



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:10 am BST

PDB ID : 5IQB
Title : Aminoglycoside Phosphotransferase (2'')-Ia (CTD of AAC(6')-Ie/APH(2'')-Ia)
in complex with GMPPNP, Magnesium, and Kanamycin A
Authors : Caldwell, S.J.; Berghuis, A.M.
Deposited on : 2016-03-10
Resolution : 2.30 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

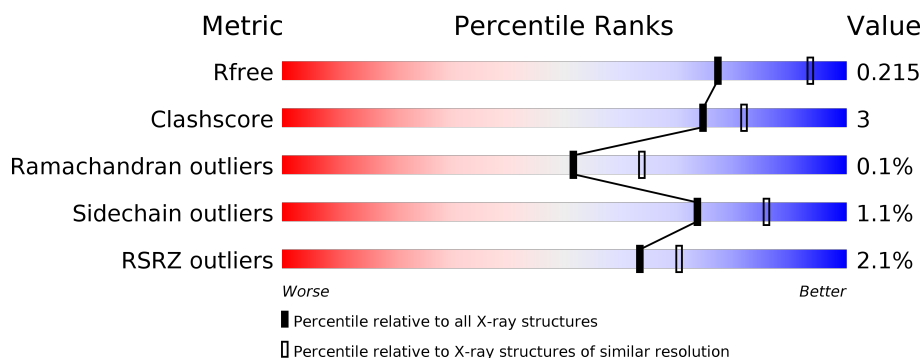
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 89%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 89% 7% . </div> </div>
1	B	305	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 89%, yellow 7%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 89% 7% . </div> </div>
1	C	305	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 89%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 89% 6% 5% </div> </div>
1	D	305	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 1%, yellow 1%, green 89%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 6% 89% 6% 5% </div> </div>

2 Entry composition [i](#)

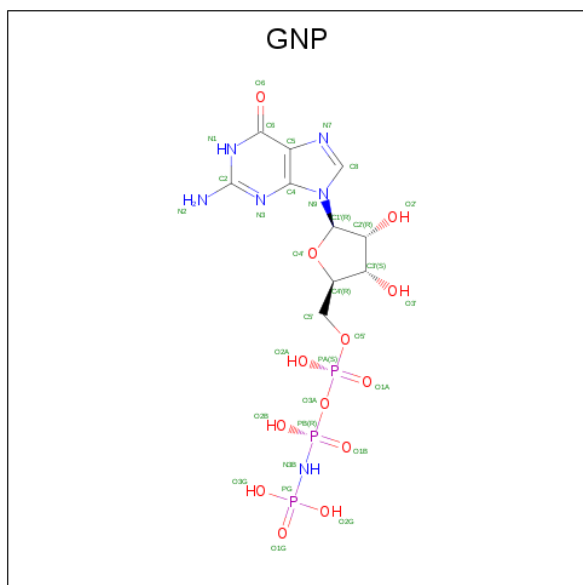
There are 6 unique types of molecules in this entry. The entry contains 10672 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	292	Total	C	N	O	S	0	1	0
			2411	1541	375	485	10			
1	B	292	Total	C	N	O	S	0	1	0
			2410	1542	372	486	10			
1	C	290	Total	C	N	O	S	0	1	0
			2398	1534	372	482	10			
1	D	289	Total	C	N	O	S	0	1	0
			2380	1520	373	477	10			

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



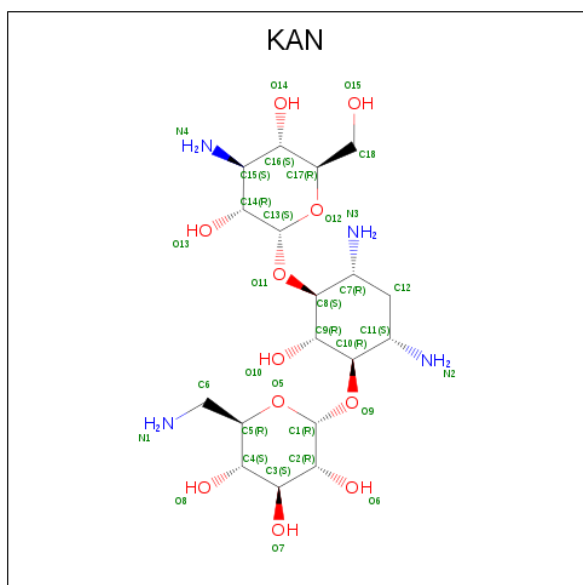
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	1
			41	10	7	19	5		
2	B	1	Total	C	N	O	P	0	1
			41	10	7	19	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	1
			41	10	7	19		
2	D	1	Total	C	N	O	0	1
			41	10	7	19		

- Molecule 3 is KANAMYCIN A (three-letter code: KAN) (formula: $C_{18}H_{36}N_4O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	18	4	11		
3	B	1	Total	C	N	O	0	0
			33	18	4	11		
3	C	1	Total	C	N	O	0	0
			33	18	4	11		
3	D	1	Total	C	N	O	0	0
			33	18	4	11		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total 3	Mg 3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

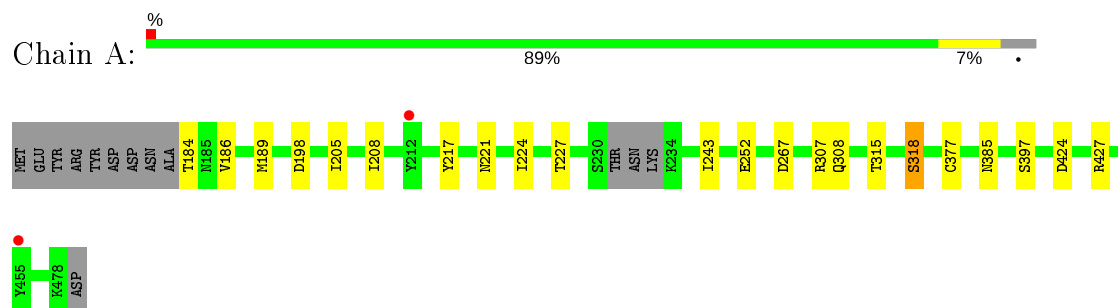
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	210	Total 210	O 210	0	0
6	B	230	Total 230	O 230	0	0
6	C	177	Total 177	O 177	0	0
6	D	149	Total 149	O 149	0	0

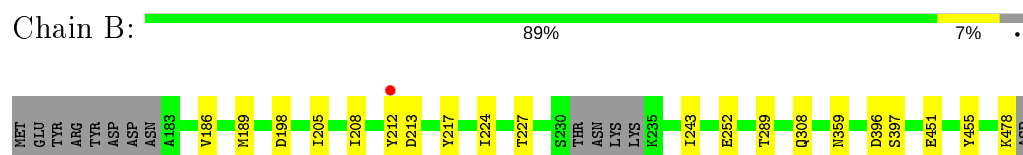
3 Residue-property plots [i](#)

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.

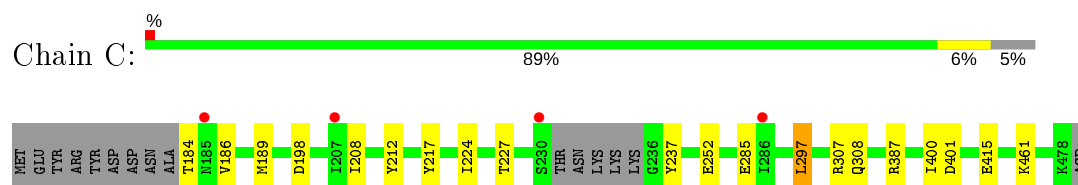
- Molecule 1: Bifunctional AAC/APH



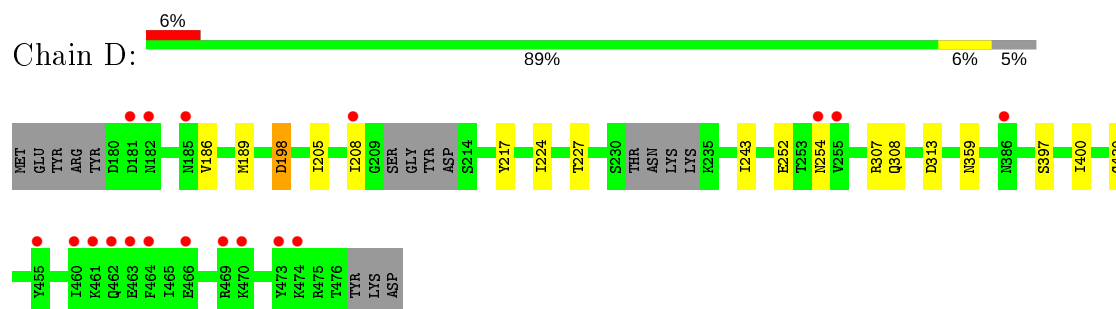
- Molecule 1: Bifunctional AAC/APH



- Molecule 1: Bifunctional AAC/APH



- Molecule 1: Bifunctional AAC/APH



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.43 Å 99.22 Å 93.51 Å 90.00° 105.46° 90.00°	Depositor
Resolution (Å)	90.13 – 2.30 55.36 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (90.13-2.30) 98.9 (55.36-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.167 , 0.211 0.172 , 0.215	Depositor DCC
R_{free} test set	3504 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10672	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: MG, GNP, KAN, 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	0.78	1/2457 (0.0%)	0.77	0/3313
1	B	0.75	0/2456	0.75	0/3311
1	C	0.76	0/2444	0.78	0/3295
1	D	0.66	0/2423	0.73	0/3266
All	All	0.74	1/9780 (0.0%)	0.76	0/13185

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	CYS	CB-SG	-5.43	1.73	1.81

There are no bond angle outliers.

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	2411	0	2322	10	0
1	B	2410	0	2325	13	0
1	C	2398	0	2314	16	0
1	D	2380	0	2297	12	0
2	A	41	0	2	5	0
2	B	41	0	2	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	41	0	2	0	0
2	D	41	0	2	2	0
3	A	33	0	36	0	0
3	B	33	0	36	2	0
3	C	33	0	36	1	0
3	D	33	0	36	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	1	0
6	A	210	0	0	7	0
6	B	230	0	0	6	1
6	C	177	0	0	4	1
6	D	149	0	0	4	0
All	All	10672	0	9410	61	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 3.

All (61) 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)
2:A:500[A]:GNP:O3G	6:A:926:HOH:O	1.55	1.21
2:B:500[A]:GNP:O3G	6:B:924:HOH:O	1.59	1.20
2:A:500[A]:GNP:O1G	6:A:924:HOH:O	1.81	0.96
1:C:184:THR:HG23	1:C:186:VAL:HG22	1.62	0.82
2:B:500[B]:GNP:O1G	6:B:924:HOH:O	1.98	0.81
2:A:500[A]:GNP:PG	6:A:924:HOH:O	2.39	0.78
1:B:289:THR:HG22	6:B:1371:HOH:O	1.86	0.75
2:A:500[B]:GNP:O1G	6:A:926:HOH:O	2.05	0.74
1:C:184:THR:CG2	1:C:186:VAL:HG22	2.18	0.74
2:A:500[A]:GNP:O3G	6:A:924:HOH:O	2.09	0.71
1:C:307[A]:ARG:NH2	6:C:1030:HOH:O	2.06	0.71
1:C:237:TYR:HA	6:C:1384:HOH:O	1.91	0.71
1:C:297:LEU:HD23	1:C:387:ARG:NE	2.08	0.68
2:D:500[A]:GNP:O2G	6:D:901:HOH:O	0.68	0.68
1:A:315:THR:O	1:A:318:SER:OG	2.15	0.63
1:B:213:ASP:OD1	1:B:455:TYR:OH	2.16	0.62
1:B:359:ASN:OD1	6:B:1050:HOH:O	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307[A]:ARG:NH2	6:C:995:HOH:O	2.36	0.57
1:B:213:ASP:OD2	6:B:1538:HOH:O	2.17	0.56
1:C:189:MET:HG2	1:C:217:TYR:CE2	2.41	0.56
1:C:297:LEU:HD23	1:C:387:ARG:CD	2.37	0.54
1:A:243:ILE:HD13	1:A:397:SER:HB2	1.91	0.53
1:A:307[A]:ARG:NH1	6:A:1030:HOH:O	2.20	0.53
6:A:1062:HOH:O	1:D:198:ASP:CB	2.57	0.52
1:A:424:ASP:OD1	1:A:427:ARG:NH1	2.42	0.52
1:D:359:ASN:OD1	6:D:1050:HOH:O	2.19	0.52
1:A:186:VAL:HG13	1:A:205:ILE:HG23	1.92	0.51
1:B:186:VAL:HG13	1:B:205:ILE:HG23	1.92	0.51
1:D:254:ASN:HB2	6:D:1500:HOH:O	2.09	0.51
1:D:186:VAL:HG13	1:D:205:ILE:HG23	1.93	0.50
1:B:252:GLU:O	1:B:308:GLN:NE2	2.44	0.49
1:B:243:ILE:HD13	1:B:397:SER:HB2	1.95	0.49
1:B:189:MET:HG2	1:B:217:TYR:CE1	2.48	0.49
1:C:297:LEU:HD23	1:C:387:ARG:CZ	2.42	0.48
2:D:500[A]:GNP:O2G	3:D:600:KAN:O13	2.30	0.48
1:D:243:ILE:HD13	1:D:397:SER:HB2	1.96	0.48
1:A:184:THR:N	6:B:1394:HOH:O	2.46	0.47
1:D:189:MET:HG2	1:D:217:TYR:CE1	2.49	0.47
1:B:396:ASP:OD2	3:B:600:KAN:N4	2.37	0.47
1:D:307[B]:ARG:NH1	1:D:430:GLY:O	2.48	0.47
1:A:189:MET:HG2	1:A:217:TYR:CE1	2.50	0.46
1:C:252:GLU:O	1:C:308:GLN:NE2	2.46	0.46
5:C:802:CL:CL	6:C:1107:HOH:O	2.58	0.45
1:D:252:GLU:O	1:D:308:GLN:NE2	2.49	0.45
1:B:189:MET:SD	1:B:227:THR:HG21	2.57	0.44
1:D:189:MET:SD	1:D:227:THR:HG21	2.57	0.44
1:D:208:ILE:CD1	1:D:224:ILE:HD12	2.48	0.43
1:C:415:GLU:OE2	3:C:600:KAN:N2	2.52	0.43
1:C:212:TYR:OH	1:C:461:LYS:CD	2.67	0.43
1:A:208:ILE:CD1	1:A:224:ILE:HD12	2.49	0.43
1:D:208:ILE:HD11	1:D:224:ILE:HD12	2.01	0.43
1:C:208:ILE:CD1	1:C:224:ILE:HD12	2.49	0.42
1:B:208:ILE:CD1	1:B:224:ILE:HD12	2.50	0.42
1:C:189:MET:SD	1:C:227:THR:HG21	2.60	0.41
1:D:313:ASP:HA	6:D:966:HOH:O	2.19	0.41
1:A:189:MET:SD	1:A:227:THR:HG21	2.61	0.41
1:B:208:ILE:HD11	1:B:224:ILE:HD12	2.03	0.41
1:A:252:GLU:O	1:A:308:GLN:NE2	2.48	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:THR:O	1:C:184:THR:HG22	2.21	0.40
1:B:451:GLU:OE1	3:B:600:KAN:C18	2.69	0.40
1:C:400:ILE:HG12	1:C:401:ASP:H	1.87	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)
6:B:1391:HOH:O	6:C:1240:HOH:O[2_746]	2.12	0.08

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	289/305 (95%)	278 (96%)	11 (4%)	0	100	100
1	B	289/305 (95%)	279 (96%)	10 (4%)	0	100	100
1	C	287/305 (94%)	277 (96%)	10 (4%)	0	100	100
1	D	284/305 (93%)	273 (96%)	10 (4%)	1 (0%)	34	42
All	All	1149/1220 (94%)	1107 (96%)	41 (4%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	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	267/281 (95%)	262 (98%)	5 (2%)	57	73
1	B	267/281 (95%)	264 (99%)	3 (1%)	73	86
1	C	266/281 (95%)	263 (99%)	3 (1%)	73	86
1	D	263/281 (94%)	262 (100%)	1 (0%)	91	96
All	All	1063/1124 (95%)	1051 (99%)	12 (1%)	73	86

All (12) 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	318	SER
1	A	385	ASN
1	B	198	ASP
1	B	212	TYR
1	B	478	LYS
1	C	198	ASP
1	C	285	GLU
1	C	297	LEU
1	D	198	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	221	ASN
1	A	341	ASN
1	A	359	ASN
1	A	385	ASN
1	C	296	ASN
1	C	327	ASN
1	C	341	ASN
1	D	295	GLN
1	D	296	ASN
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 23 ligands modelled in this entry, 11 are monoatomic - leaving 12 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	D	500[A]	4	28,34,34	2.03	6 (21%)	30,54,54	1.89	4 (13%)
2	GNP	C	500[B]	4	28,34,34	2.18	7 (25%)	30,54,54	2.02	7 (23%)
3	KAN	D	600	-	35,35,35	0.40	0	46,52,52	1.11	3 (6%)
2	GNP	B	500[B]	4	28,34,34	2.12	7 (25%)	30,54,54	1.87	5 (16%)
3	KAN	A	600	-	35,35,35	0.40	0	46,52,52	0.87	1 (2%)
3	KAN	B	600	-	35,35,35	0.46	0	46,52,52	0.95	3 (6%)
2	GNP	B	500[A]	4	28,34,34	2.09	7 (25%)	30,54,54	2.02	6 (20%)
3	KAN	C	600	-	35,35,35	0.41	0	46,52,52	0.84	2 (4%)
2	GNP	D	500[B]	4	28,34,34	2.00	6 (21%)	30,54,54	1.85	4 (13%)
2	GNP	A	500[A]	4	28,34,34	2.56	5 (17%)	30,54,54	1.81	5 (16%)
2	GNP	C	500[A]	4	28,34,34	2.24	7 (25%)	30,54,54	1.95	6 (20%)
2	GNP	A	500[B]	4	28,34,34	2.61	6 (21%)	30,54,54	1.80	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	D	500[A]	4	-	6/17/38/38	0/3/3/3
2	GNP	C	500[B]	4	-	4/17/38/38	0/3/3/3
3	KAN	D	600	-	-	2/12/72/72	0/3/3/3
2	GNP	B	500[B]	4	-	6/17/38/38	0/3/3/3
3	KAN	A	600	-	-	4/12/72/72	0/3/3/3
3	KAN	B	600	-	-	4/12/72/72	0/3/3/3
2	GNP	B	500[A]	4	-	4/17/38/38	0/3/3/3
3	KAN	C	600	-	-	4/12/72/72	0/3/3/3
2	GNP	D	500[B]	4	-	6/17/38/38	0/3/3/3
2	GNP	A	500[A]	4	-	6/17/38/38	0/3/3/3
2	GNP	C	500[A]	4	-	5/17/38/38	0/3/3/3
2	GNP	A	500[B]	4	-	4/17/38/38	0/3/3/3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500[B]	GNP	C5-C6	-9.52	1.36	1.52
2	A	500[A]	GNP	C5-C6	-9.52	1.36	1.52
2	C	500[B]	GNP	C4-N9	-8.05	1.37	1.47
2	C	500[A]	GNP	C4-N9	-8.05	1.37	1.47
2	A	500[B]	GNP	C4-N9	-7.79	1.37	1.47
2	A	500[A]	GNP	C4-N9	-7.79	1.37	1.47
2	D	500[B]	GNP	C4-N9	-7.56	1.37	1.47
2	D	500[A]	GNP	C4-N9	-7.56	1.37	1.47
2	B	500[A]	GNP	C4-N9	-7.22	1.38	1.47
2	B	500[B]	GNP	C4-N9	-7.22	1.38	1.47
2	C	500[B]	GNP	C5-C6	-5.53	1.43	1.52
2	C	500[A]	GNP	C5-C6	-5.53	1.43	1.52
2	B	500[B]	GNP	PB-O3A	4.73	1.65	1.59
2	B	500[A]	GNP	PB-O3A	4.26	1.64	1.59
2	D	500[B]	GNP	C5-C6	-3.92	1.46	1.52
2	D	500[A]	GNP	C5-C6	-3.92	1.46	1.52
2	B	500[A]	GNP	C5-C6	-3.53	1.46	1.52
2	B	500[B]	GNP	C5-C6	-3.53	1.46	1.52
2	A	500[B]	GNP	C6-N1	3.31	1.38	1.33
2	A	500[A]	GNP	C6-N1	3.31	1.38	1.33
2	D	500[B]	GNP	C6-N1	3.29	1.38	1.33
2	D	500[A]	GNP	C6-N1	3.29	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500[A]	GNP	C6-N1	2.89	1.38	1.33
2	B	500[B]	GNP	C6-N1	2.89	1.38	1.33
2	B	500[A]	GNP	C5-C4	-2.77	1.35	1.53
2	B	500[B]	GNP	C5-C4	-2.77	1.35	1.53
2	D	500[B]	GNP	PG-O3G	2.77	1.64	1.56
2	C	500[B]	GNP	C6-N1	2.74	1.37	1.33
2	C	500[A]	GNP	C6-N1	2.74	1.37	1.33
2	C	500[A]	GNP	PB-O3A	2.71	1.62	1.59
2	A	500[B]	GNP	PB-O2B	-2.70	1.49	1.56
2	A	500[B]	GNP	C5-C4	-2.67	1.36	1.53
2	A	500[A]	GNP	C5-C4	-2.67	1.36	1.53
2	C	500[B]	GNP	C5-C4	-2.64	1.36	1.53
2	C	500[A]	GNP	C5-C4	-2.64	1.36	1.53
2	C	500[B]	GNP	PB-O2B	-2.51	1.50	1.56
2	B	500[A]	GNP	C8-N9	-2.50	1.37	1.45
2	B	500[B]	GNP	C8-N9	-2.50	1.37	1.45
2	D	500[A]	GNP	PB-O3A	2.45	1.62	1.59
2	A	500[B]	GNP	C8-N9	-2.44	1.37	1.45
2	A	500[A]	GNP	C8-N9	-2.44	1.37	1.45
2	D	500[B]	GNP	C5-C4	-2.42	1.38	1.53
2	D	500[A]	GNP	C5-C4	-2.42	1.38	1.53
2	B	500[B]	GNP	PB-O2B	-2.39	1.50	1.56
2	D	500[B]	GNP	C8-N9	-2.37	1.37	1.45
2	D	500[A]	GNP	C8-N9	-2.37	1.37	1.45
2	C	500[B]	GNP	C8-N9	-2.21	1.38	1.45
2	C	500[A]	GNP	C8-N9	-2.21	1.38	1.45
2	C	500[B]	GNP	C2-N1	-2.15	1.35	1.44
2	C	500[A]	GNP	C2-N1	-2.15	1.35	1.44
2	B	500[A]	GNP	PG-O2G	2.08	1.62	1.56

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500[B]	GNP	C4-C5-N7	6.37	110.91	102.46
2	A	500[A]	GNP	C4-C5-N7	6.37	110.91	102.46
2	B	500[A]	GNP	C4-C5-N7	6.33	110.85	102.46
2	B	500[B]	GNP	C4-C5-N7	6.33	110.85	102.46
2	C	500[B]	GNP	C4-C5-N7	6.19	110.66	102.46
2	C	500[A]	GNP	C4-C5-N7	6.19	110.66	102.46
2	D	500[B]	GNP	C4-C5-N7	5.99	110.40	102.46
2	D	500[A]	GNP	C4-C5-N7	5.99	110.40	102.46
2	D	500[B]	GNP	C5-C6-N1	-5.48	111.43	118.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500[A]	GNP	C5-C6-N1	-5.48	111.43	118.19
2	C	500[B]	GNP	C5-C6-N1	-5.16	111.82	118.19
2	C	500[A]	GNP	C5-C6-N1	-5.16	111.82	118.19
2	B	500[A]	GNP	C5-C6-N1	-4.87	112.18	118.19
2	B	500[B]	GNP	C5-C6-N1	-4.87	112.18	118.19
2	C	500[B]	GNP	O6-C6-C5	4.52	129.08	119.86
2	C	500[A]	GNP	O6-C6-C5	4.52	129.08	119.86
2	A	500[B]	GNP	C5-C6-N1	-4.35	112.82	118.19
2	A	500[A]	GNP	C5-C6-N1	-4.35	112.82	118.19
2	B	500[A]	GNP	O3G-PG-O1G	-4.21	102.87	113.45
2	D	500[B]	GNP	O6-C6-C5	4.10	128.22	119.86
2	D	500[A]	GNP	O6-C6-C5	4.10	128.22	119.86
3	D	600	KAN	O9-C10-C9	3.53	116.68	107.28
2	B	500[B]	GNP	O1G-PG-N3B	3.48	116.90	111.77
2	B	500[A]	GNP	O6-C6-C5	3.37	126.73	119.86
2	B	500[B]	GNP	O6-C6-C5	3.37	126.73	119.86
2	B	500[A]	GNP	O1G-PG-N3B	3.35	116.70	111.77
2	A	500[B]	GNP	O6-C6-C5	3.20	126.39	119.86
2	A	500[A]	GNP	O6-C6-C5	3.20	126.39	119.86
3	D	600	KAN	O9-C10-C11	-3.19	101.56	109.18
2	A	500[A]	GNP	O3G-PG-O1G	-3.04	105.81	113.45
2	B	500[B]	GNP	O2G-PG-O1G	-2.70	106.65	113.45
2	C	500[B]	GNP	O6-C6-N1	-2.68	119.09	122.69
2	C	500[A]	GNP	O6-C6-N1	-2.68	119.09	122.69
3	A	600	KAN	O9-C10-C11	-2.67	102.81	109.18
3	B	600	KAN	C11-C12-C7	-2.65	105.74	111.18
2	C	500[B]	GNP	O1G-PG-N3B	2.57	115.56	111.77
2	D	500[A]	GNP	O2G-PG-O1G	-2.51	107.16	113.45
3	B	600	KAN	O5-C5-C6	2.48	110.63	106.01
3	D	600	KAN	O11-C8-C9	2.46	113.84	107.28
2	C	500[A]	GNP	O3G-PG-O1G	-2.45	107.29	113.45
2	B	500[A]	GNP	O3A-PB-N3B	2.45	113.38	106.59
2	A	500[A]	GNP	O1G-PG-N3B	2.43	115.36	111.77
2	D	500[B]	GNP	O1G-PG-N3B	-2.40	108.23	111.77
2	C	500[B]	GNP	O3G-PG-O1G	-2.32	107.62	113.45
2	C	500[B]	GNP	O5'-PA-O1A	2.30	118.06	109.07
2	C	500[A]	GNP	O5'-PA-O1A	2.30	118.06	109.07
3	C	600	KAN	O14-C16-C17	-2.28	103.64	109.30
3	C	600	KAN	O9-C10-C11	-2.27	103.77	109.18
2	A	500[B]	GNP	O2G-PG-O1G	-2.25	107.80	113.45
3	B	600	KAN	O11-C8-C7	-2.14	104.07	109.18
2	A	500[B]	GNP	O2B-PB-O1B	-2.02	105.69	109.92

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	500[B]	GNP	PB-N3B-PG-O1G
2	C	500[B]	GNP	C2'-C1'-N9-C8
2	C	500[B]	GNP	C2'-C1'-N9-C4
2	B	500[A]	GNP	PB-N3B-PG-O1G
2	B	500[A]	GNP	PG-N3B-PB-O1B
2	B	500[A]	GNP	C2'-C1'-N9-C8
2	B	500[A]	GNP	C2'-C1'-N9-C4
2	D	500[B]	GNP	PB-N3B-PG-O1G
2	D	500[B]	GNP	PG-N3B-PB-O1B
2	D	500[B]	GNP	PG-N3B-PB-O3A
2	D	500[B]	GNP	O4'-C1'-N9-C4
2	D	500[B]	GNP	C2'-C1'-N9-C8
2	D	500[B]	GNP	C2'-C1'-N9-C4
2	B	500[B]	GNP	PB-N3B-PG-O1G
2	B	500[B]	GNP	PA-O3A-PB-O1B
2	B	500[B]	GNP	C2'-C1'-N9-C8
2	B	500[B]	GNP	C2'-C1'-N9-C4
2	D	500[A]	GNP	PB-N3B-PG-O1G
2	D	500[A]	GNP	PG-N3B-PB-O1B
2	D	500[A]	GNP	O4'-C1'-N9-C4
2	D	500[A]	GNP	C2'-C1'-N9-C8
2	D	500[A]	GNP	C2'-C1'-N9-C4
2	A	500[B]	GNP	PB-N3B-PG-O1G
2	A	500[B]	GNP	C5'-O5'-PA-O1A
2	A	500[B]	GNP	C2'-C1'-N9-C8
2	A	500[B]	GNP	C2'-C1'-N9-C4
2	A	500[A]	GNP	PB-N3B-PG-O1G
2	A	500[A]	GNP	PG-N3B-PB-O1B
2	A	500[A]	GNP	C5'-O5'-PA-O1A
2	A	500[A]	GNP	C2'-C1'-N9-C8
2	A	500[A]	GNP	C2'-C1'-N9-C4
2	C	500[A]	GNP	PB-N3B-PG-O1G
2	C	500[A]	GNP	PG-N3B-PB-O1B
2	C	500[A]	GNP	C2'-C1'-N9-C8
2	C	500[A]	GNP	C2'-C1'-N9-C4
3	D	600	KAN	C9-C10-O9-C1
3	B	600	KAN	C9-C10-O9-C1
3	C	600	KAN	C9-C10-O9-C1
3	A	600	KAN	O5-C1-O9-C10
3	A	600	KAN	C9-C10-O9-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	600	KAN	O5-C1-O9-C10
3	B	600	KAN	C11-C10-O9-C1
3	C	600	KAN	C11-C10-O9-C1
3	D	600	KAN	C11-C10-O9-C1
3	A	600	KAN	C11-C10-O9-C1
2	D	500[A]	GNP	PG-N3B-PB-O3A
2	A	500[A]	GNP	PG-N3B-PB-O3A
3	B	600	KAN	O5-C1-O9-C10
2	B	500[B]	GNP	PB-O3A-PA-O1A
3	C	600	KAN	C2-C1-O9-C10
3	A	600	KAN	C2-C1-O9-C10
3	B	600	KAN	C2-C1-O9-C10
2	B	500[B]	GNP	PB-O3A-PA-O2A
2	C	500[B]	GNP	C5'-O5'-PA-O1A
2	C	500[A]	GNP	C5'-O5'-PA-O1A

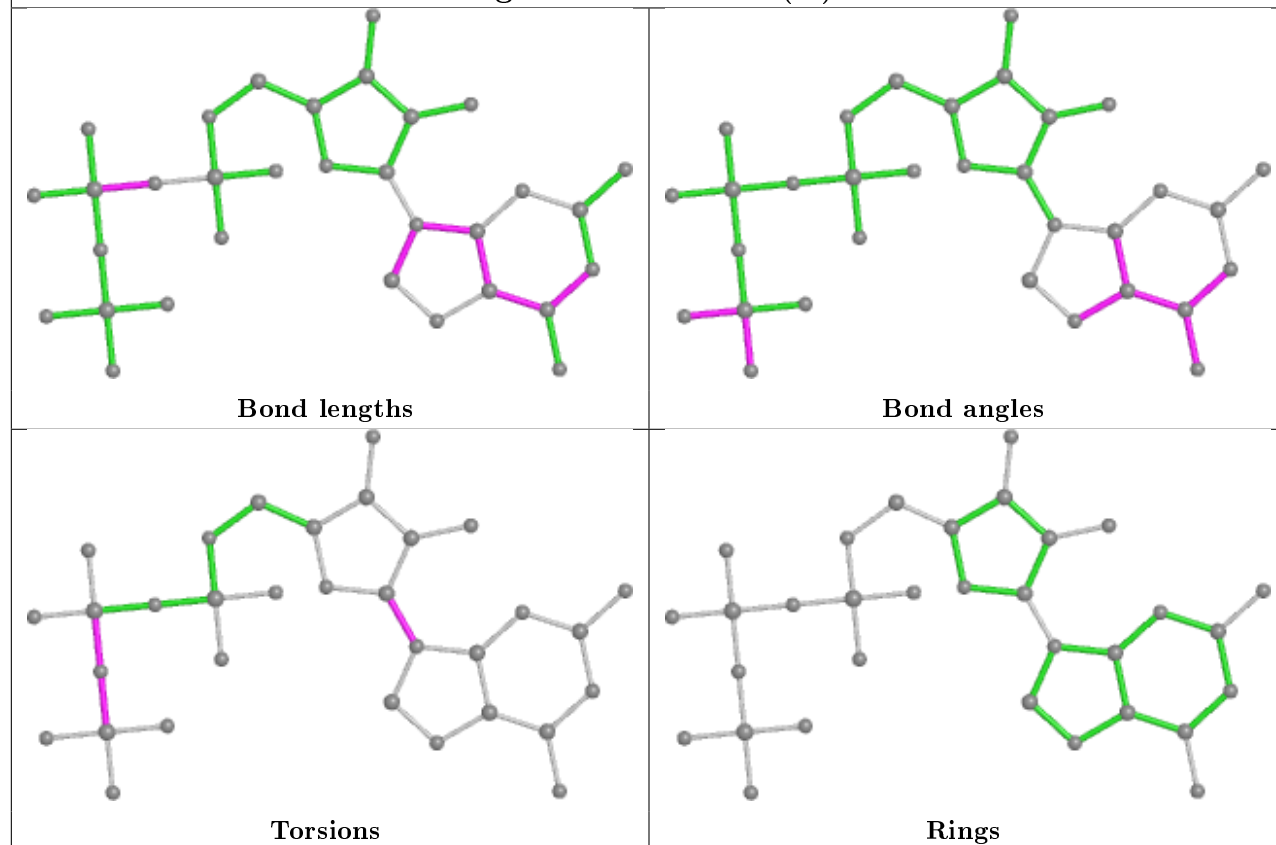
There are no ring outliers.

8 monomers are involved in 12 short contacts:

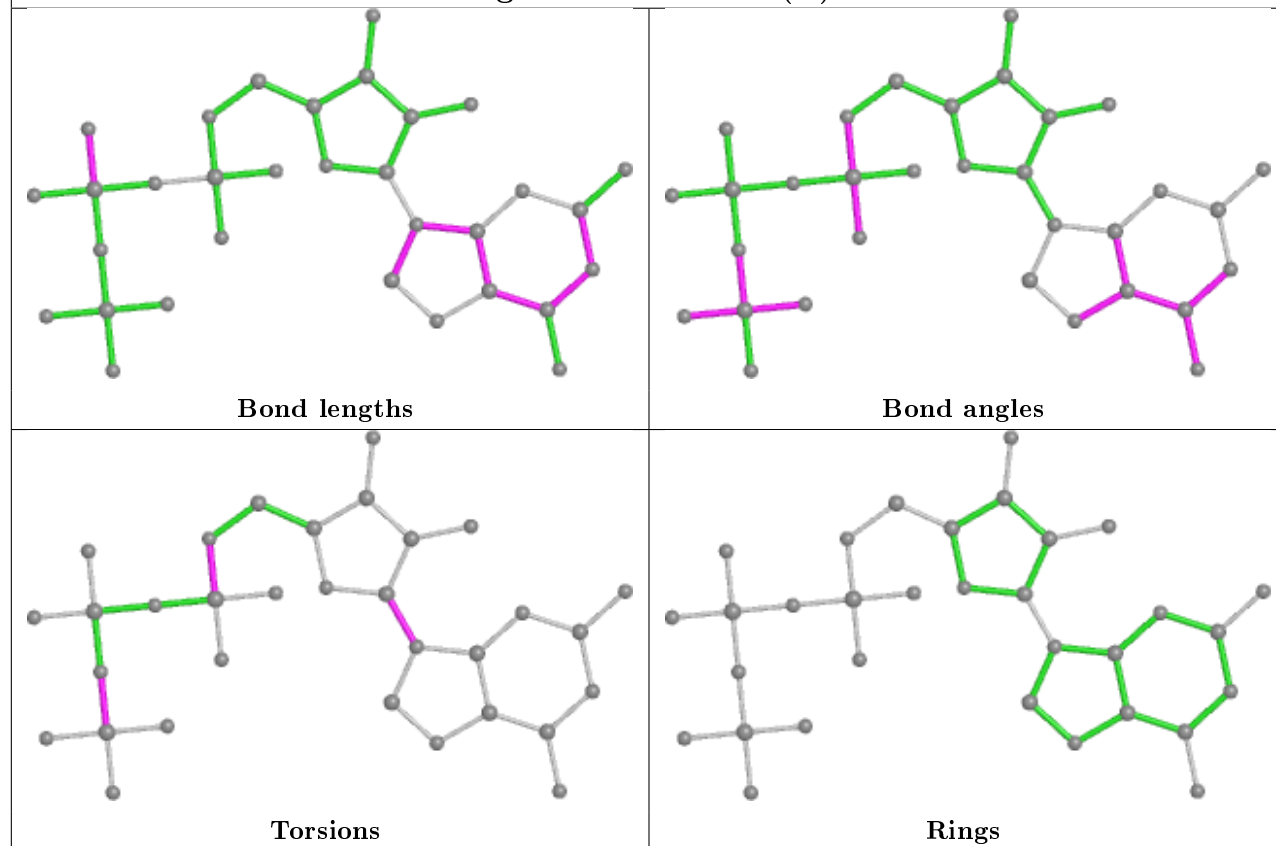
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500[A]	GNP	2	0
3	D	600	KAN	1	0
2	B	500[B]	GNP	1	0
3	B	600	KAN	2	0
2	B	500[A]	GNP	1	0
3	C	600	KAN	1	0
2	A	500[A]	GNP	4	0
2	A	500[B]	GNP	1	0

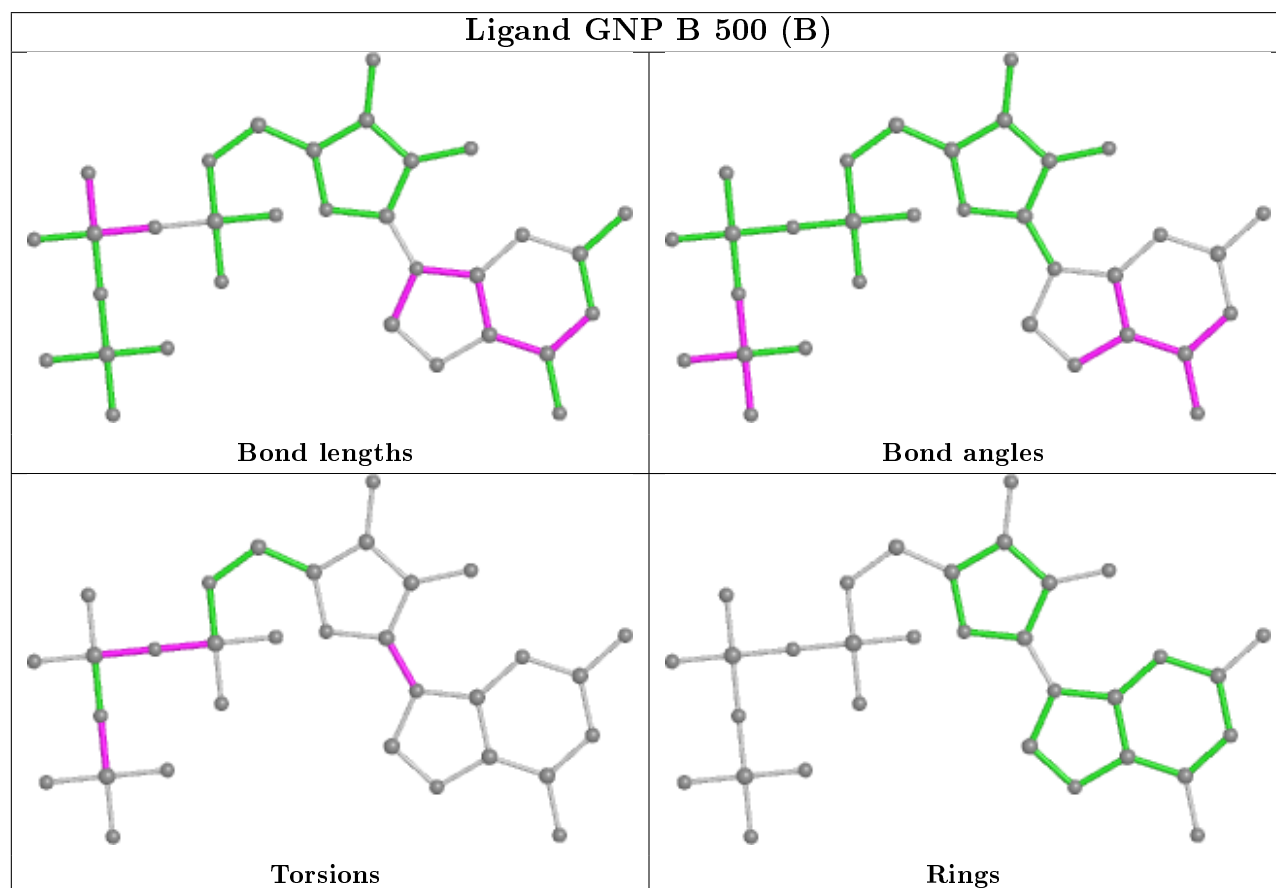
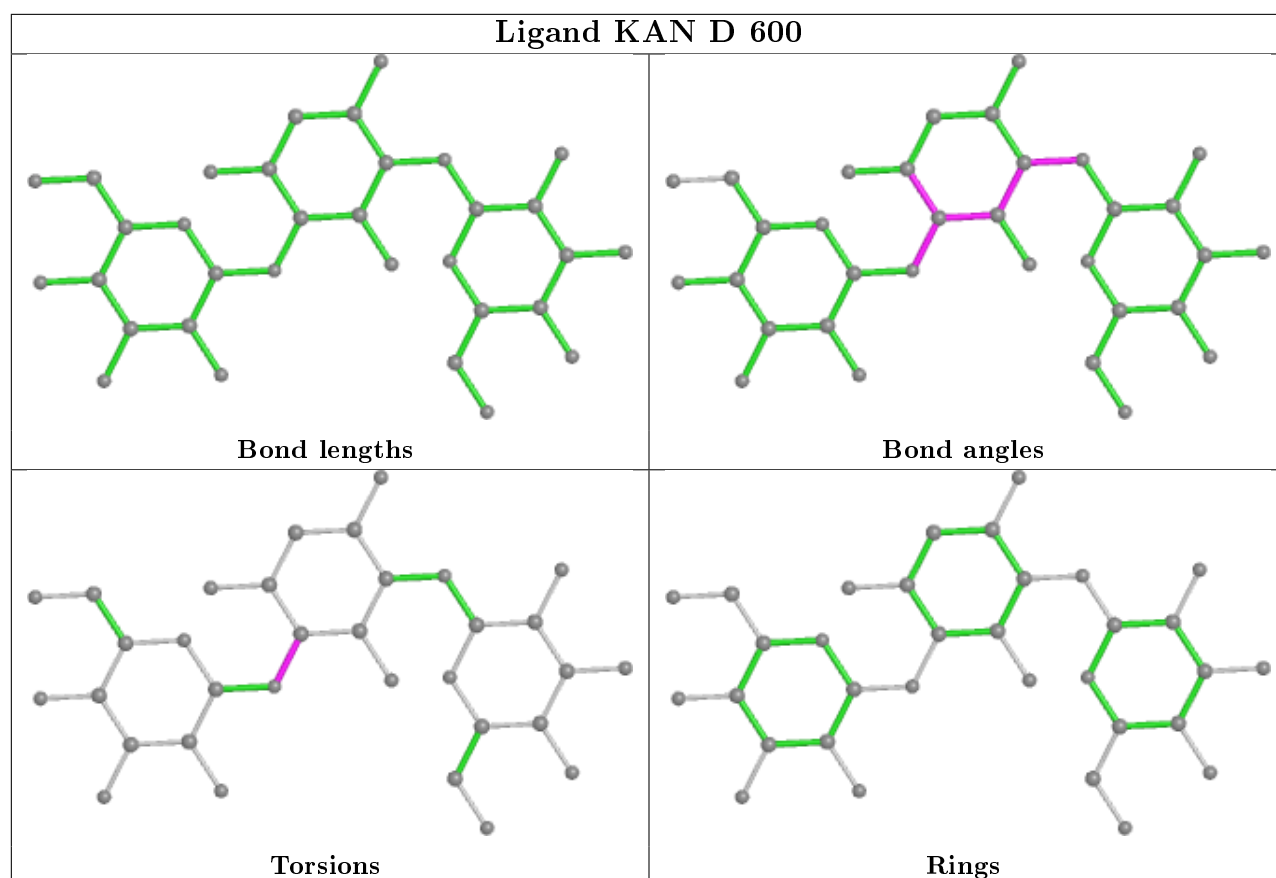
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

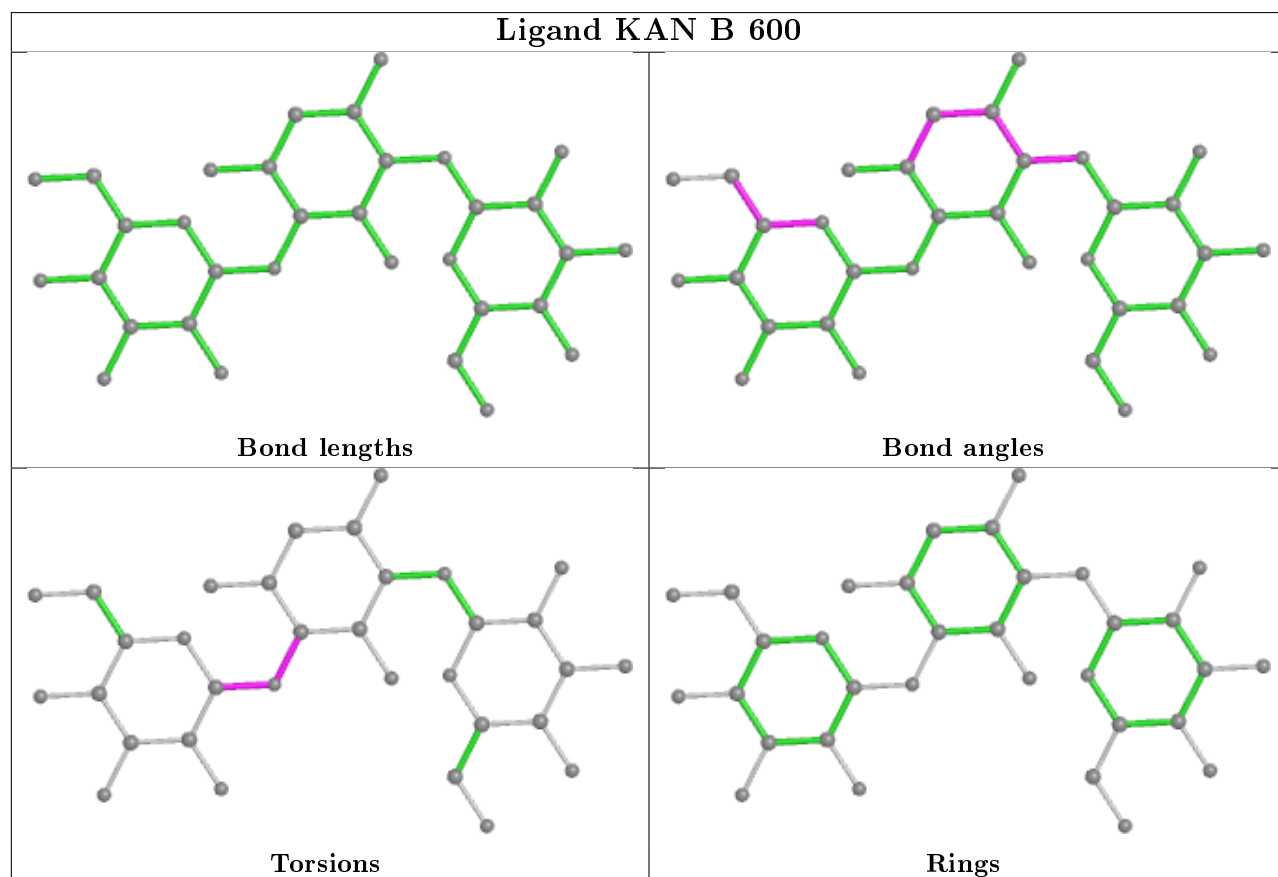
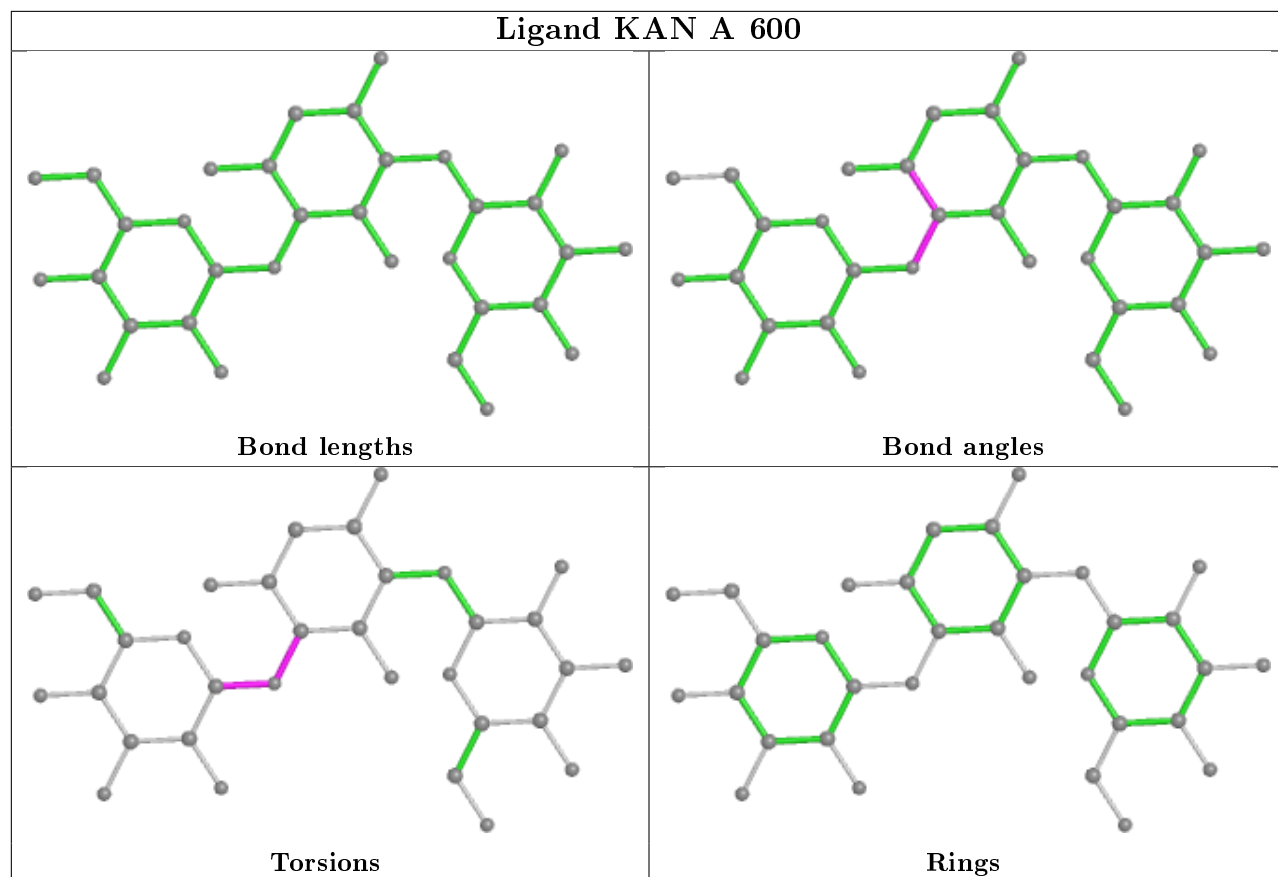
Ligand GNP D 500 (A)



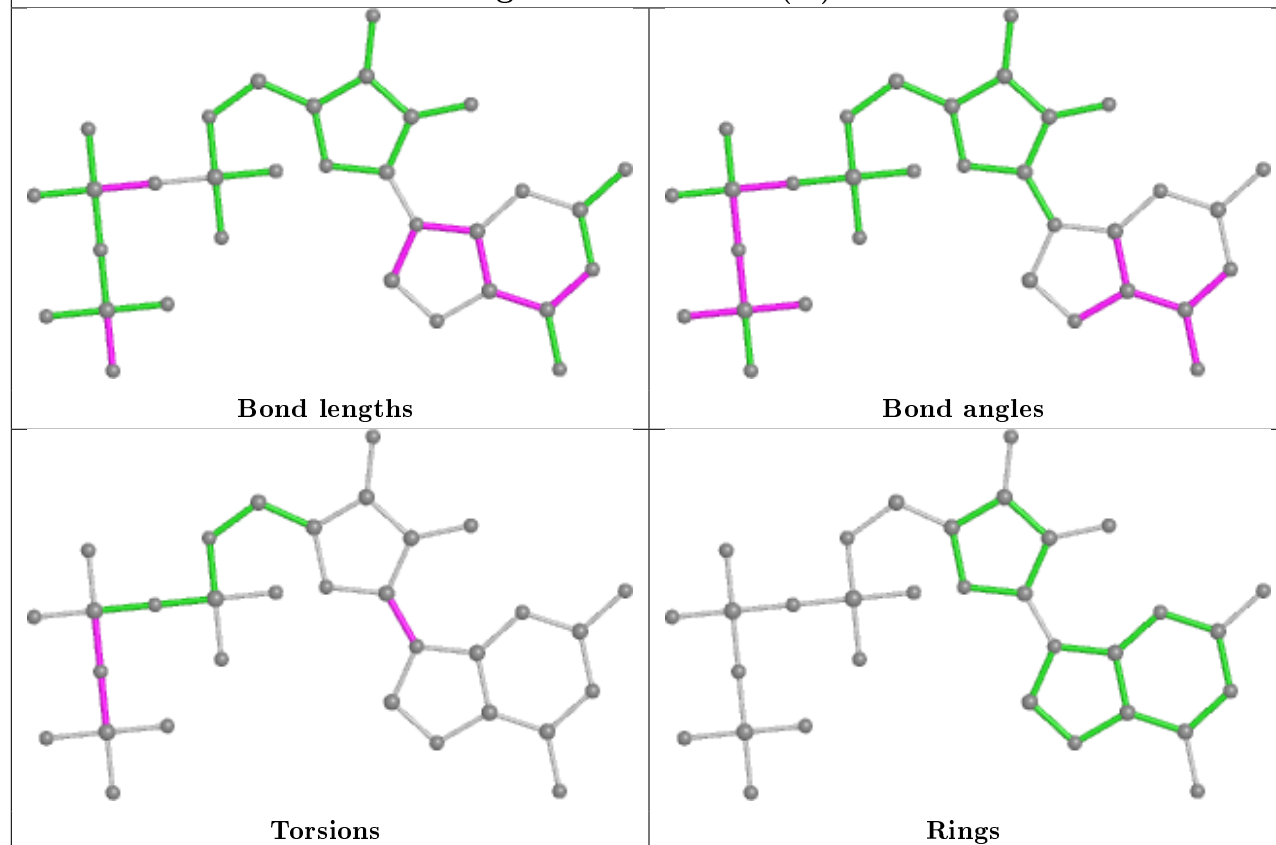
Ligand GNP C 500 (B)



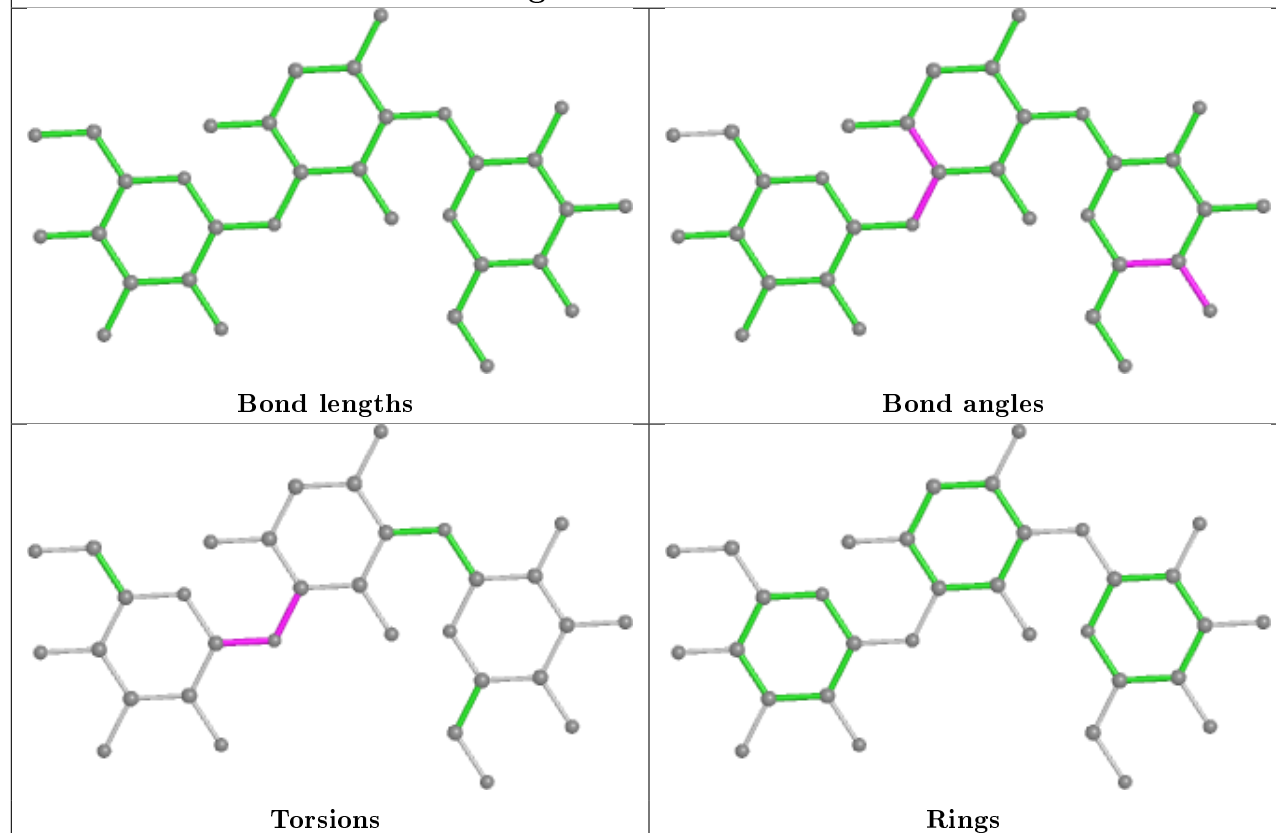




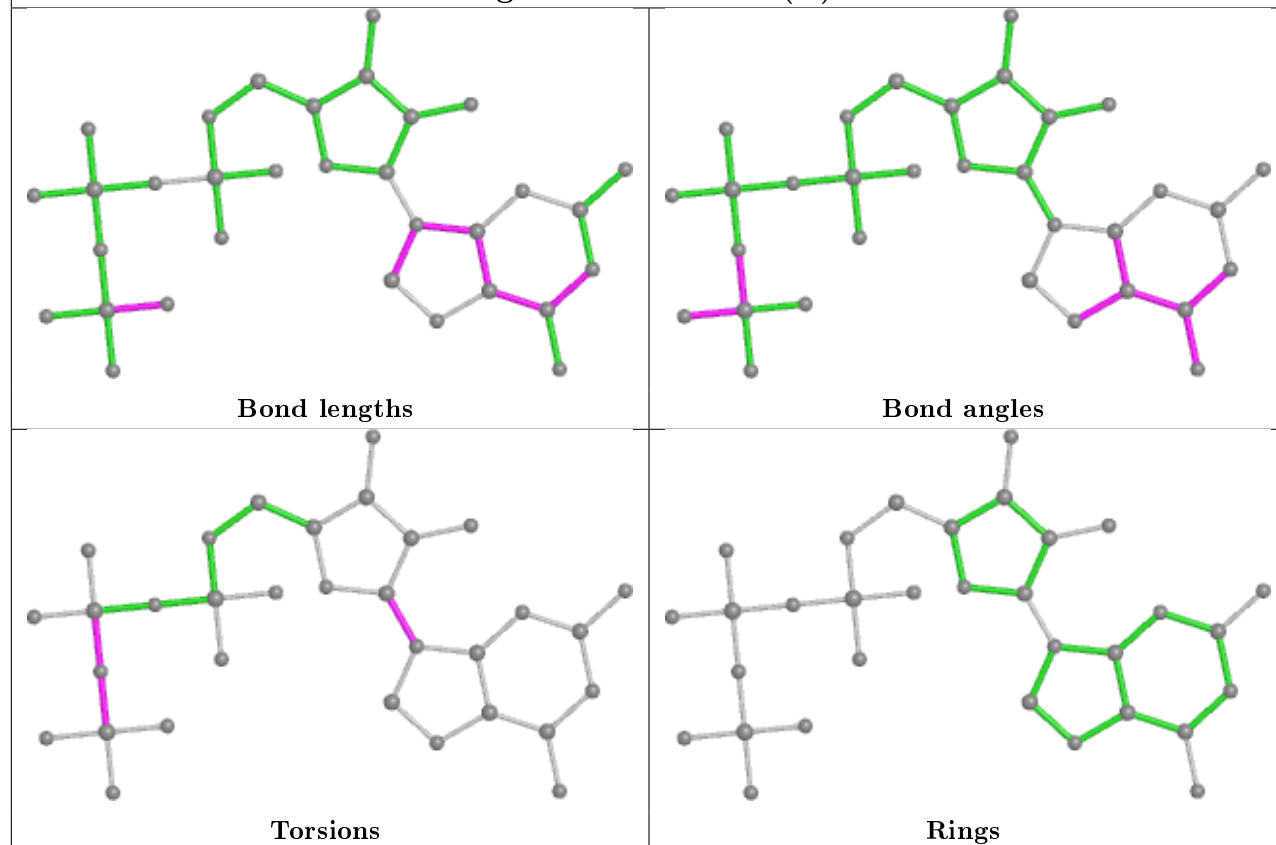
Ligand GNP B 500 (A)



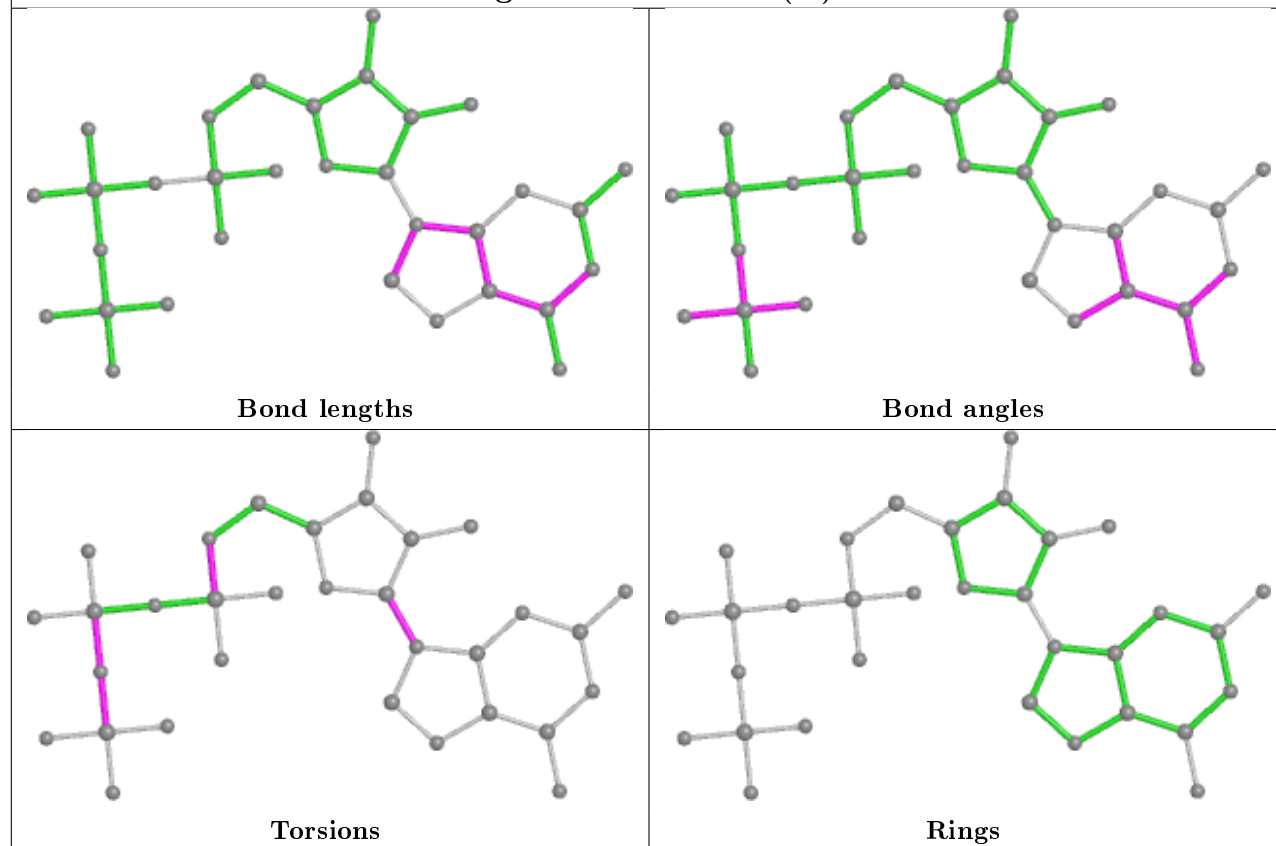
Ligand KAN C 600



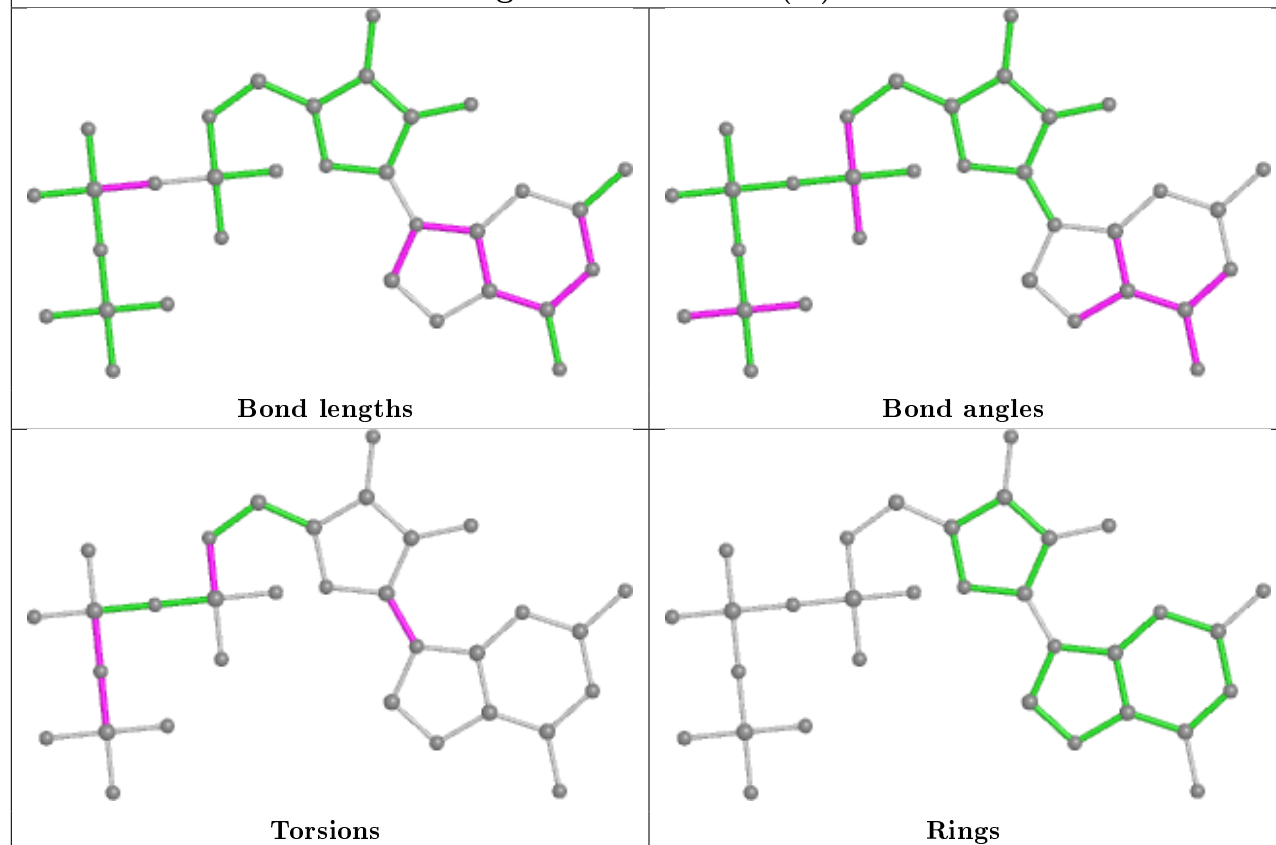
Ligand GNP D 500 (B)



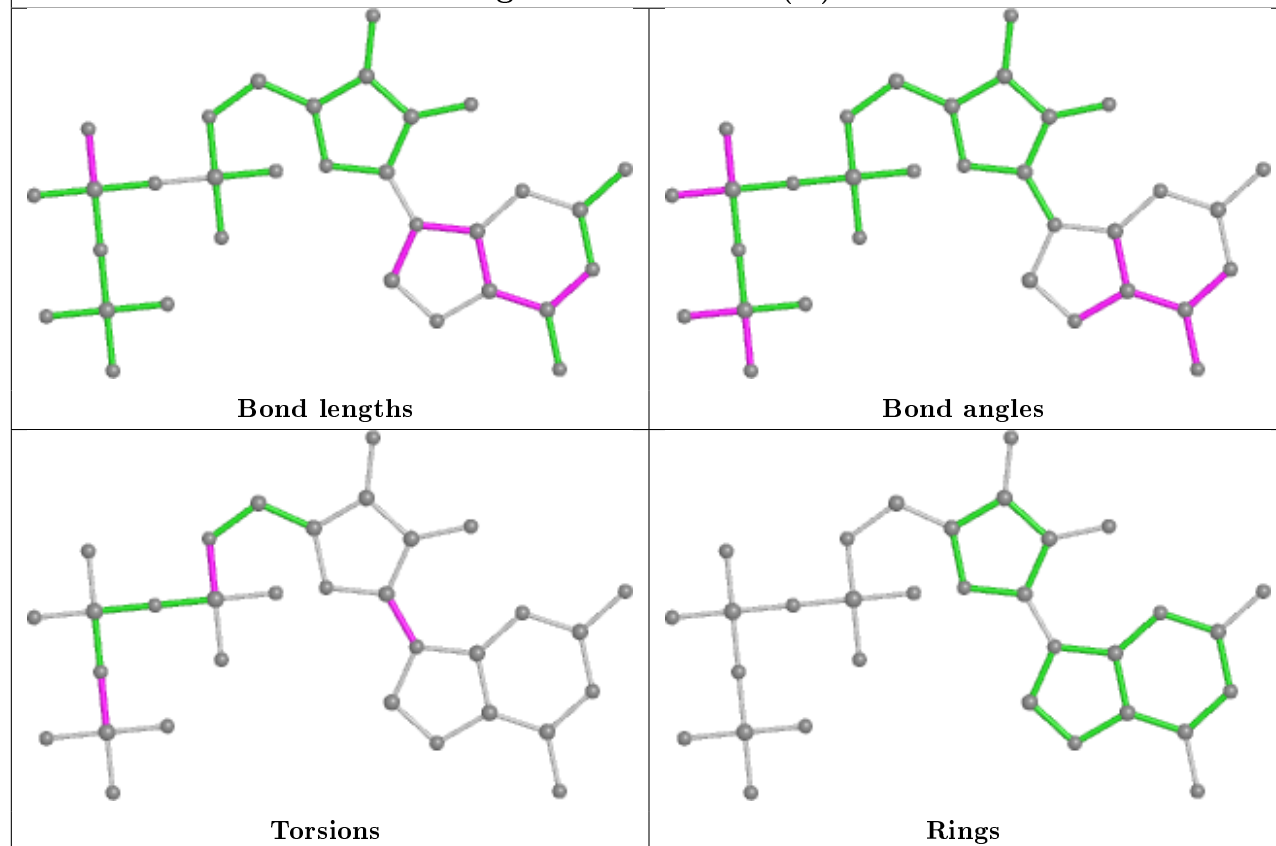
Ligand GNP A 500 (A)



Ligand GNP C 500 (A)



Ligand GNP A 500 (B)



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	292/305 (95%)	0.05	2 (0%) 87 91	34, 52, 80, 101	0
1	B	292/305 (95%)	0.02	1 (0%) 94 96	36, 54, 83, 110	0
1	C	290/305 (95%)	0.14	4 (1%) 75 80	32, 55, 89, 113	0
1	D	289/305 (94%)	0.30	18 (6%) 20 26	43, 64, 101, 123	0
All	All	1163/1220 (95%)	0.13	25 (2%) 63 70	32, 56, 90, 123	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	473	TYR	5.0
1	A	212	TYR	3.9
1	D	464	PHE	3.7
1	D	181	ASP	3.2
1	D	474	LYS	3.0
1	D	462	GLN	2.9
1	D	255	VAL	2.7
1	C	207	ILE	2.7
1	D	460	ILE	2.6
1	D	254	ASN	2.6
1	D	182	ASN	2.3
1	D	463	GLU	2.3
1	C	230	SER	2.3
1	C	185	ASN	2.3
1	C	286	ILE	2.2
1	D	461	LYS	2.2
1	B	212	TYR	2.2
1	D	466	GLU	2.2
1	D	208	ILE	2.2
1	A	455	TYR	2.1
1	D	455	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	386	ASN	2.1
1	D	185	ASN	2.1
1	D	470	LYS	2.0
1	D	469	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.

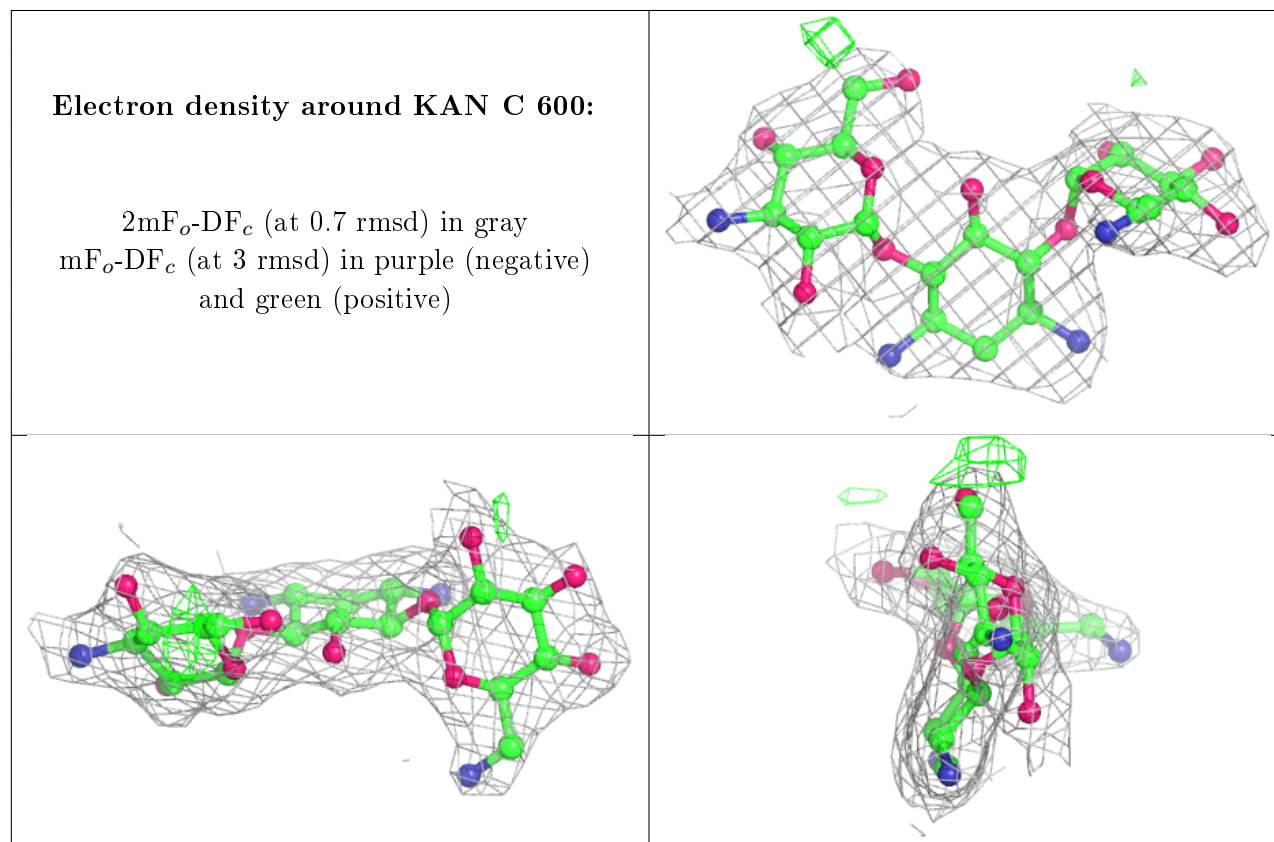
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CL	A	802	1/1	0.87	0.17	84,84,84,84	0
3	KAN	C	600	33/33	0.90	0.13	64,70,75,79	0
4	MG	A	700	1/1	0.94	0.17	35,35,35,35	0
4	MG	C	800	1/1	0.95	0.05	76,76,76,76	0
3	KAN	B	600	33/33	0.95	0.13	49,55,63,70	0
2	GNP	D	500[A]	32/32	0.96	0.12	47,57,63,63	9
2	GNP	D	500[B]	32/32	0.96	0.12	47,56,63,63	9
4	MG	C	702	1/1	0.97	0.07	49,49,49,49	0
4	MG	A	702	1/1	0.97	0.08	46,46,46,46	0
2	GNP	B	500[B]	32/32	0.97	0.13	40,43,46,50	9
3	KAN	D	600	33/33	0.97	0.12	48,51,59,64	0
2	GNP	B	500[A]	32/32	0.97	0.13	40,43,48,50	9
3	KAN	A	600	33/33	0.97	0.13	40,49,57,64	0
4	MG	D	702	1/1	0.97	0.06	47,47,47,47	0
2	GNP	C	500[B]	32/32	0.97	0.11	39,47,52,58	9
2	GNP	C	500[A]	32/32	0.97	0.11	43,48,52,58	9
4	MG	D	700	1/1	0.98	0.09	36,36,36,36	0
4	MG	C	700	1/1	0.98	0.10	37,37,37,37	0
5	CL	C	802	1/1	0.98	0.11	69,69,69,69	0

Continued on next page...

Continued from previous page...

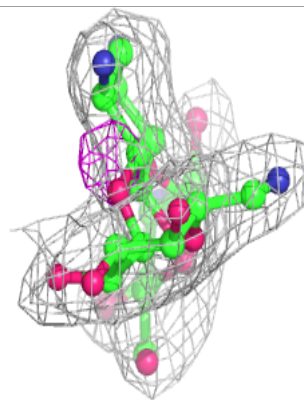
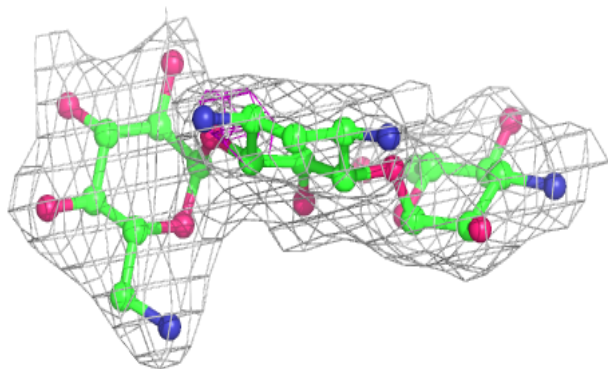
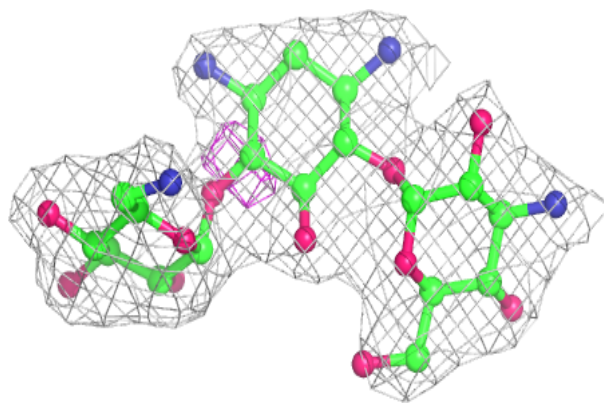
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GNP	A	500[A]	32/32	0.98	0.14	37,43,47,53	9
2	GNP	A	500[B]	32/32	0.98	0.14	37,45,50,53	9
4	MG	B	702	1/1	0.99	0.09	44,44,44,44	0
4	MG	B	700	1/1	0.99	0.13	33,33,33,33	0

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.

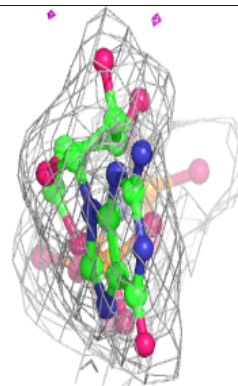
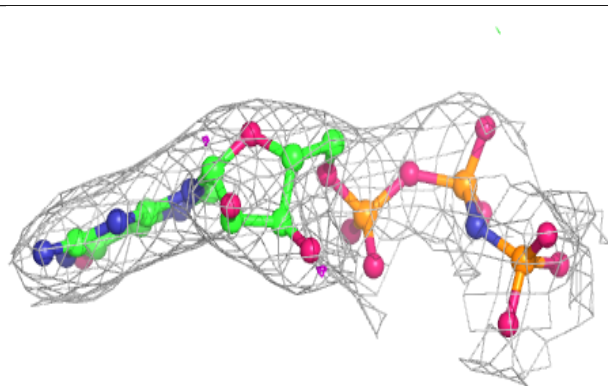
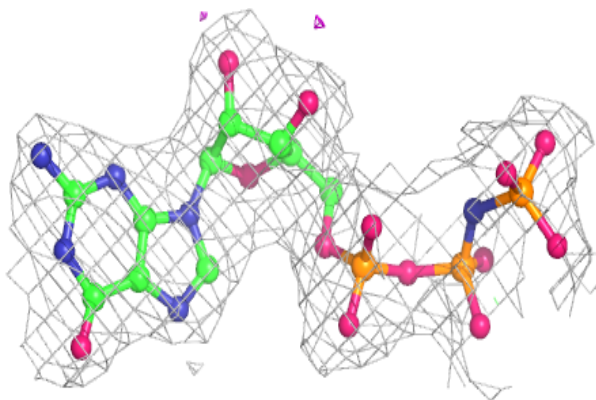


Electron density around KAN B 600:

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

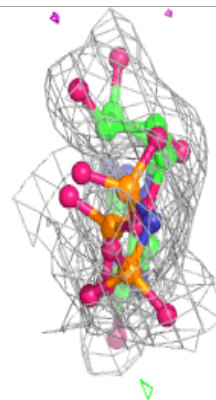
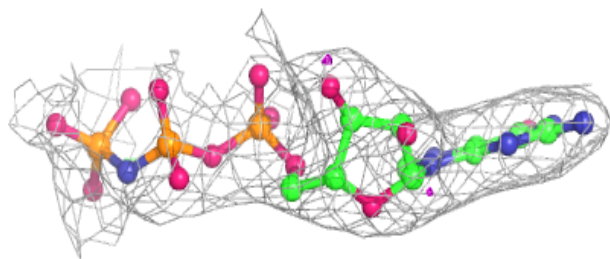
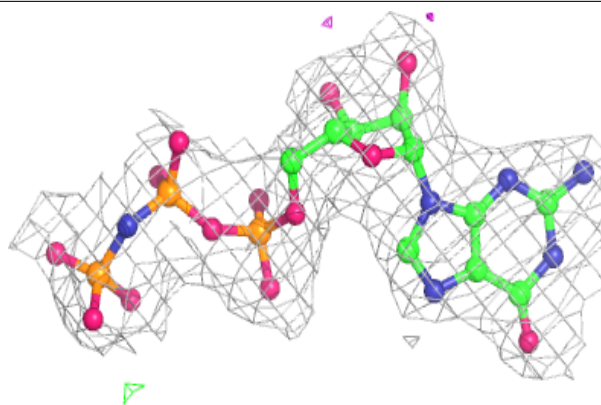
**Electron density around GNP D 500 (A):**

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

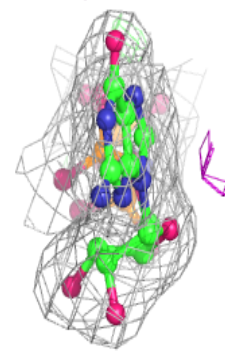
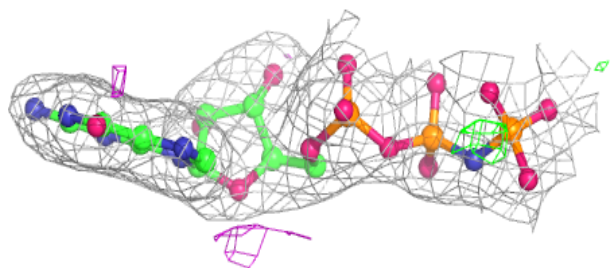
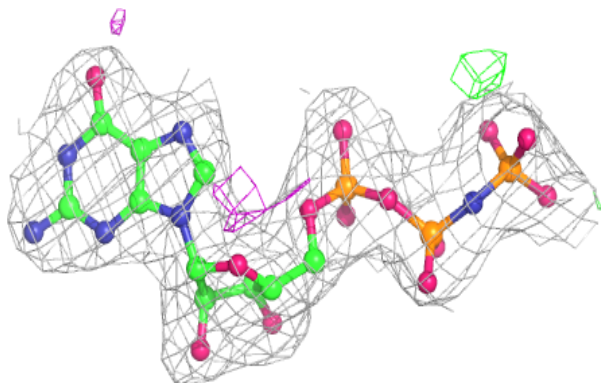


Electron density around GNP D 500 (B):

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

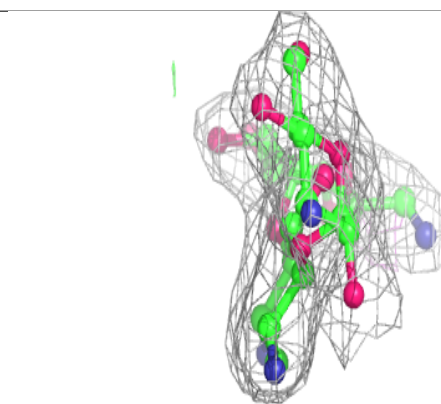
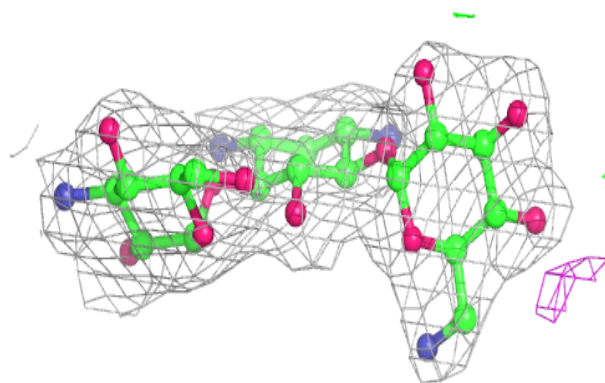
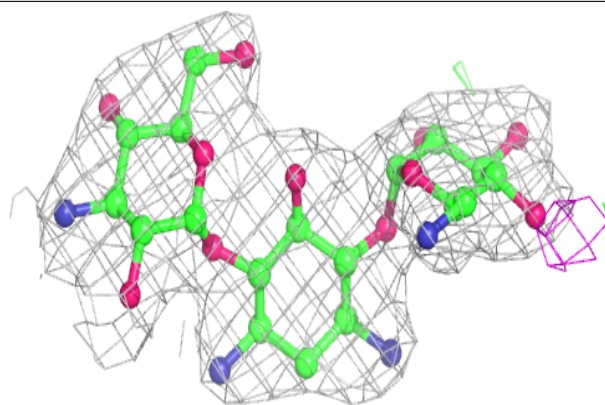
**Electron density around GNP B 500 (B):**

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

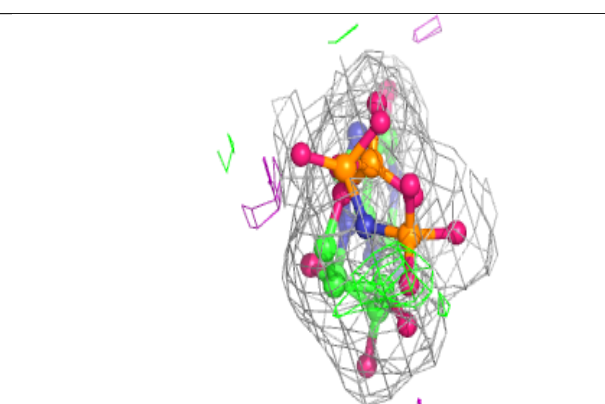
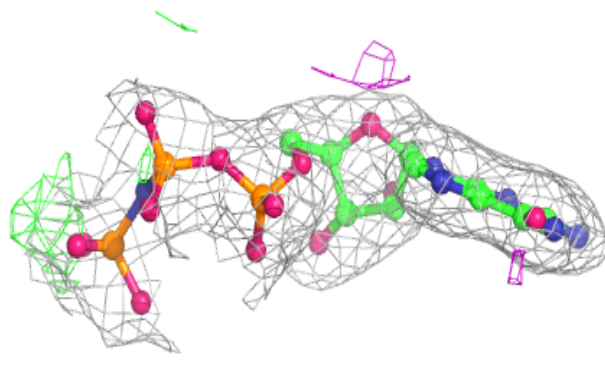
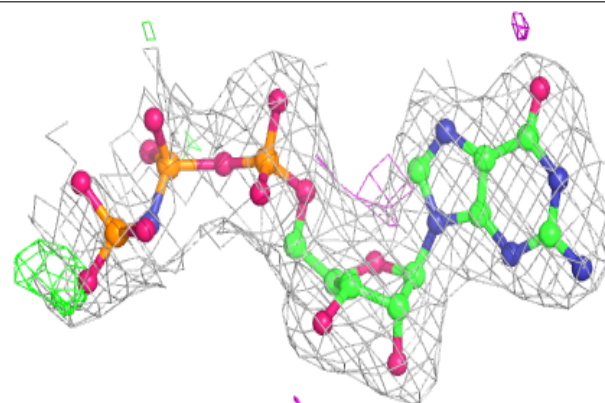


Electron density around KAN D 600:

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

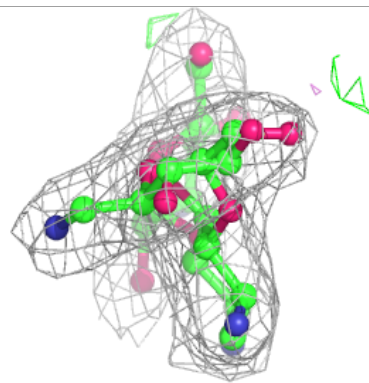
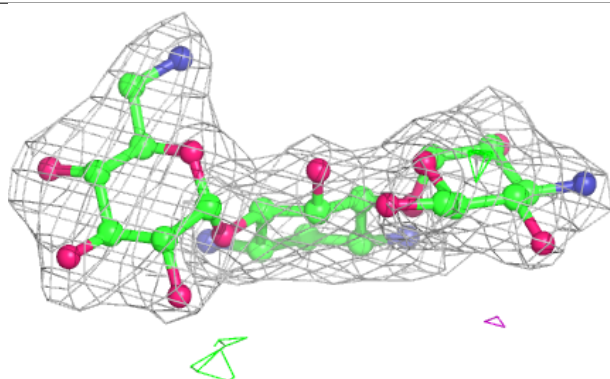
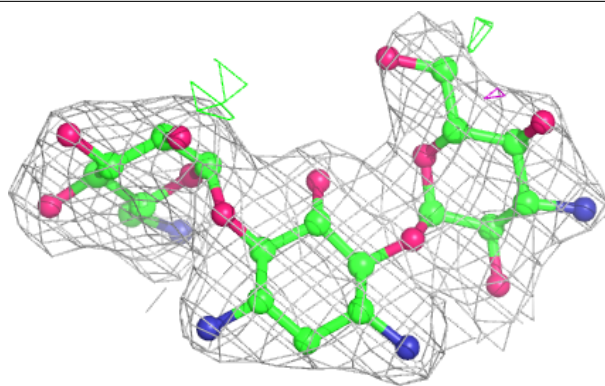
**Electron density around GNP B 500 (A):**

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

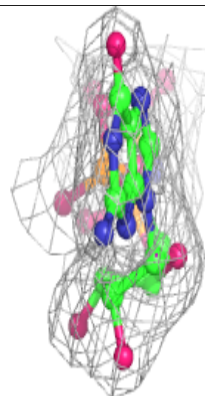
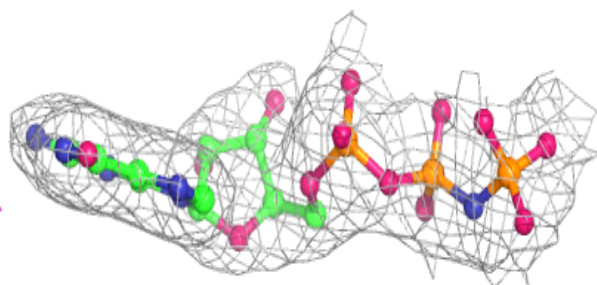
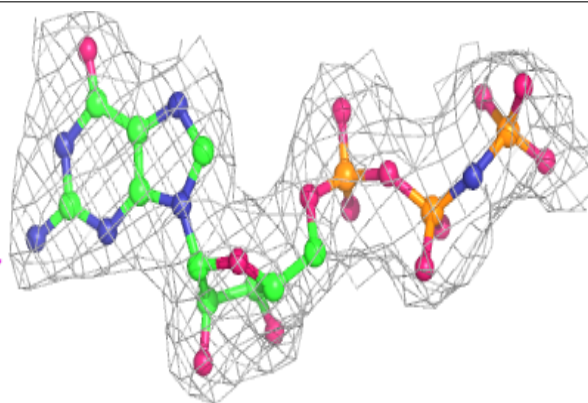


Electron density around KAN A 600:

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

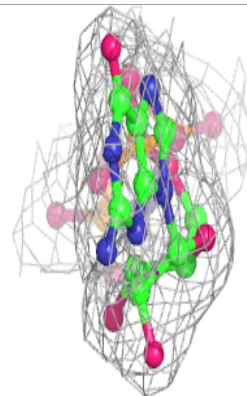
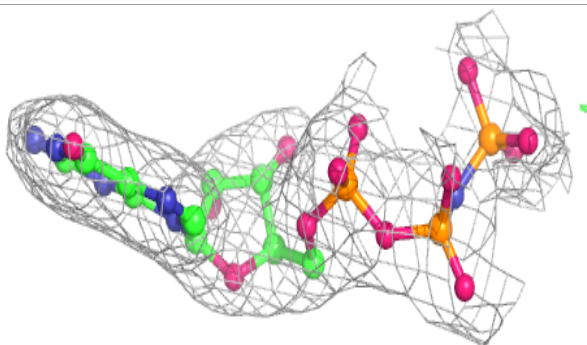
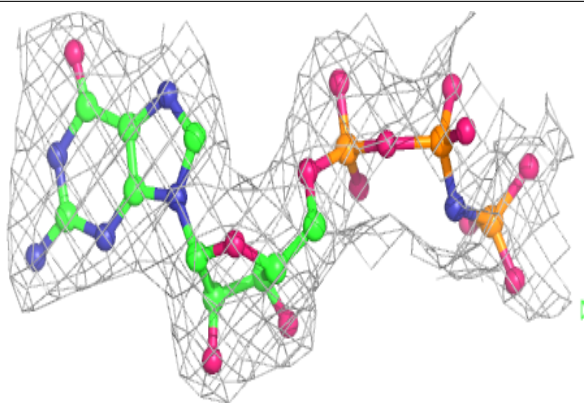
**Electron density around GNP C 500 (B):**

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

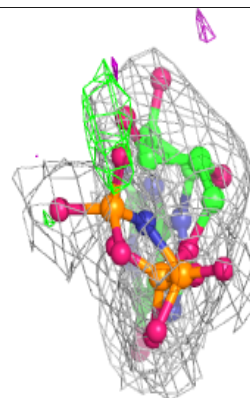
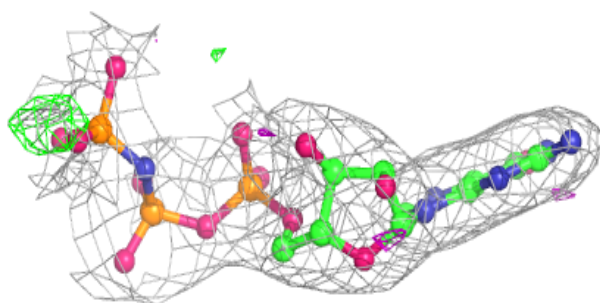
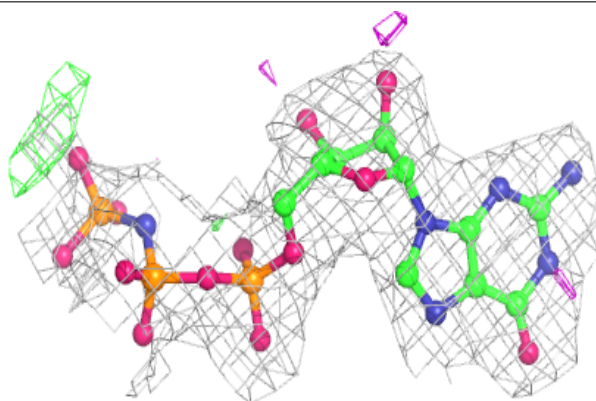


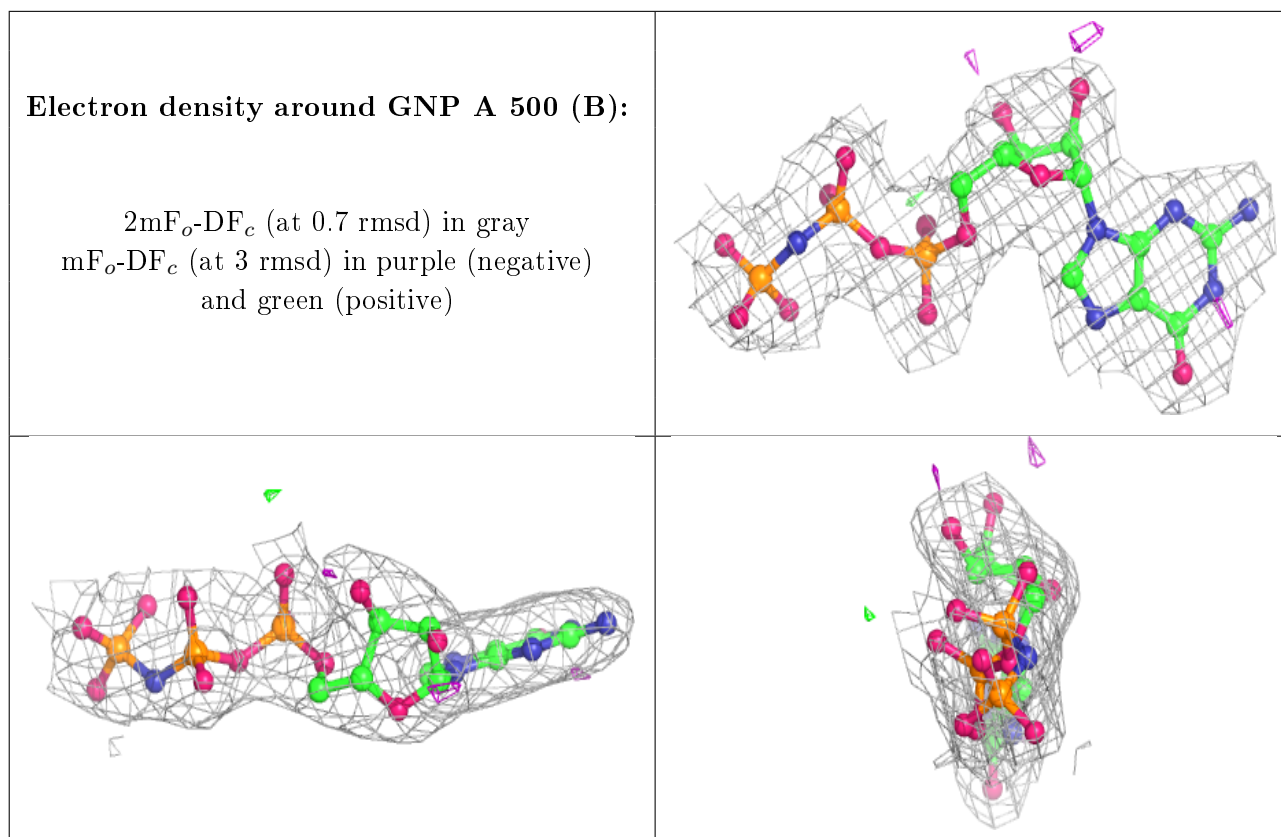
Electron density around GNP C 500 (A):

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

**Electron density around GNP 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.