Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:34 PM UTC

PDB ID	:	6C5U / pdb_00006c5u
Title	:	Aminoglycoside Phosphotransferase (2")-Ia in complex with GMPPNP, Magnesium, and Ribostamycin, Alternate form
Authors	:	Caldwell, S.J.; Berghuis, A.M.
Deposited on	:	2018-01-16
Resolution	:	2.41 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:

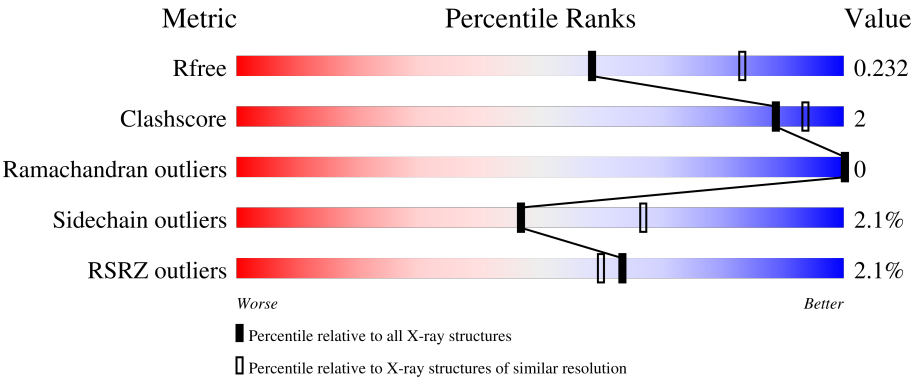
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	305	3% 87% 9% .
1	B	305	2% 88% 8% .
1	C	305	% 88% 7% 6%
1	D	305	3% 89% 6% 5%

2 Entry composition

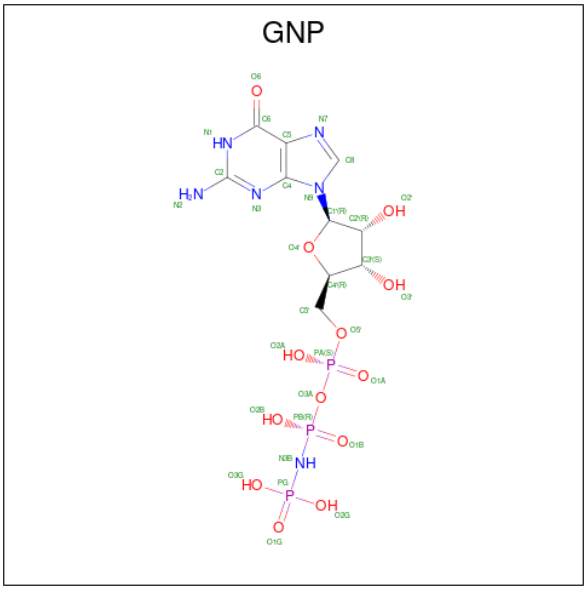
There are 6 unique types of molecules in this entry. The entry contains 10345 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	293	Total	C	N	O	S	0	3	0
			2424	1547	377	490	10			
1	B	292	Total	C	N	O	S	0	2	0
			2418	1546	373	489	10			
1	C	287	Total	C	N	O	S	0	2	0
			2382	1524	369	479	10			
1	D	291	Total	C	N	O	S	0	1	0
			2376	1512	372	482	10			

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



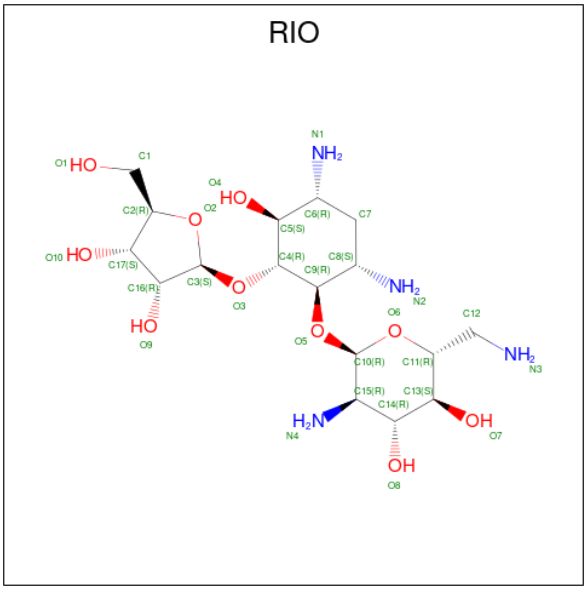
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is RIBOSTAMYCIN (CCD ID: RIO) (formula: $C_{17}H_{34}N_4O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 31 17 4 10	0	0
3	B	1	Total C N O 31 17 4 10	0	0
3	D	1	Total C N O 31 17 4 10	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
4	D	2	Total Mg 2 2	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is water.

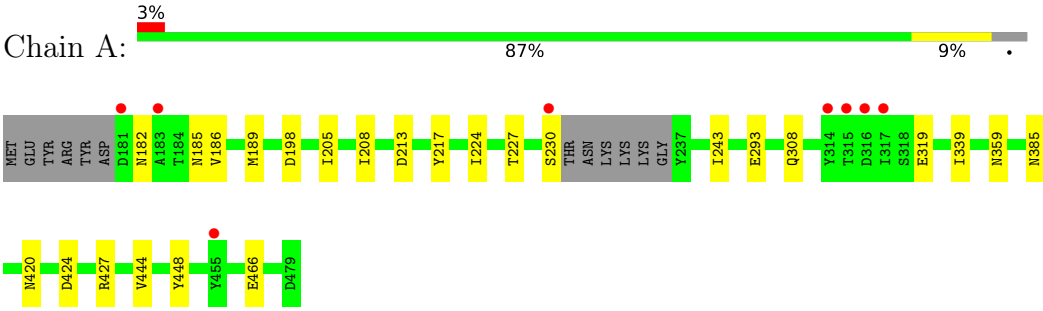
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	144	Total O 144 144	0	0
6	B	167	Total O 167 167	0	0
6	C	124	Total O 124 124	0	0
6	D	78	Total O 78 78	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

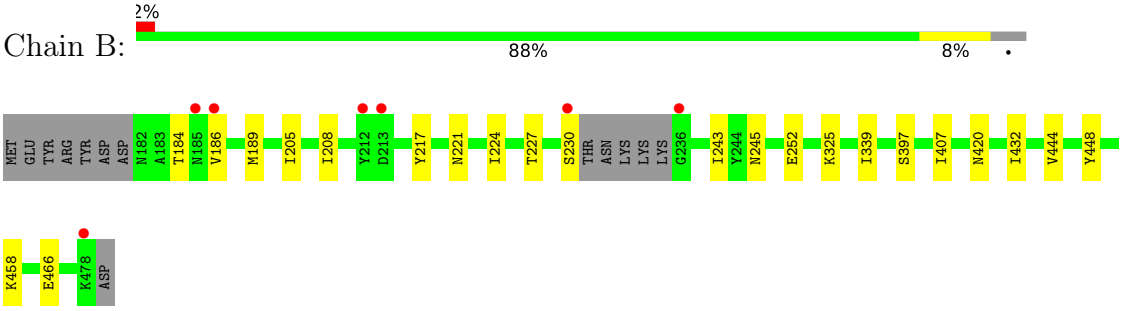
• Molecule 1: Bifunctional AAC/APH

Chain A:



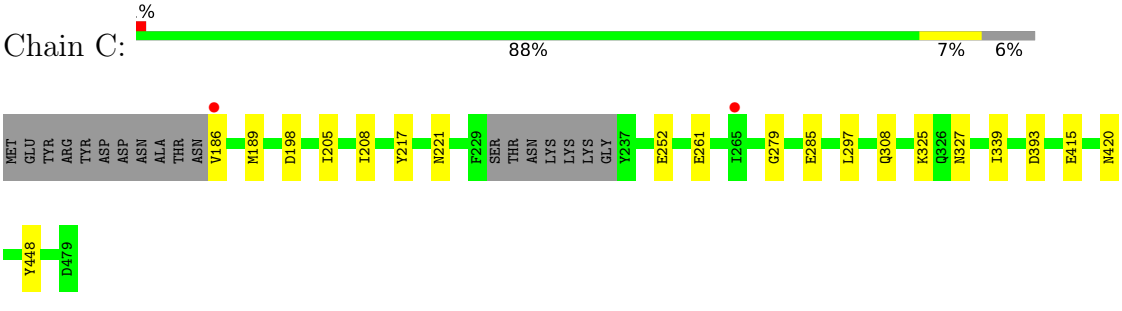
• Molecule 1: Bifunctional AAC/APH

Chain B:



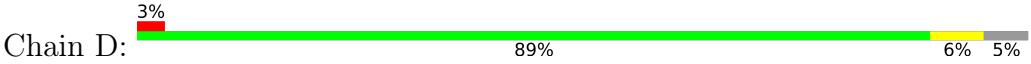
• Molecule 1: Bifunctional AAC/APH

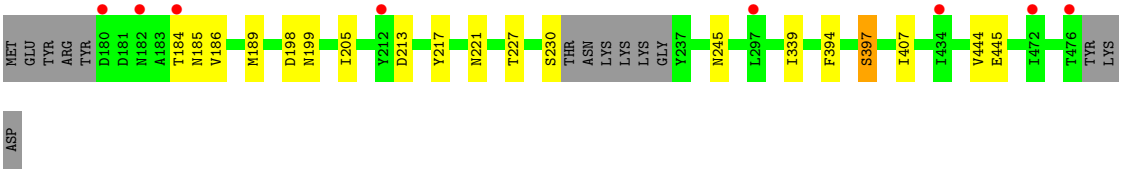
Chain C:



• Molecule 1: Bifunctional AAC/APH

Chain D:




MET
GLU
TYR
ARG
TYR
D180
D181
N182
A183
T184
N185
V186
M189
D198
N199
I205
Y212
D213
Y217
N221
T227
S230
THR
ASN
LYS
LYS
LYS
GLY
Y237
N245
L297
I339
F394
S397
I407
I434
V444
E445
I472
T476
TYR
LYS
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.25Å 100.28Å 94.04Å 90.00° 105.29° 90.00°	Depositor
Resolution (Å)	90.71 – 2.41 90.71 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.9 (90.71-2.41) 99.9 (90.71-2.42)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.180 , 0.227 (Not available) , 0.232	Depositor DCC
R_{free} test set	3119 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	60.9	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 40.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.020 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10345	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	1.16	2/2475 (0.1%)	1.06	4/3338 (0.1%)
1	B	1.15	2/2467 (0.1%)	1.01	1/3326 (0.0%)
1	C	1.16	4/2431 (0.2%)	1.04	4/3278 (0.1%)
1	D	1.05	1/2419 (0.0%)	1.01	2/3264 (0.1%)
All	All	1.13	9/9792 (0.1%)	1.03	11/13206 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	393	ASP	CA-C	-6.78	1.47	1.53
1	C	261	GLU	C-O	-6.37	1.15	1.24
1	A	385	ASN	CB-CG	-5.85	1.37	1.52
1	B	432	ILE	C-O	-5.48	1.17	1.24
1	A	448	TYR	C-O	-5.19	1.19	1.24
1	D	445	GLU	C-O	-5.13	1.18	1.24
1	B	448	TYR	C-O	-5.05	1.19	1.24
1	C	279	GLY	N-CA	-5.05	1.40	1.45
1	C	448	TYR	C-O	-5.03	1.19	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	ASP	N-CA-C	7.04	119.85	111.33
1	D	339	ILE	N-CA-C	6.28	119.04	112.83
1	C	198	ASP	N-CA-C	6.24	118.59	111.11
1	B	339	ILE	N-CA-C	6.03	118.80	112.83
1	A	339	ILE	N-CA-C	5.89	118.66	112.83
1	D	198	ASP	N-CA-CB	5.73	118.38	109.85
1	A	319	GLU	CB-CG-CD	5.44	121.84	112.60
1	C	308	GLN	CA-CB-CG	-5.25	103.60	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	308	GLN	CA-CB-CG	5.20	124.51	114.10
1	C	198	ASP	CB-CA-C	-5.18	102.52	110.81
1	C	339	ILE	N-CA-C	5.04	117.82	112.83

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	2424	0	2333	10	1
1	B	2418	0	2333	10	0
1	C	2382	0	2292	6	0
1	D	2376	0	2267	9	0
2	A	32	0	13	1	0
2	B	32	0	13	0	0
2	C	32	0	13	0	0
2	D	32	0	13	0	0
3	A	31	0	34	0	0
3	B	31	0	34	0	0
3	D	31	0	34	0	0
4	A	2	0	0	1	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
5	C	1	0	0	0	0
6	A	144	0	0	4	0
6	B	167	0	0	2	0
6	C	124	0	0	4	1
6	D	78	0	0	0	0
All	All	10345	0	9379	37	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 (37) 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:GNP:O2B	6:A:901:HOH:O	1.75	1.01
4:A:700:MG:MG	6:A:901:HOH:O	1.25	0.79
1:A:243:ILE:HD13	1:A:397:SER:HB2	1.81	0.62
1:D:185:ASN:ND2	1:D:217:TYR:OH	2.37	0.58
1:D:394:PHE:O	1:D:397:SER:OG	2.23	0.56
1:A:185:ASN:ND2	1:A:217:TYR:OH	2.39	0.54
1:D:186:VAL:HG13	1:D:205:ILE:HG23	1.91	0.52
1:D:186:VAL:CG1	1:D:205:ILE:HG23	2.40	0.51
1:C:325:LYS:NZ	6:C:1258:HOH:O	2.44	0.51
1:B:189:MET:HG2	1:B:217:TYR:CE1	2.45	0.51
1:C:189:MET:HG2	1:C:217:TYR:CE1	2.46	0.51
1:B:208:ILE:CD1	1:B:224:ILE:HD12	2.41	0.51
1:B:243:ILE:HD13	1:B:397:SER:HB2	1.94	0.50
1:A:208:ILE:CD1	1:A:224:ILE:HD12	2.42	0.49
1:D:407:ILE:HD12	1:D:444:VAL:HG11	1.94	0.49
1:A:189:MET:HG2	1:A:217:TYR:CE1	2.48	0.48
1:C:415:GLU:HG3	6:C:1560:HOH:O	2.13	0.48
1:C:415:GLU:N	6:C:1560:HOH:O	2.47	0.48
1:B:458:LYS:NZ	6:B:1156:HOH:O	2.47	0.48
1:A:359:ASN:ND2	6:A:1050:HOH:O	2.47	0.47
1:A:424:ASP:OD1	1:A:427:ARG:NH1	2.42	0.47
1:B:186:VAL:CG1	1:B:205:ILE:HG23	2.45	0.47
1:D:189:MET:HG2	1:D:217:TYR:CE1	2.49	0.46
1:A:186:VAL:CG1	1:A:205:ILE:HG23	2.46	0.45
6:A:1587:HOH:O	1:D:199:ASN:ND2	2.49	0.45
1:C:186:VAL:CG1	1:C:205:ILE:HG23	2.46	0.45
1:D:189:MET:SD	1:D:227:THR:HG21	2.56	0.45
1:B:466:GLU:HG3	5:B:802:CL:CL	2.56	0.43
1:A:189:MET:SD	1:A:227:THR:HG21	2.59	0.43
1:B:189:MET:SD	1:B:227:THR:HG21	2.58	0.43
1:D:394:PHE:HB3	1:D:397:SER:OG	2.19	0.42
1:B:407:ILE:HD12	1:B:444:VAL:HG11	2.01	0.41
1:A:407:ILE:HD12	1:A:444:VAL:HG11	2.03	0.41
1:A:420:ASN:HD22	1:A:420:ASN:HA	1.72	0.41
1:C:327:ASN:ND2	6:C:1181:HOH:O	2.54	0.40
1:B:208:ILE:HD11	1:B:224:ILE:HD12	2.03	0.40
1:B:325:LYS:NZ	6:B:1347:HOH:O	2.55	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLU:OE1	6:C:1080:HOH:O[2_747]	2.14	0.06

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	292/305 (96%)	280 (96%)	12 (4%)	0	100	100
1	B	290/305 (95%)	281 (97%)	9 (3%)	0	100	100
1	C	285/305 (93%)	275 (96%)	10 (4%)	0	100	100
1	D	288/305 (94%)	277 (96%)	11 (4%)	0	100	100
All	All	1155/1220 (95%)	1113 (96%)	42 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/281 (96%)	265 (98%)	4 (2%)	57	75
1	B	269/281 (96%)	263 (98%)	6 (2%)	45	66
1	C	264/281 (94%)	258 (98%)	6 (2%)	44	64
1	D	261/281 (93%)	255 (98%)	6 (2%)	44	64
All	All	1063/1124 (95%)	1041 (98%)	22 (2%)	47	67

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	213	ASP
1	A	230	SER
1	A	466	GLU
1	B	184	THR
1	B	221	ASN
1	B	230	SER
1	B	245	ASN
1	B	252	GLU
1	B	420	ASN
1	C	208	ILE
1	C	221	ASN
1	C	252	GLU
1	C	285	GLU
1	C	297	LEU
1	C	420	ASN
1	D	184	THR
1	D	213	ASP
1	D	221	ASN
1	D	230	SER
1	D	245	ASN
1	D	397	SER

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	185	ASN
1	A	341	ASN
1	A	420	ASN
1	A	467	ASN
1	B	467	ASN
1	C	327	ASN
1	C	462	GLN
1	D	185	ASN
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 (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, 11 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
3	RIO	A	600	-	32,33,33	0.51	0	46,49,49	1.18	5 (10%)
2	GNP	D	500	4	34,34,34	1.53	3 (8%)	47,54,54	0.97	5 (10%)
2	GNP	B	500	4	34,34,34	1.76	2 (5%)	47,54,54	1.54	6 (12%)
3	RIO	B	600	-	32,33,33	0.64	0	46,49,49	1.86	14 (30%)
3	RIO	D	600	-	32,33,33	0.49	0	46,49,49	2.34	10 (21%)
2	GNP	C	500	4	34,34,34	1.15	1 (2%)	47,54,54	0.96	3 (6%)
2	GNP	A	500	4	34,34,34	1.99	5 (14%)	47,54,54	1.07	4 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RIO	A	600	-	-	6/12/68/68	0/3/3/3
2	GNP	D	500	4	-	5/18/38/38	0/3/3/3
2	GNP	B	500	4	-	2/18/38/38	0/3/3/3
3	RIO	B	600	-	-	7/12/68/68	0/3/3/3
3	RIO	D	600	-	-	5/12/68/68	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GNP	C	500	4	-	4/18/38/38	0/3/3/3
2	GNP	A	500	4	-	3/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	GNP	PG-O2G	7.66	1.77	1.56
2	A	500	GNP	PG-O2G	6.06	1.72	1.56
2	C	500	GNP	PG-O2G	5.84	1.72	1.56
2	B	500	GNP	PG-O3G	5.79	1.72	1.56
2	A	500	GNP	PB-O3A	-5.68	1.52	1.59
2	D	500	GNP	PG-O2G	5.12	1.70	1.56
2	D	500	GNP	PB-O2B	4.91	1.69	1.56
2	D	500	GNP	PG-O3G	4.76	1.69	1.56
2	A	500	GNP	PB-O2B	4.49	1.68	1.56
2	A	500	GNP	PG-O3G	4.09	1.67	1.56
2	A	500	GNP	C5-C6	-3.49	1.31	1.44

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	600	RIO	O3-C3-O2	-8.41	102.78	111.37
3	D	600	RIO	O5-C10-C15	7.63	120.56	108.08
2	B	500	GNP	O1G-PG-N3B	-5.99	102.94	111.77
3	D	600	RIO	O3-C4-C5	-5.58	93.05	107.23
2	B	500	GNP	O2B-PB-O3A	4.84	120.79	104.64
3	B	600	RIO	O3-C4-C5	-4.75	95.16	107.23
3	B	600	RIO	O3-C3-O2	-4.65	106.62	111.37
3	B	600	RIO	C3-O3-C4	4.53	128.72	117.98
2	B	500	GNP	O2B-PB-O1B	-3.91	101.48	109.87
2	A	500	GNP	O1B-PB-N3B	-3.46	106.68	111.77
3	D	600	RIO	O3-C4-C9	-3.42	98.76	107.42
2	C	500	GNP	O2B-PB-O1B	3.34	117.03	109.87
3	D	600	RIO	C10-C15-N4	3.21	115.99	110.20
3	A	600	RIO	O5-C9-C8	-3.08	101.83	109.18
3	D	600	RIO	C5-C4-C9	3.03	118.53	111.72
3	B	600	RIO	O10-C17-C2	-2.97	102.54	111.08
2	C	500	GNP	O5'-PA-O1A	2.95	120.63	108.94
2	A	500	GNP	O3A-PB-N3B	-2.95	98.41	106.59
3	B	600	RIO	C4-C5-C6	2.92	116.97	109.93
2	B	500	GNP	O3G-PG-O1G	2.91	120.75	113.45
3	A	600	RIO	C14-C15-N4	2.90	117.00	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	600	RIO	O5-C9-C4	2.90	114.80	107.42
3	B	600	RIO	C8-C7-C6	-2.86	106.12	111.02
3	D	600	RIO	C3-O3-C4	2.63	124.21	117.98
2	D	500	GNP	O3A-PB-N3B	2.60	113.81	106.59
3	A	600	RIO	O3-C4-C9	2.60	114.02	107.42
3	A	600	RIO	O5-C10-C15	2.58	112.30	108.08
3	B	600	RIO	C4-C9-C8	2.53	116.00	111.31
2	D	500	GNP	O2G-PG-O1G	-2.53	107.11	113.45
3	A	600	RIO	C8-C7-C6	-2.47	106.79	111.02
2	A	500	GNP	O5'-PA-O1A	2.46	118.68	108.94
2	B	500	GNP	O3A-PA-O1A	-2.41	103.44	110.70
3	B	600	RIO	O10-C17-C16	2.34	119.33	111.82
2	D	500	GNP	O2G-PG-O3G	2.34	113.86	107.59
3	B	600	RIO	O5-C9-C4	2.32	113.32	107.42
2	D	500	GNP	O1G-PG-N3B	-2.30	108.39	111.77
3	B	600	RIO	C10-O6-C11	2.26	118.14	113.72
3	D	600	RIO	C4-C9-C8	2.25	115.48	111.31
3	B	600	RIO	O5-C10-C15	2.20	111.69	108.08
2	C	500	GNP	O2G-PG-O1G	-2.19	107.95	113.45
2	A	500	GNP	O5'-C5'-C4'	-2.19	101.53	108.99
2	B	500	GNP	O2A-PA-O3A	2.17	113.14	107.27
3	D	600	RIO	C10-O6-C11	2.13	117.87	113.72
3	B	600	RIO	C3-O2-C2	2.12	113.84	105.76
3	B	600	RIO	C5-C4-C9	2.09	116.43	111.72
2	D	500	GNP	O2B-PB-O3A	2.06	111.52	104.64
3	B	600	RIO	C10-O5-C9	2.02	122.77	117.98

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	GNP	PG-N3B-PB-O1B
2	B	500	GNP	PG-N3B-PB-O1B
2	C	500	GNP	PB-N3B-PG-O1G
2	C	500	GNP	PG-N3B-PB-O3A
2	D	500	GNP	PB-N3B-PG-O1G
2	D	500	GNP	PG-N3B-PB-O1B
2	D	500	GNP	PA-O3A-PB-O2B
3	A	600	RIO	O2-C3-O3-C4
3	A	600	RIO	C16-C3-O3-C4
3	B	600	RIO	O2-C3-O3-C4
3	B	600	RIO	C16-C3-O3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	600	RIO	O6-C11-C12-N3
3	D	600	RIO	O2-C3-O3-C4
3	D	600	RIO	C16-C3-O3-C4
3	D	600	RIO	O6-C11-C12-N3
3	A	600	RIO	C5-C4-O3-C3
3	B	600	RIO	O1-C1-C2-O2
3	B	600	RIO	O6-C10-O5-C9
3	B	600	RIO	O1-C1-C2-C17
3	D	600	RIO	O6-C10-O5-C9
2	B	500	GNP	PB-O3A-PA-O1A
3	A	600	RIO	C4-C9-O5-C10
3	D	600	RIO	C4-C9-O5-C10
3	B	600	RIO	C4-C9-O5-C10
3	A	600	RIO	C8-C9-O5-C10
2	A	500	GNP	PG-N3B-PB-O3A
2	A	500	GNP	PB-O3A-PA-O1A
2	D	500	GNP	PB-O3A-PA-O1A
2	C	500	GNP	PB-O3A-PA-O2A
2	D	500	GNP	PB-O3A-PA-O2A
3	A	600	RIO	C9-C4-O3-C3
2	C	500	GNP	PB-O3A-PA-O1A

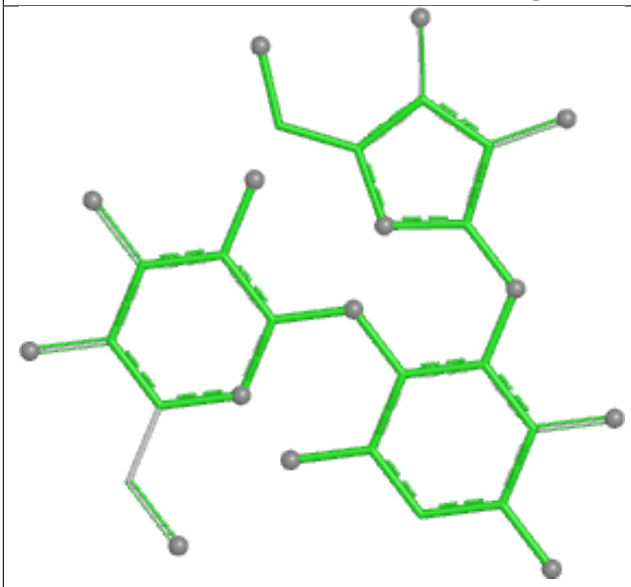
There are no ring outliers.

1 monomer is involved in 1 short contact:

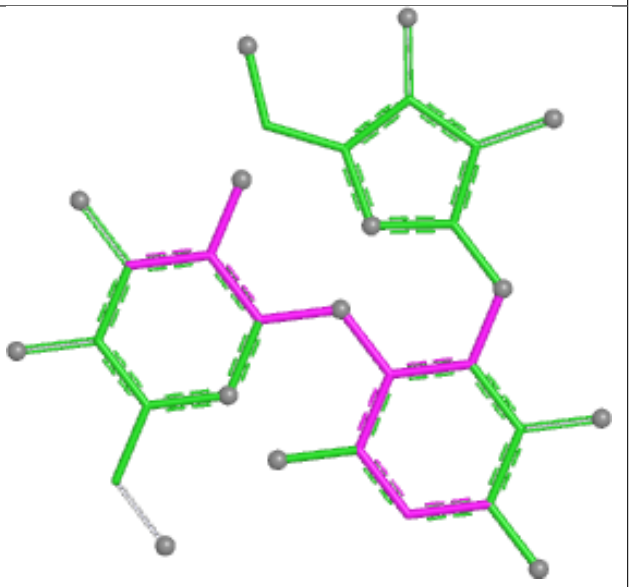
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	GNP	1	0

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

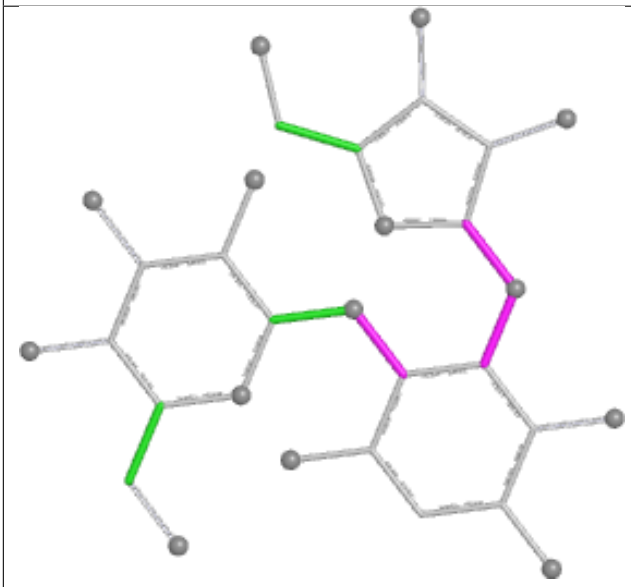
Ligand RIO A 600



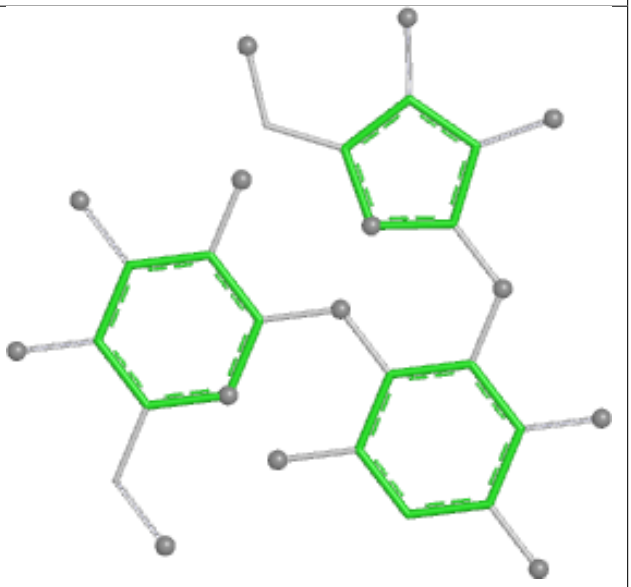
Bond lengths



Bond angles

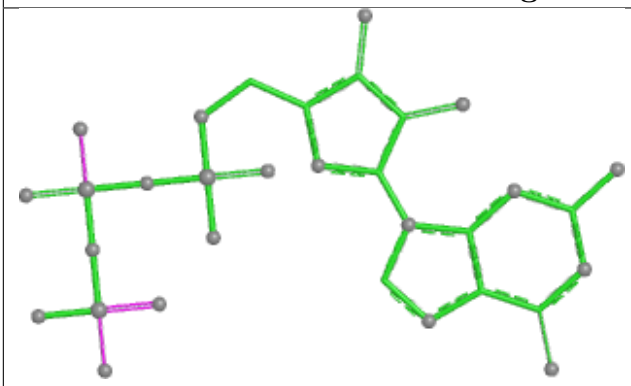


Torsions

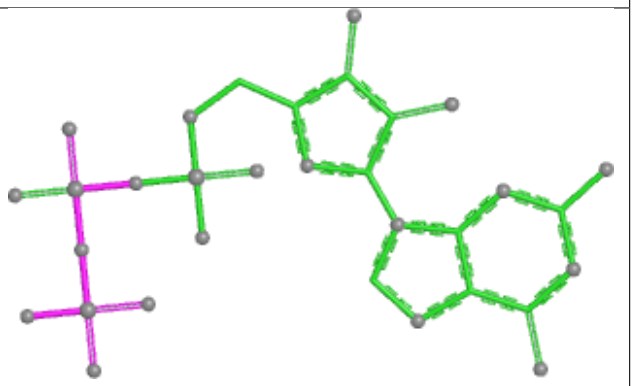


Rings

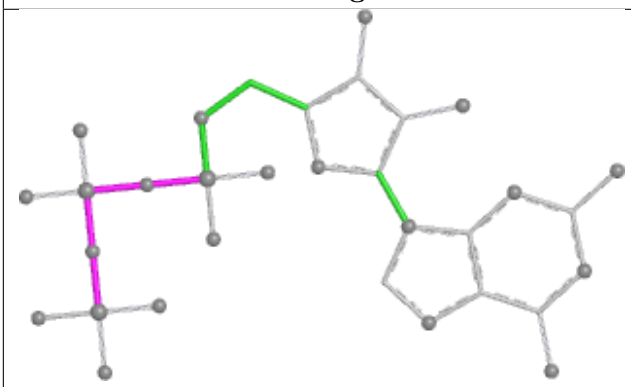
Ligand GNP D 500



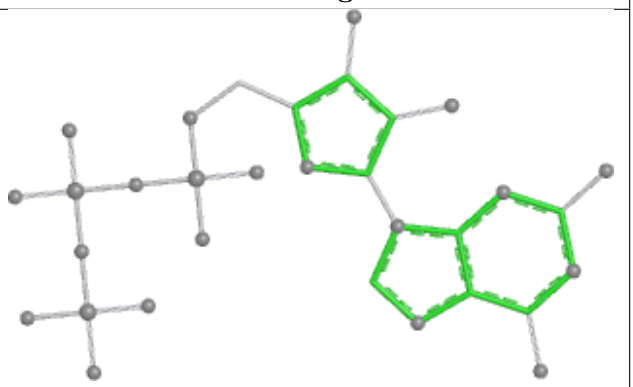
Bond lengths



Bond angles

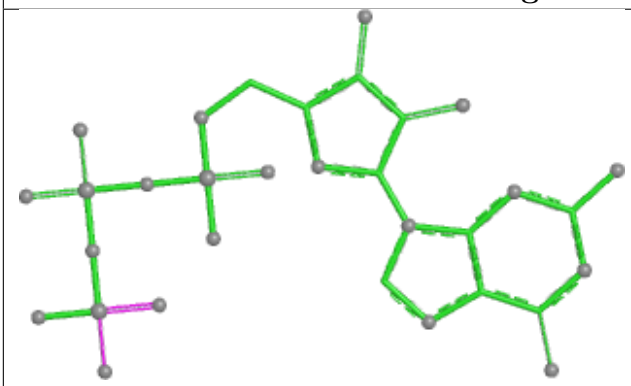


Torsions

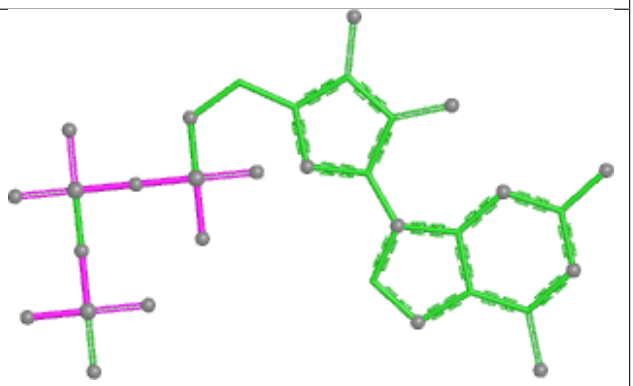


Rings

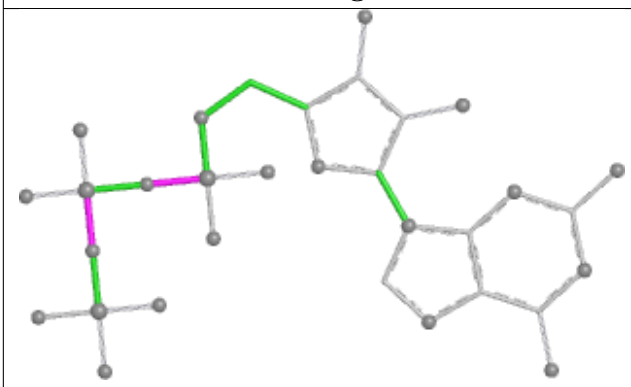
Ligand GNP B 500



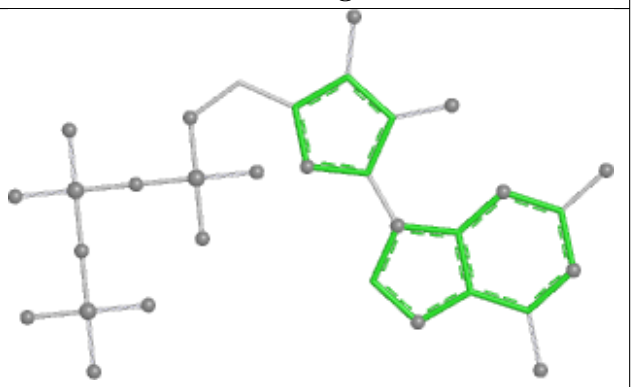
Bond lengths



Bond angles

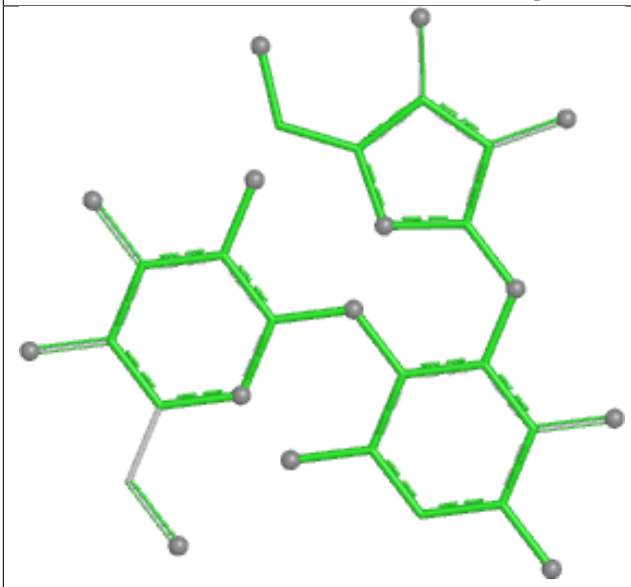


Torsions

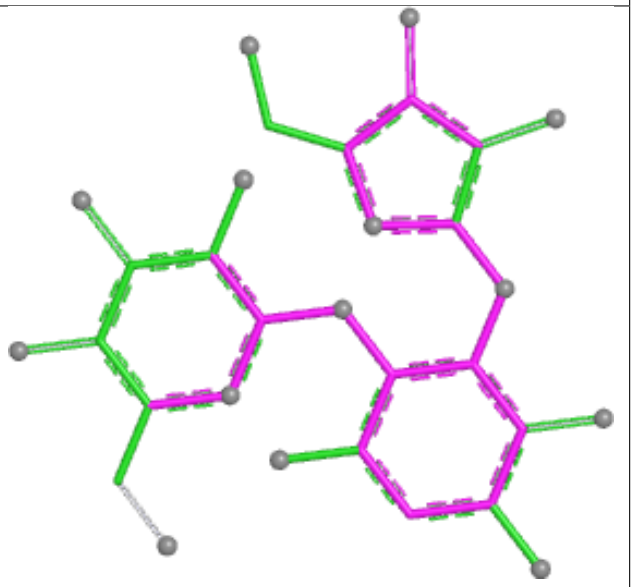


Rings

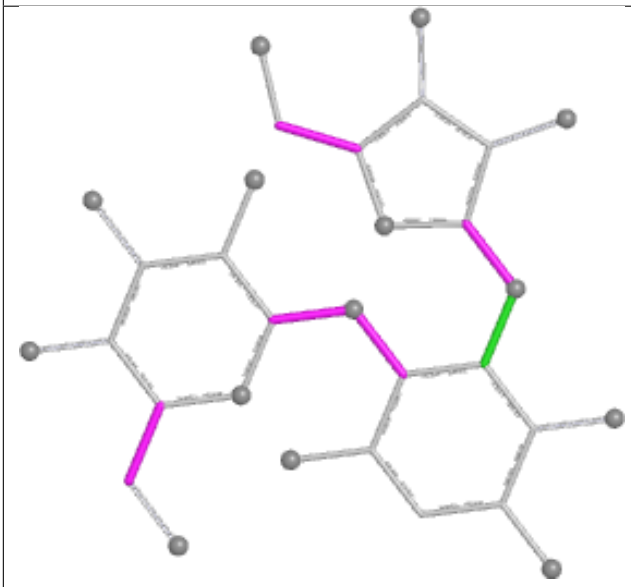
Ligand RIO B 600



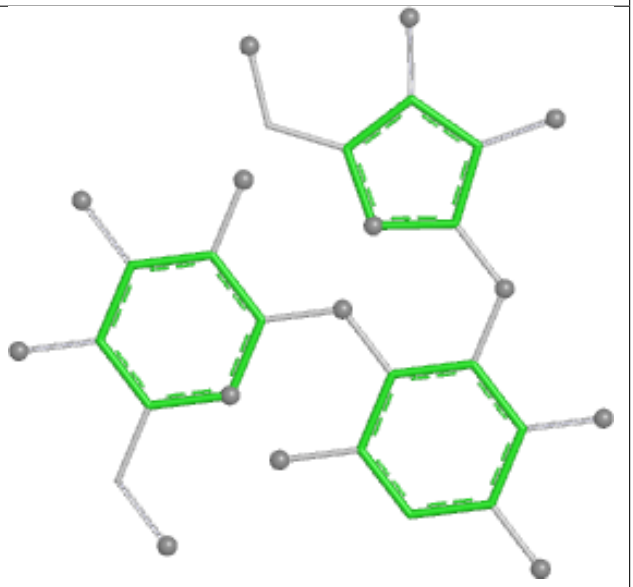
Bond lengths



Bond angles

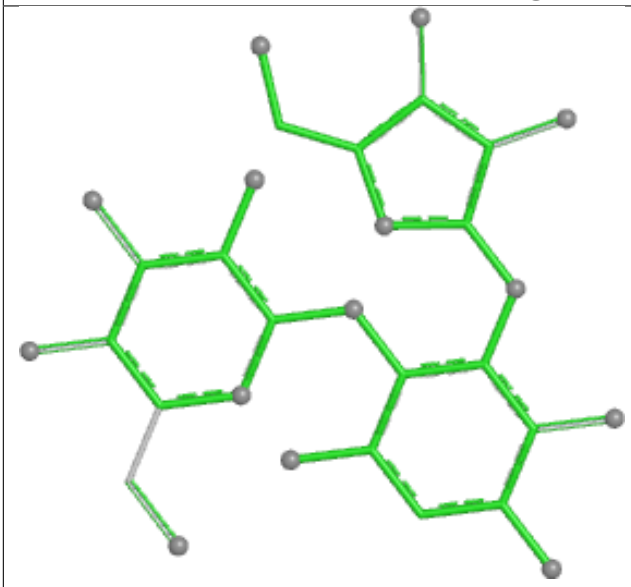


Torsions

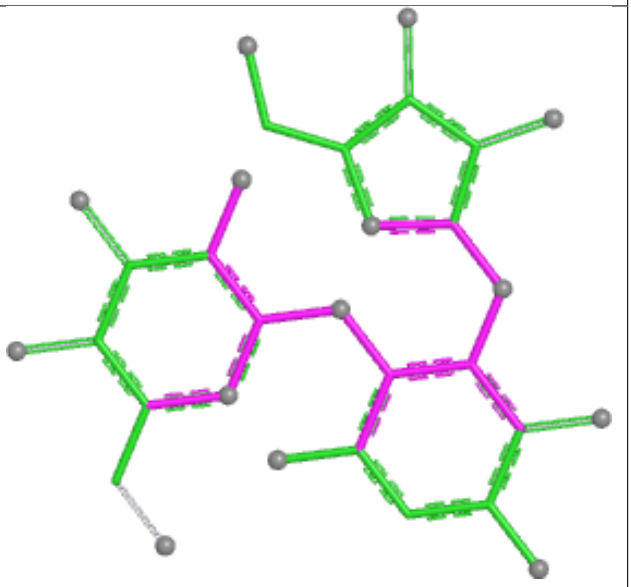


Rings

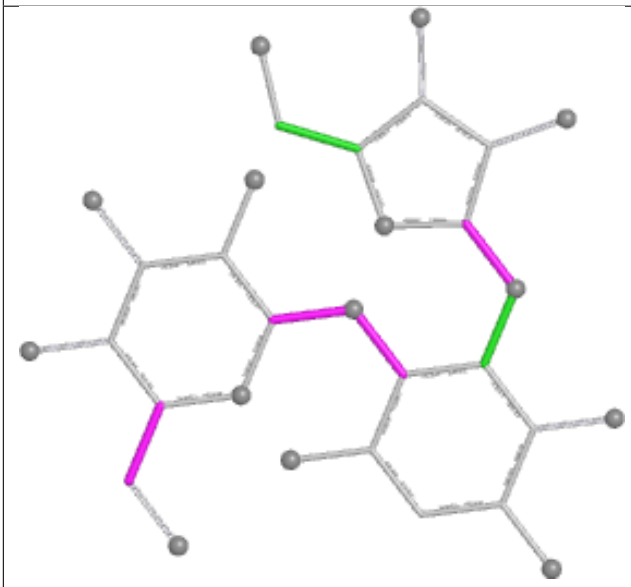
Ligand RIO D 600



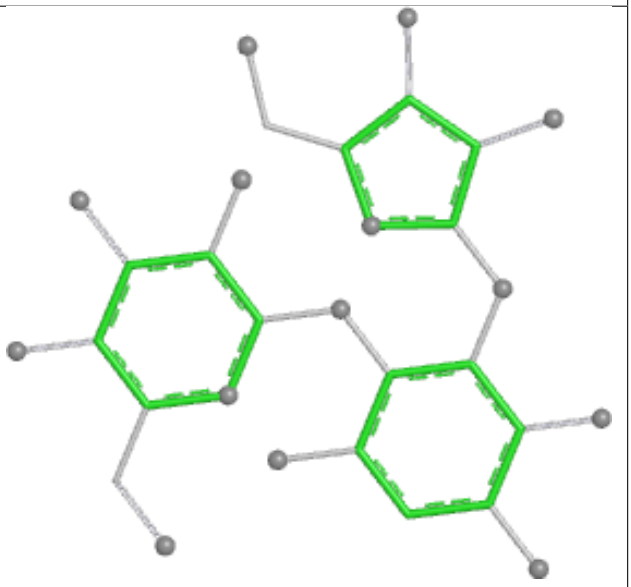
Bond lengths



Bond angles

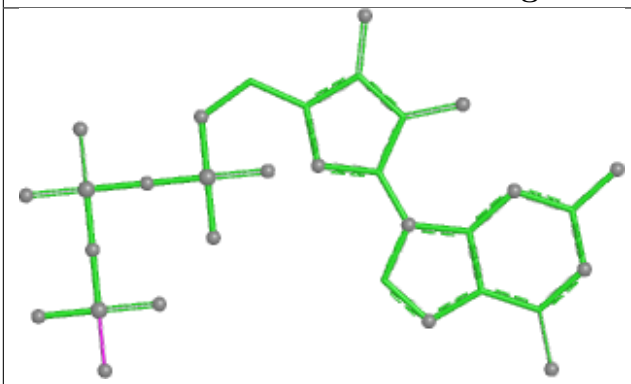


Torsions

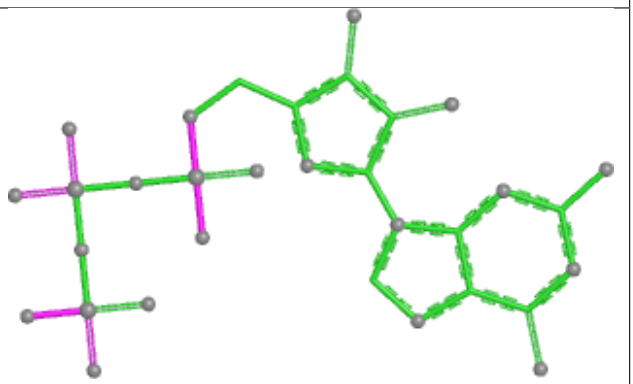


Rings

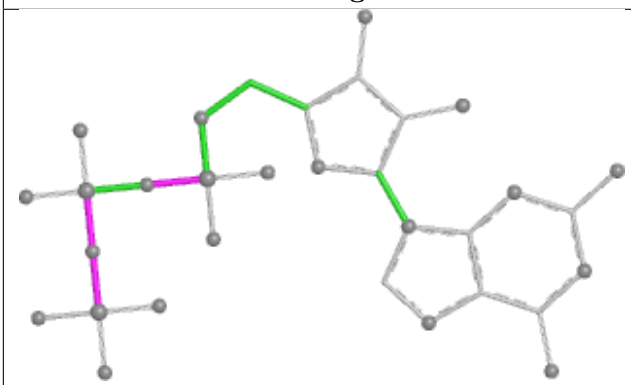
Ligand GNP C 500



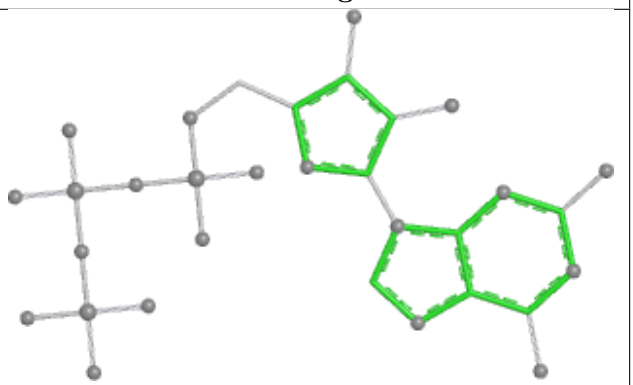
Bond lengths



Bond angles

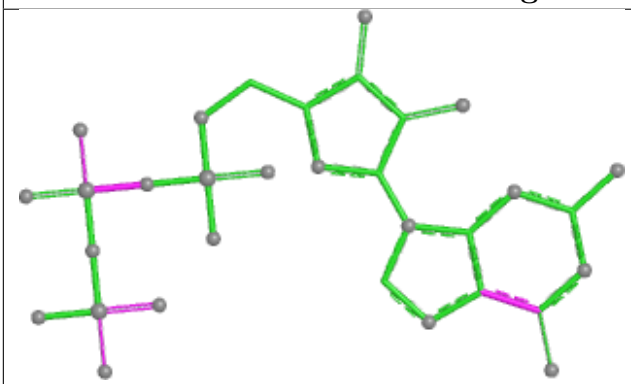


Torsions

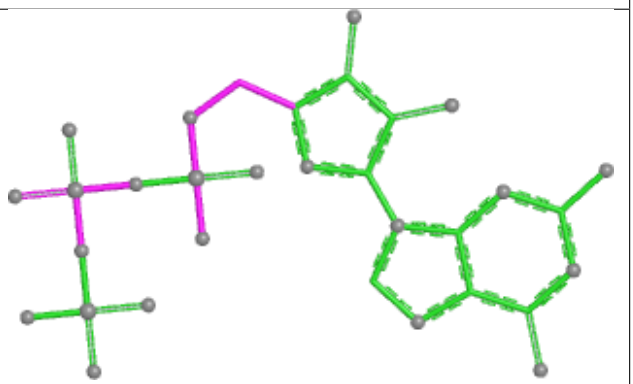


Rings

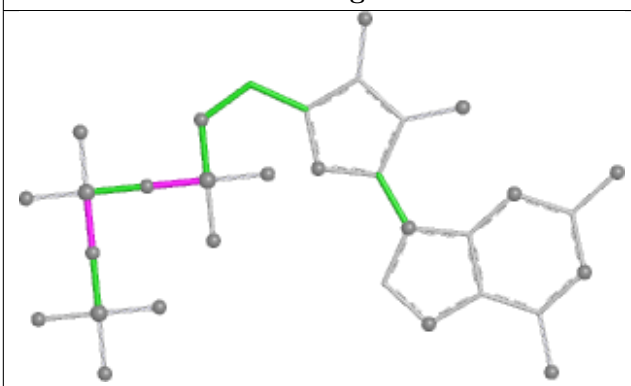
Ligand GNP A 500



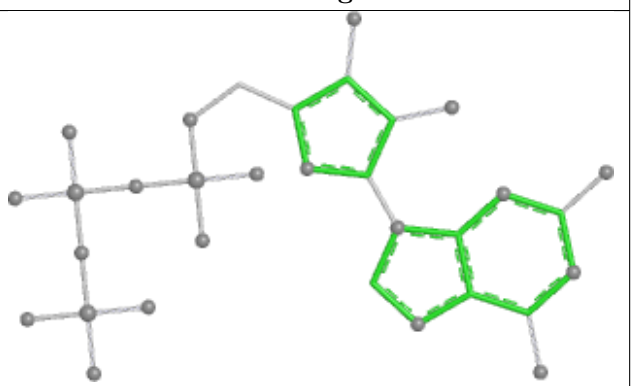
Bond lengths



Bond angles



Torsions



Rings

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	293/305 (96%)	-0.23	8 (2%)	56	52	33, 67, 91, 143	3 (1%)
1	B	292/305 (95%)	-0.25	7 (2%)	59	56	34, 63, 95, 128	2 (0%)
1	C	287/305 (94%)	-0.13	2 (0%)	84	82	39, 70, 106, 138	2 (0%)
1	D	291/305 (95%)	0.06	8 (2%)	56	52	46, 84, 118, 134	1 (0%)
All	All	1163/1220 (95%)	-0.14	25 (2%)	63	60	33, 71, 109, 143	8 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	236	GLY	5.7
1	A	181	ASP	4.0
1	B	185	ASN	3.4
1	A	315	THR	3.4
1	D	182	ASN	3.3
1	B	230	SER	2.9
1	A	316	ASP	2.9
1	D	472	ILE	2.8
1	D	434	ILE	2.8
1	A	230	SER	2.6
1	D	180	ASP	2.6
1	D	184	THR	2.5
1	B	186	VAL	2.5
1	A	314	TYR	2.3
1	C	265	ILE	2.3
1	A	317	ILE	2.3
1	B	478	LYS	2.3
1	A	183	ALA	2.2
1	B	212	TYR	2.2
1	D	297	LEU	2.1
1	D	476	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	455	TYR	2.1
1	C	186	VAL	2.0
1	B	213	ASP	2.0
1	D	212	TYR	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 oligosaccharides in this entry.

6.4 Ligands (i)

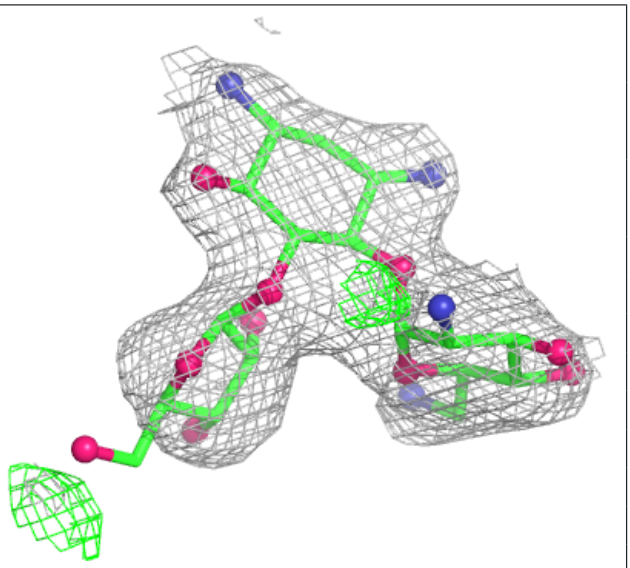
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

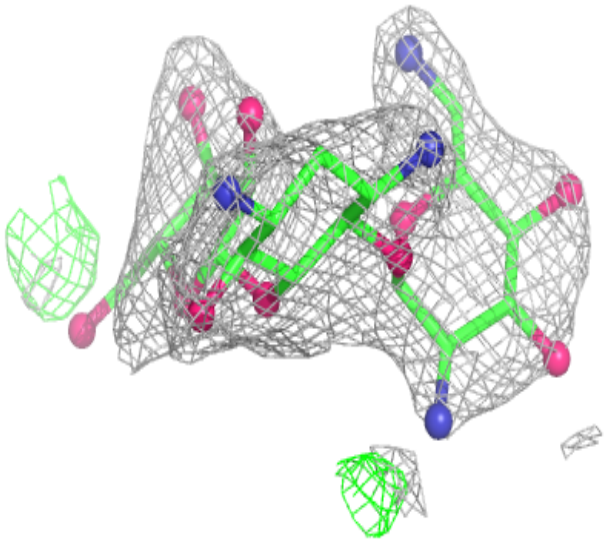
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	RIO	A	600	31/31	0.86	0.10	77,99,123,139	0
3	RIO	B	600	31/31	0.86	0.11	82,96,104,109	0
3	RIO	D	600	31/31	0.89	0.09	83,94,107,114	0
5	CL	B	802	1/1	0.92	0.11	89,89,89,89	0
5	CL	C	802	1/1	0.93	0.09	76,76,76,76	0
5	CL	A	802	1/1	0.94	0.06	98,98,98,98	0
2	GNP	A	500	32/32	0.95	0.09	60,68,78,83	0
2	GNP	C	500	32/32	0.95	0.07	56,68,87,93	0
2	GNP	D	500	32/32	0.95	0.06	65,71,109,118	0
4	MG	A	700	1/1	0.97	0.05	87,87,87,87	0
2	GNP	B	500	32/32	0.97	0.05	53,57,79,87	0
4	MG	D	702	1/1	0.98	0.05	90,90,90,90	0
4	MG	C	702	1/1	0.99	0.06	85,85,85,85	0
4	MG	D	700	1/1	0.99	0.04	62,62,62,62	0
4	MG	C	700	1/1	0.99	0.03	76,76,76,76	0
4	MG	B	700	1/1	1.00	0.01	57,57,57,57	0
4	MG	B	702	1/1	1.00	0.05	73,73,73,73	0
4	MG	A	702	1/1	1.00	0.03	75,75,75,75	0

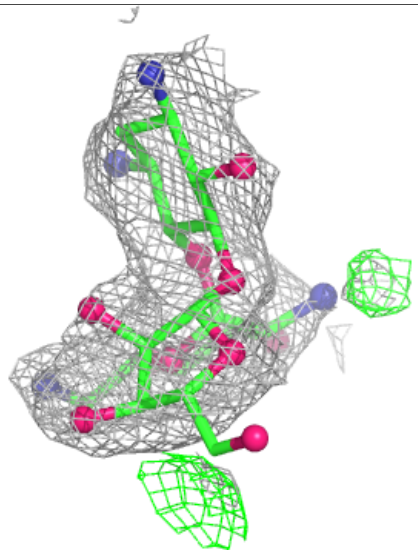
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RIO 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)

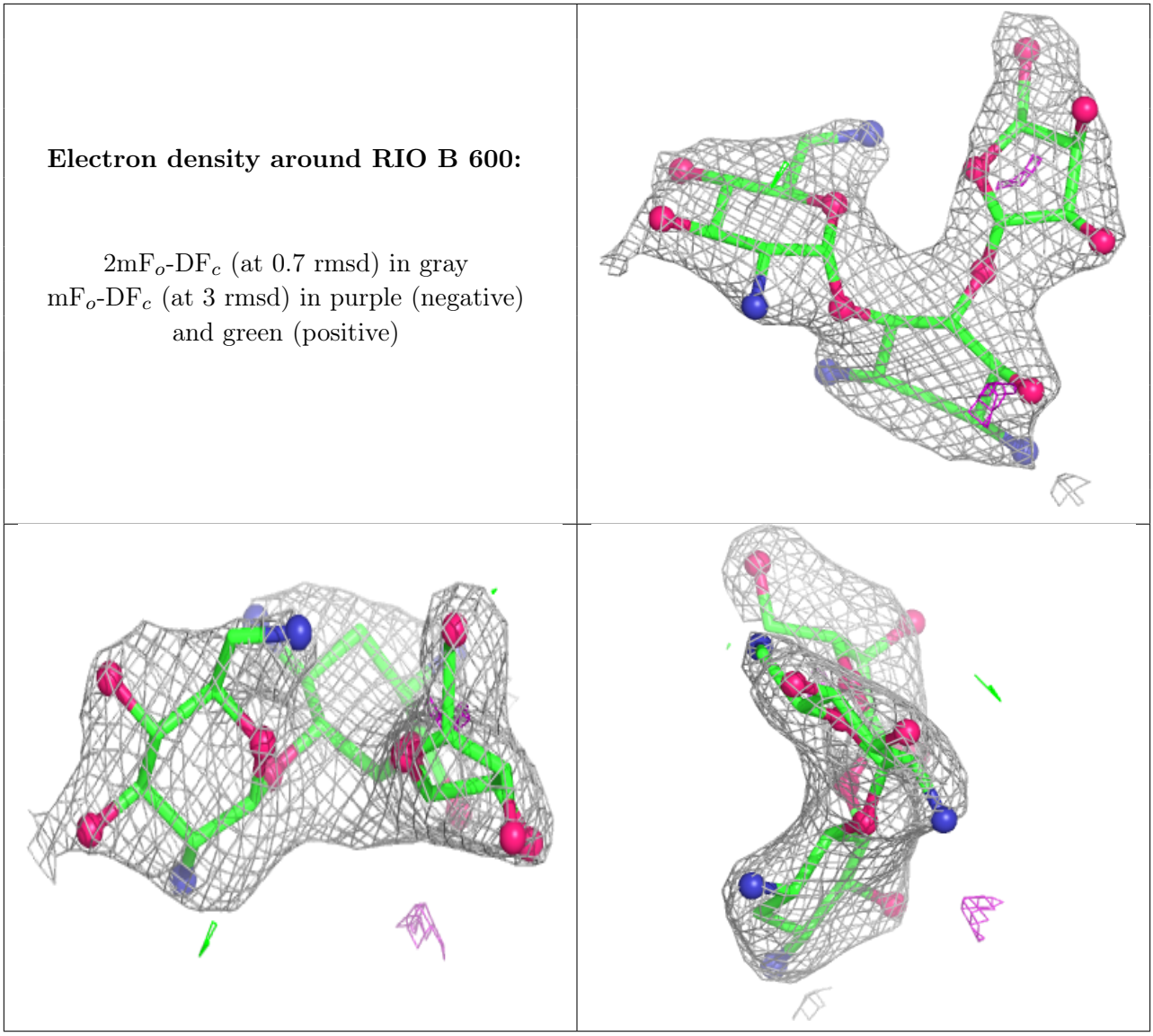






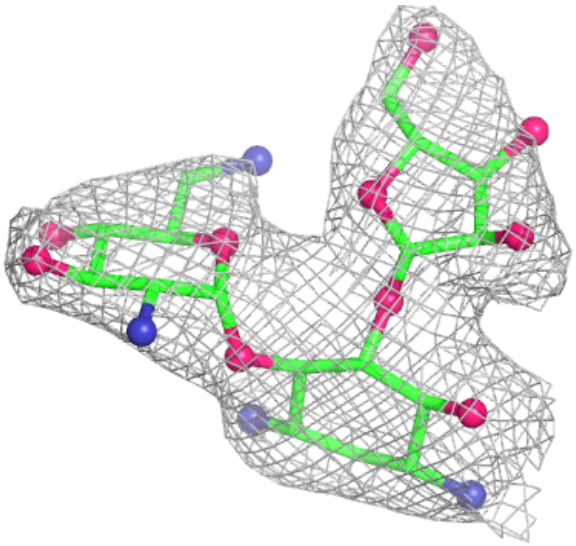
Electron density around RIO B 600:

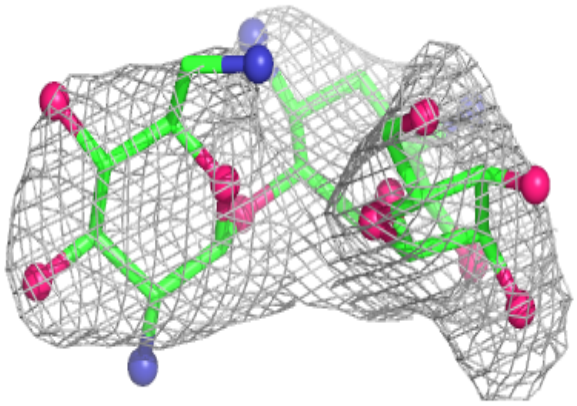
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

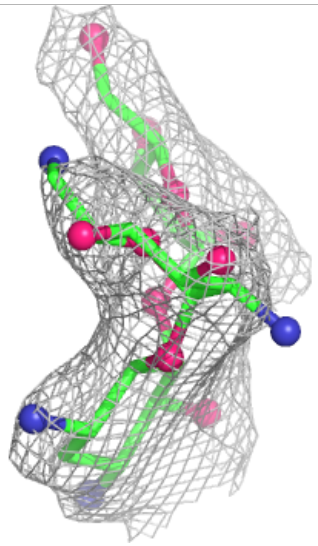


Electron density around RIO D 600:

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

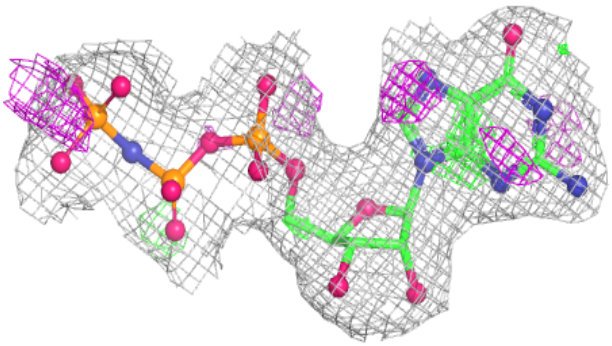


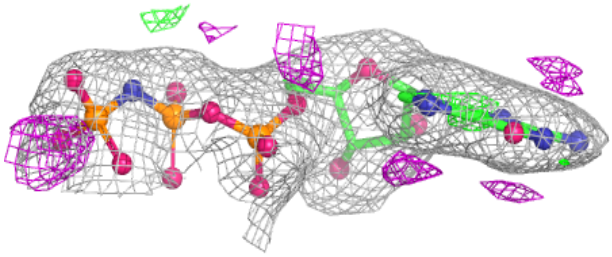


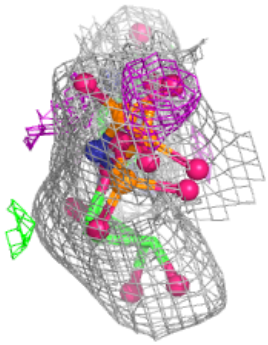


Electron density around GNP A 500:

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

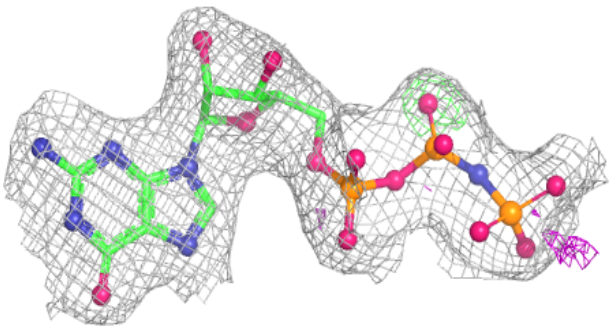


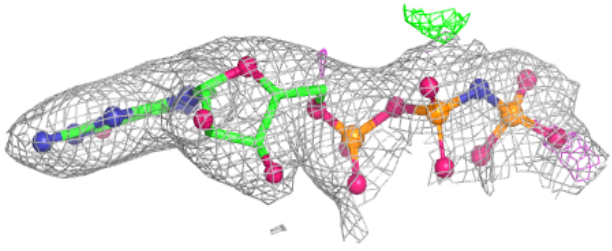


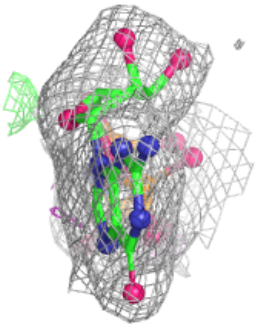


Electron density around GNP C 500:

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

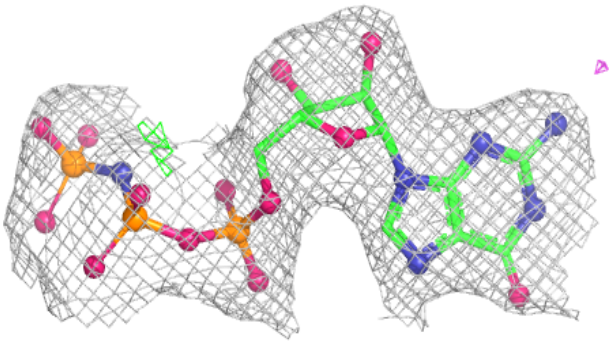


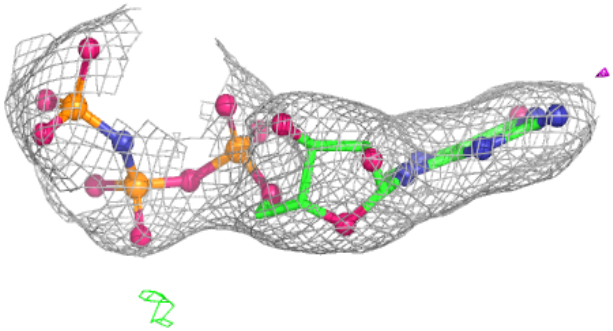


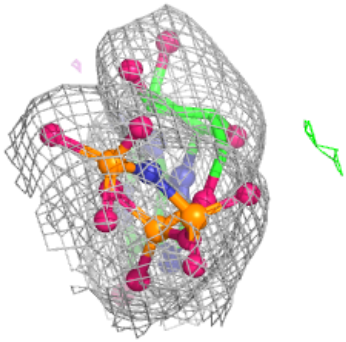


Electron density around GNP D 500:

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

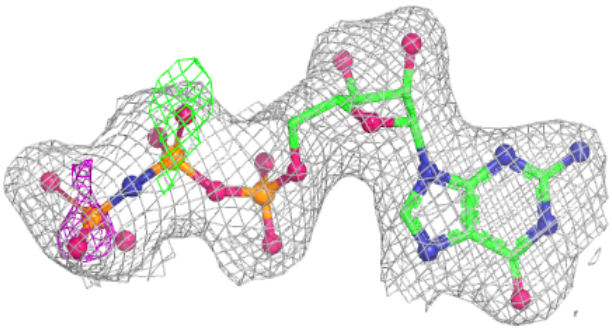


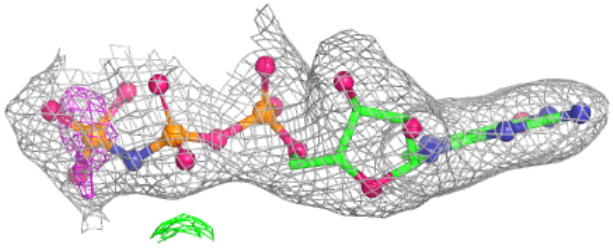


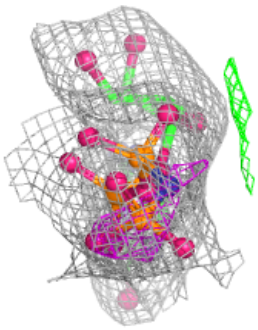


Electron density around GNP B 500:

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







6.5 Other polymers (i)

There are no such residues in this entry.