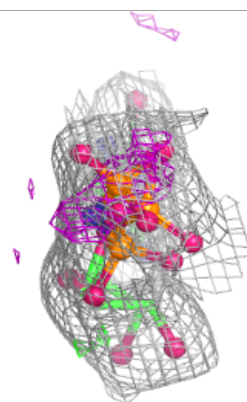
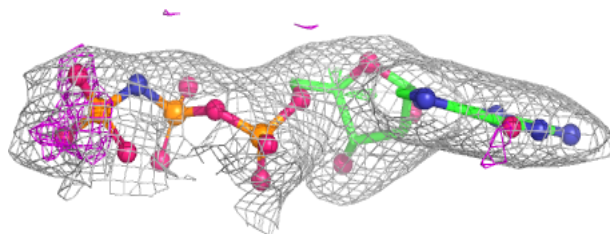
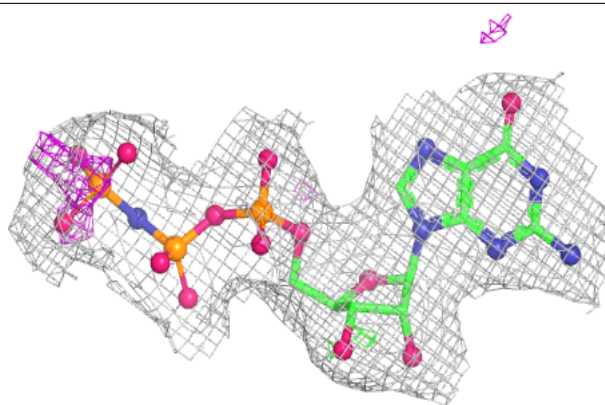
**Electron density around NMY D 600:**

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

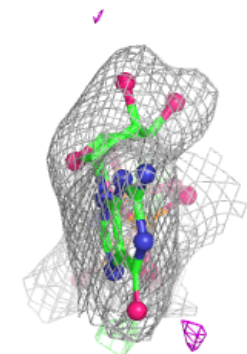
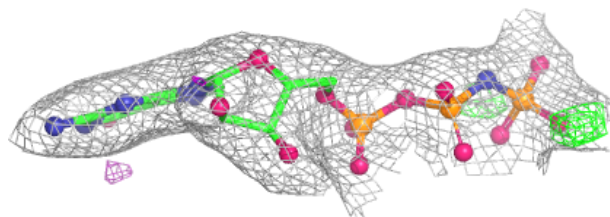
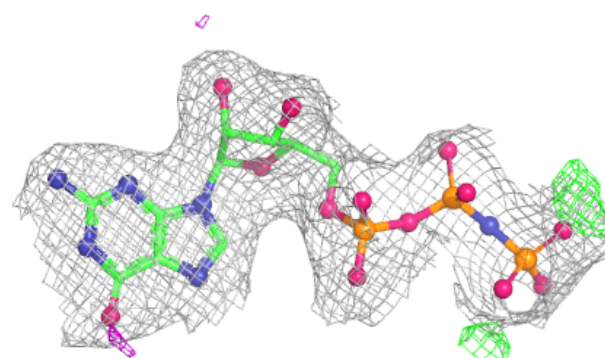


Electron density around GNP A 500:

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

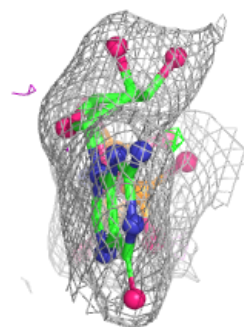
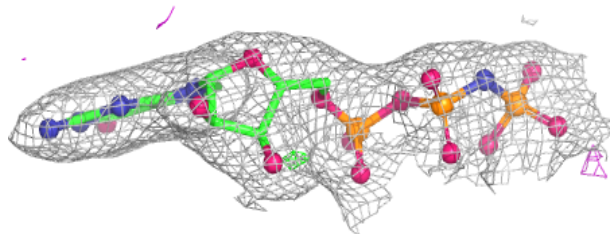
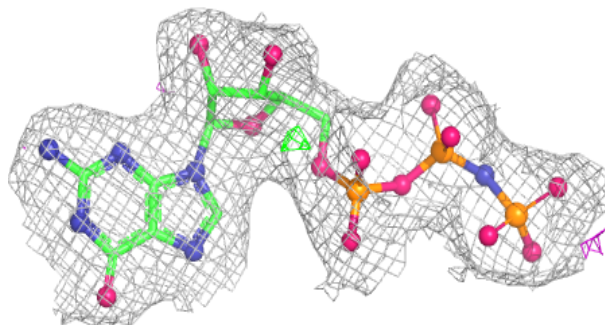
**Electron density around GNP B 500 (B):**

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

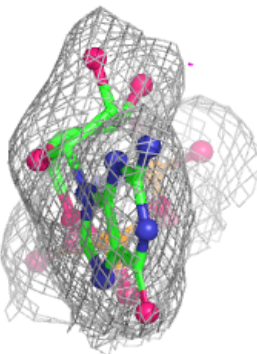
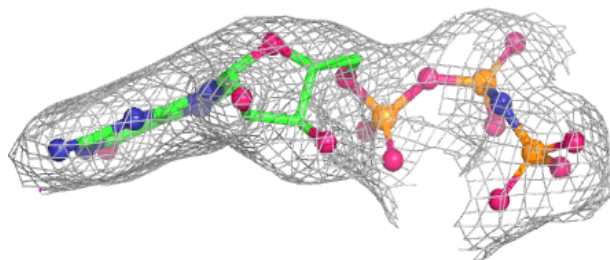
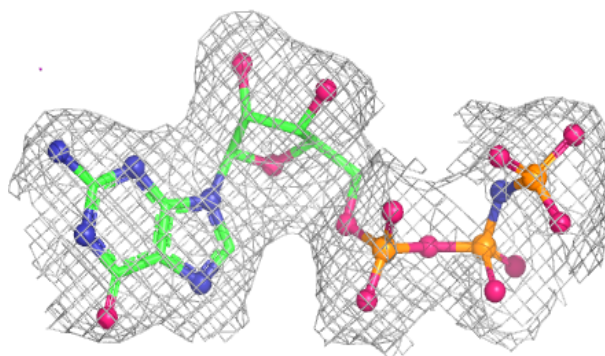


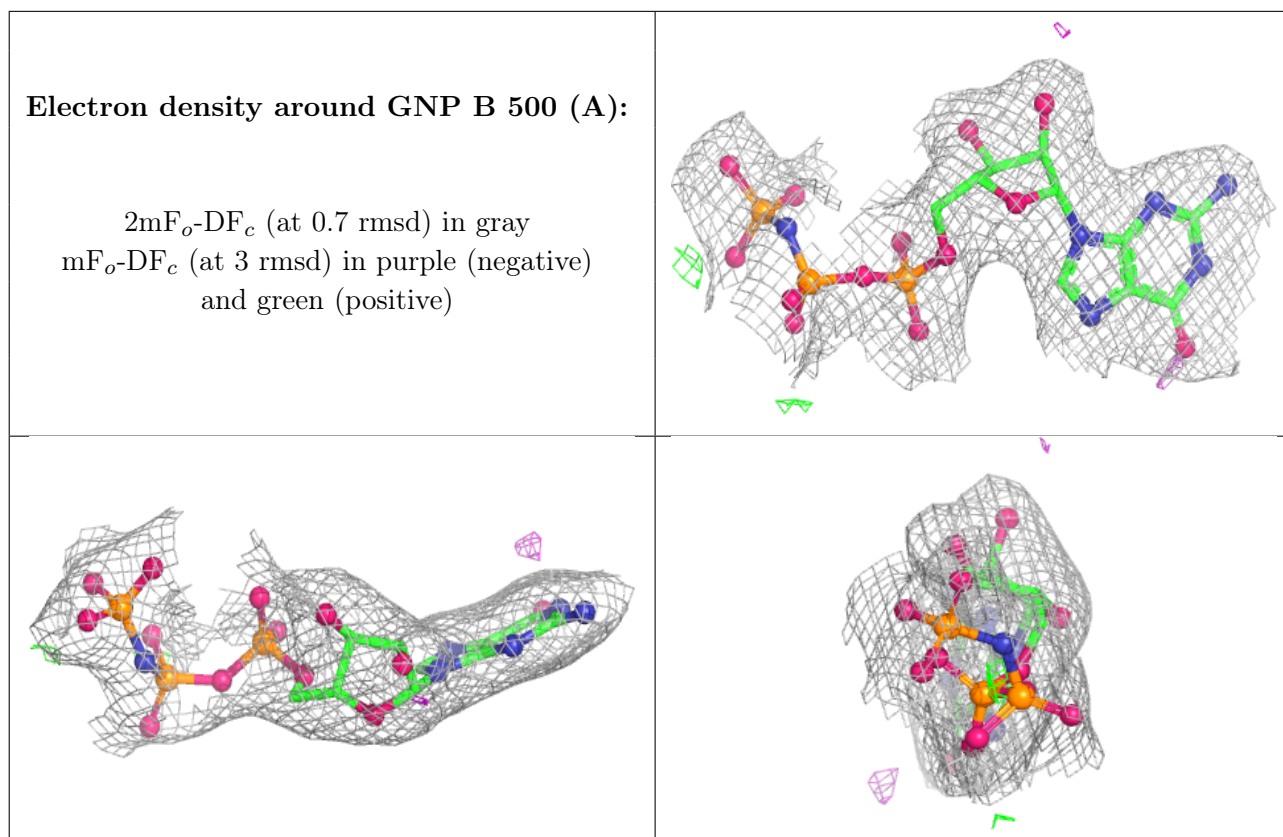
Electron density around GNP C 500:

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

**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.