



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 10:30 PM EDT

PDB ID : 6CH4  
Title : Aminoglycoside Phosphotransferase (2'')-Ia S376N mutant in complex with GMPPNP and Magnesium  
Authors : Caldwell, S.J.; Berghuis, A.M.  
Deposited on : 2018-02-21  
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](mailto: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>.

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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 : 2.35.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

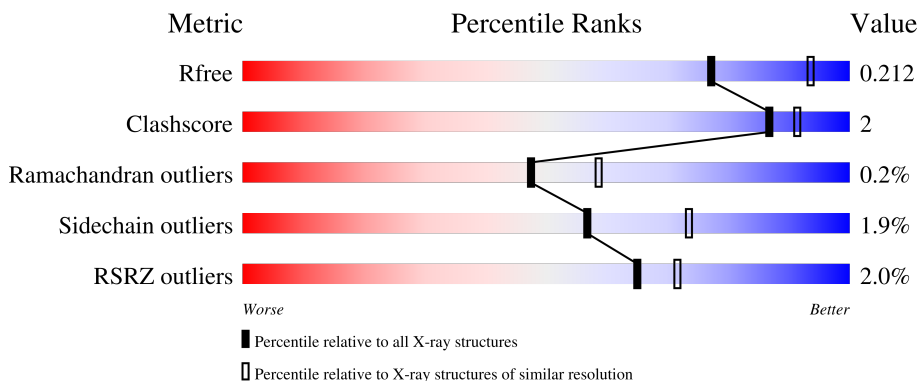
# 1 Overall quality at a glance

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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% 87% 10% .
1	B	305	 % 88% 9% ..
1	C	305	 3% 86% 10% ..
1	D	305	 2% 84% 8% 8%

## 2 Entry composition

There are 5 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
			Total	C	N	O	S			
1	A	298	2448	1561	381	496	10	0	0	0
1	B	297	2462	1570	383	499	10	0	1	0
1	C	297	2451	1563	383	495	10	0	1	0
1	D	282	2271	1451	353	457	10	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	376	ASN	SER	engineered mutation	UNP P0A0C1
B	376	ASN	SER	engineered mutation	UNP P0A0C1
C	376	ASN	SER	engineered mutation	UNP P0A0C1
D	376	ASN	SER	engineered mutation	UNP P0A0C1

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		
3	D	1	Total	Mg	0	0
			1	1		

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

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

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

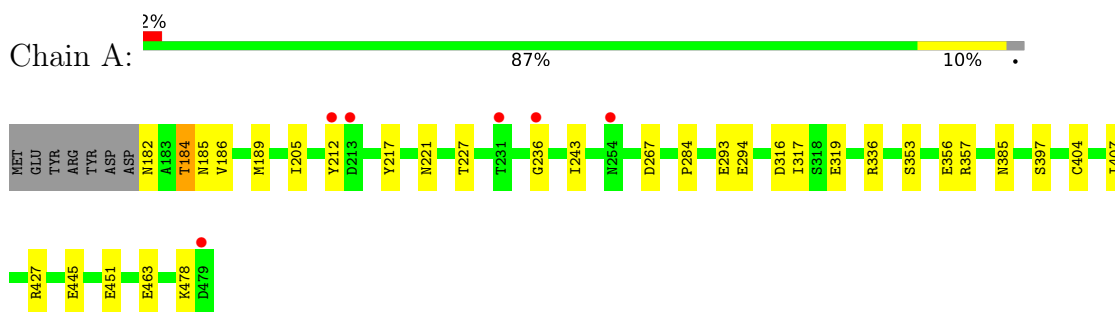
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	154	Total 154	O 154	0	0
5	B	184	Total 184	O 184	0	0
5	C	149	Total 149	O 149	0	0
5	D	92	Total 92	O 92	0	0

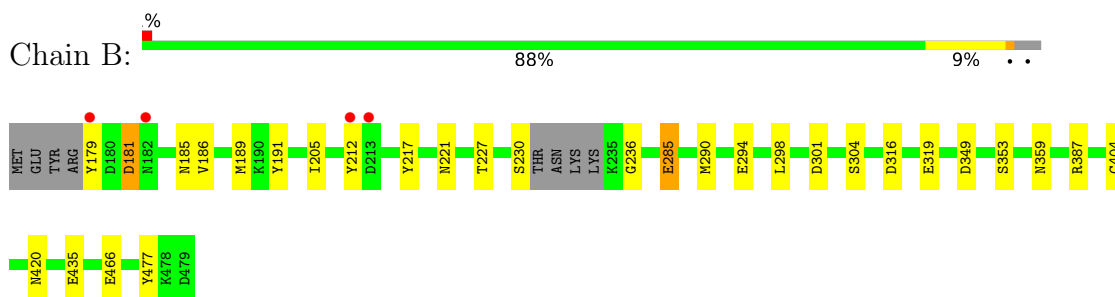
### 3 Residue-property plots [i](#)

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.

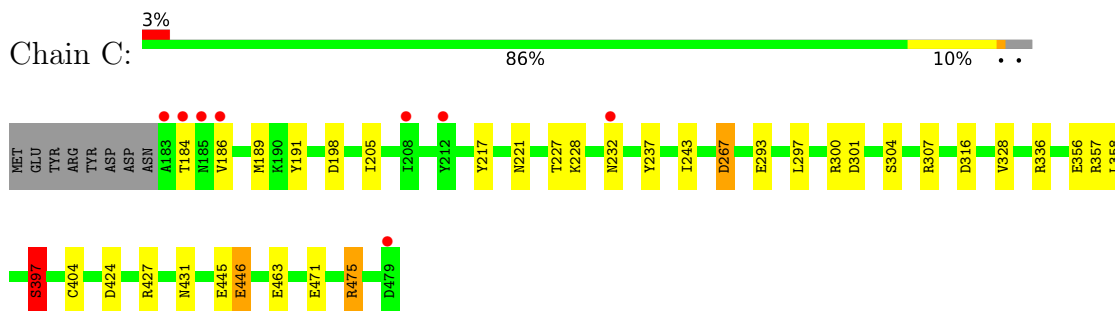
- Molecule 1: Bifunctional AAC/APH



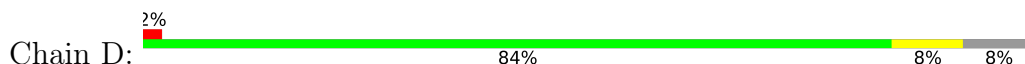
- Molecule 1: Bifunctional AAC/APH

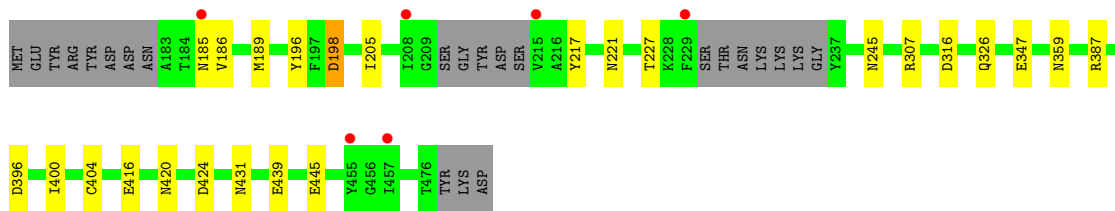


- Molecule 1: Bifunctional AAC/APH



- Molecule 1: Bifunctional AAC/APH





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.43Å 99.91Å 93.20Å 90.00° 105.17° 90.00°	Depositor
Resolution (Å)	58.89 – 2.30 55.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (58.89-2.30) 100.0 (55.77-2.30)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.170 , 0.210 0.176 , 0.212	Depositor DCC
$R_{free}$ test set	3596 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtrriage
Anisotropy	0.058	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.016 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10345	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, MG, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.15	7/2492 (0.3%)	1.05	8/3362 (0.2%)
1	B	1.18	12/2509 (0.5%)	1.03	8/3382 (0.2%)
1	C	1.15	9/2498 (0.4%)	1.06	13/3369 (0.4%)
1	D	1.02	3/2312 (0.1%)	1.00	8/3125 (0.3%)
All	All	1.13	31/9811 (0.3%)	1.04	37/13238 (0.3%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	466	GLU	CD-OE2	7.83	1.34	1.25
1	C	356	GLU	CD-OE1	7.16	1.33	1.25
1	C	445	GLU	CD-OE1	7.01	1.33	1.25
1	C	293	GLU	CD-OE1	6.90	1.33	1.25
1	C	304	SER	CB-OG	-6.83	1.33	1.42
1	B	319	GLU	CG-CD	6.67	1.61	1.51
1	D	416	GLU	CD-OE1	6.47	1.32	1.25
1	A	445	GLU	CG-CD	6.01	1.60	1.51
1	C	446	GLU	CD-OE2	6.00	1.32	1.25
1	C	356	GLU	CD-OE2	5.92	1.32	1.25
1	A	353	SER	CB-OG	-5.88	1.34	1.42
1	B	236	GLY	CA-C	5.85	1.61	1.51
1	B	285	GLU	CD-OE2	5.85	1.32	1.25
1	D	439	GLU	CD-OE2	5.80	1.32	1.25
1	B	477	TYR	CG-CD1	-5.71	1.31	1.39
1	D	445	GLU	CG-CD	5.62	1.60	1.51
1	A	445	GLU	CD-OE1	5.61	1.31	1.25
1	B	353	SER	CB-OG	-5.49	1.35	1.42
1	C	397	SER	CB-OG	-5.46	1.35	1.42
1	B	191	TYR	CE2-CZ	-5.43	1.31	1.38
1	B	301	ASP	CB-CG	5.42	1.63	1.51
1	A	236	GLY	C-O	5.37	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	463	GLU	CD-OE2	5.31	1.31	1.25
1	B	304	SER	CB-OG	-5.28	1.35	1.42
1	A	319	GLU	CD-OE2	5.26	1.31	1.25
1	B	466	GLU	CD-OE1	5.24	1.31	1.25
1	B	435	GLU	CD-OE2	5.17	1.31	1.25
1	B	435	GLU	CD-OE1	5.11	1.31	1.25
1	A	356	GLU	CD-OE1	5.11	1.31	1.25
1	A	294	GLU	CD-OE2	-5.11	1.20	1.25
1	C	237	TYR	CE1-CZ	5.03	1.45	1.38

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	475	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	C	404	CYS	CA-CB-SG	-8.63	98.47	114.00
1	A	404	CYS	CA-CB-SG	-8.12	99.38	114.00
1	B	301	ASP	CB-CG-OD1	7.83	125.34	118.30
1	A	451	GLU	OE1-CD-OE2	-7.37	114.45	123.30
1	C	301	ASP	CB-CG-OD1	6.91	124.52	118.30
1	C	228	LYS	CD-CE-NZ	6.85	127.46	111.70
1	D	316	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	A	316	ASP	CB-CG-OD1	6.73	124.36	118.30
1	B	316	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	357	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	C	475	ARG	NH1-CZ-NH2	-6.32	112.45	119.40
1	D	445	GLU	OE1-CD-OE2	-6.25	115.80	123.30
1	B	404	CYS	CA-CB-SG	-6.13	102.96	114.00
1	D	404	CYS	CA-CB-SG	-6.09	103.05	114.00
1	D	424	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	C	336	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	D	387	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	316	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	D	396	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	349	ASP	CB-CG-OD1	5.78	123.50	118.30
1	D	316	ASP	CB-CG-OD1	5.74	123.47	118.30
1	C	267	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	C	301	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	C	427	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	301	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	B	316	ASP	CB-CG-OD1	5.51	123.26	118.30
1	A	463	GLU	CA-CB-CG	5.44	125.37	113.40
1	C	424	ASP	CB-CG-OD1	5.40	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	336	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	C	357	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	336	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	C	316	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	D	347	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	B	181	ASP	CB-CG-OD1	5.11	122.89	118.30
1	A	427	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	B	387	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2448	0	2348	10	1
1	B	2462	0	2364	10	0
1	C	2451	0	2359	13	0
1	D	2271	0	2140	12	0
2	A	32	0	13	0	0
2	B	28	0	12	0	0
2	C	32	0	13	0	0
2	D	32	0	13	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	154	0	0	1	0
5	B	184	0	0	2	0
5	C	149	0	0	2	1
5	D	92	0	0	2	0
All	All	10345	0	9262	39	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 (39) 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:D:359:ASN:OD1	5:D:1050:HOH:O	2.00	0.79
1:B:359:ASN:OD1	5:B:1050:HOH:O	2.07	0.71
1:D:189:MET:SD	1:D:227:THR:HG21	2.31	0.70
1:C:198:ASP:OD1	5:C:1122:HOH:O	2.11	0.68
1:B:189:MET:SD	1:B:227:THR:HG21	2.33	0.68
1:C:243:ILE:HD13	1:C:397:SER:HB3	1.77	0.67
1:C:191:TYR:HH	1:D:196:TYR:HH	1.24	0.67
1:A:189:MET:SD	1:A:227:THR:HG21	2.38	0.63
1:C:184:THR:HB	1:D:185:ASN:OD1	2.00	0.62
1:D:186:VAL:HG13	1:D:205:ILE:HG23	1.82	0.62
1:A:184:THR:HB	1:B:185:ASN:ND2	2.17	0.60
1:D:326:GLN:NE2	5:D:1013:HOH:O	2.32	0.60
1:C:186:VAL:HG13	1:C:205:ILE:HG23	1.85	0.59
1:B:186:VAL:HG13	1:B:205:ILE:HG23	1.89	0.55
1:C:189:MET:HG2	1:C:217:TYR:CE1	2.42	0.54
1:C:191:TYR:OH	1:D:196:TYR:OH	2.04	0.52
1:B:189:MET:HG2	1:B:217:TYR:CE1	2.45	0.51
1:C:186:VAL:CG1	1:C:205:ILE:HG23	2.41	0.51
1:A:189:MET:HG2	1:A:217:TYR:CE1	2.45	0.51
1:B:186:VAL:CG1	1:B:205:ILE:HG23	2.42	0.49
1:B:298:LEU:HA	5:B:1268:HOH:O	2.12	0.49
1:D:186:VAL:CG1	1:D:205:ILE:HG23	2.42	0.48
1:D:189:MET:HG2	1:D:217:TYR:CE1	2.49	0.47
1:C:328:VAL:HG11	1:C:358:LEU:HD22	1.96	0.47
1:C:189:MET:SD	1:C:227:THR:HG21	2.55	0.46
1:A:186:VAL:HG13	1:A:205:ILE:HG23	1.97	0.46
5:A:1062:HOH:O	1:D:198:ASP:CB	2.62	0.46
1:C:446:GLU:OE2	5:C:1065:HOH:O	2.21	0.46
1:A:182:ASN:N	1:B:181:ASP:OD2	2.49	0.46
1:A:186:VAL:CG1	1:A:205:ILE:HG23	2.46	0.45
1:A:243:ILE:HD13	1:A:397:SER:HB2	1.99	0.45
1:A:185:ASN:ND2	1:B:179:TYR:OH	2.50	0.45
1:C:307[B]:ARG:HH12	1:C:431:ASN:HB2	1.83	0.44
1:A:317:ILE:HD12	1:A:317:ILE:HA	1.79	0.44
1:A:407:ILE:HD13	1:A:407:ILE:HG21	1.91	0.41
1:C:471:GLU:HG3	1:C:475:ARG:HD2	2.02	0.41
1:D:420:ASN:HD22	1:D:420:ASN:HA	1.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:MET:HE3	1:B:294:GLU:HB3	2.03	0.41
1:D:307[B]:ARG:NH1	1:D:431:ASN:HB2	2.37	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	5:C:1080:HOH:O[2_747]	2.13	0.07

## 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	296/305 (97%)	285 (96%)	11 (4%)	0	100	100
1	B	294/305 (96%)	283 (96%)	11 (4%)	0	100	100
1	C	296/305 (97%)	284 (96%)	12 (4%)	0	100	100
1	D	277/305 (91%)	267 (96%)	8 (3%)	2 (1%)	22	26
All	All	1163/1220 (95%)	1119 (96%)	42 (4%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	198	ASP
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	270/281 (96%)	263 (97%)	7 (3%)	46	63
1	B	273/281 (97%)	268 (98%)	5 (2%)	59	75
1	C	271/281 (96%)	265 (98%)	6 (2%)	52	69
1	D	243/281 (86%)	241 (99%)	2 (1%)	81	91
All	All	1057/1124 (94%)	1037 (98%)	20 (2%)	57	73

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	184	THR
1	A	212	TYR
1	A	221	ASN
1	A	267	ASP
1	A	284	PRO
1	A	385	ASN
1	A	478	LYS
1	B	212	TYR
1	B	221	ASN
1	B	230	SER
1	B	285	GLU
1	B	420	ASN
1	C	221	ASN
1	C	232	ASN
1	C	267	ASP
1	C	297	LEU
1	C	300	ARG
1	C	397	SER
1	D	221	ASN
1	D	245	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	341	ASN
1	A	378	ASN
1	A	467	ASN
1	B	185	ASN

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Mol	Chain	Res	Type
1	B	245	ASN
1	B	359	ASN
1	B	378	ASN
1	B	467	ASN
1	C	327	ASN
1	C	341	ASN
1	C	431	ASN
1	D	245	ASN
1	D	295	GLN
1	D	296	ASN
1	D	326	GLN
1	D	378	ASN
1	D	420	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	C	500	3	29,34,34	2.83	6 (20%)	33,54,54	2.97	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GNP	B	500	3	24,30,34	2.45	5 (20%)	27,47,54	2.35	7 (25%)
2	GNP	D	500	3	29,34,34	4.38	8 (27%)	33,54,54	2.72	13 (39%)
2	GNP	A	500	3	29,34,34	3.72	8 (27%)	33,54,54	2.56	10 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GNP	C	500	3	-	5/14/38/38	0/3/3/3
2	GNP	B	500	3	-	1/9/32/38	0/3/3/3
2	GNP	D	500	3	-	1/14/38/38	0/3/3/3
2	GNP	A	500	3	-	3/14/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	GNP	PB-O1B	17.01	1.73	1.46
2	A	500	GNP	PB-O1B	14.47	1.69	1.46
2	D	500	GNP	PG-O1G	11.80	1.64	1.46
2	A	500	GNP	PG-O1G	10.76	1.63	1.46
2	C	500	GNP	PB-O1B	9.37	1.61	1.46
2	C	500	GNP	PG-O1G	9.02	1.60	1.46
2	D	500	GNP	PB-O3A	8.38	1.69	1.59
2	B	500	GNP	PB-O1B	7.43	1.58	1.46
2	B	500	GNP	PB-O3A	7.18	1.68	1.59
2	D	500	GNP	PB-O2B	-4.16	1.45	1.56
2	B	500	GNP	PB-O2B	-4.10	1.45	1.56
2	C	500	GNP	PG-O2G	-4.02	1.45	1.56
2	C	500	GNP	PB-O2B	-3.89	1.46	1.56
2	A	500	GNP	PG-O2G	-3.78	1.46	1.56
2	D	500	GNP	PG-O2G	-3.77	1.46	1.56
2	A	500	GNP	PB-O2B	-3.64	1.47	1.56
2	A	500	GNP	C6-N1	3.23	1.38	1.33
2	A	500	GNP	C5-C6	-3.14	1.35	1.41
2	D	500	GNP	C6-N1	2.82	1.37	1.33
2	A	500	GNP	C5-C4	-2.73	1.33	1.40
2	C	500	GNP	PB-O3A	2.61	1.62	1.59
2	C	500	GNP	C5-C4	-2.54	1.34	1.40
2	D	500	GNP	PA-O5'	2.37	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	GNP	PG-O3G	2.33	1.63	1.56
2	B	500	GNP	C6-N1	2.15	1.36	1.33
2	B	500	GNP	C5-C4	-2.09	1.35	1.40
2	A	500	GNP	C4-N3	-2.06	1.32	1.35

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	GNP	C5-C6-N1	-8.35	112.00	123.43
2	D	500	GNP	C5-C6-N1	-8.04	112.44	123.43
2	C	500	GNP	C5-C6-N1	-7.52	113.14	123.43
2	C	500	GNP	O1B-PB-N3B	-7.49	100.75	111.77
2	A	500	GNP	C5-C6-N1	-7.08	113.75	123.43
2	C	500	GNP	O1G-PG-N3B	-6.84	101.70	111.77
2	D	500	GNP	C2-N1-C6	6.27	125.89	115.93
2	A	500	GNP	O2B-PB-O1B	-5.99	97.36	109.92
2	B	500	GNP	C2-N1-C6	5.65	124.91	115.93
2	D	500	GNP	O3A-PB-N3B	5.59	122.10	106.59
2	C	500	GNP	C2-N1-C6	5.37	124.47	115.93
2	D	500	GNP	O1B-PB-N3B	-5.32	103.93	111.77
2	A	500	GNP	O1G-PG-N3B	-5.24	104.06	111.77
2	C	500	GNP	O2B-PB-O3A	5.11	121.71	104.64
2	A	500	GNP	C2-N1-C6	4.59	123.22	115.93
2	C	500	GNP	O2B-PB-O1B	-4.11	101.31	109.92
2	A	500	GNP	O2G-PG-O3G	4.08	118.50	107.64
2	A	500	GNP	N3-C2-N1	-3.76	122.20	127.22
2	A	500	GNP	O2B-PB-O3A	3.74	117.13	104.64
2	D	500	GNP	C2-N3-C4	-3.19	111.72	115.36
2	A	500	GNP	O1B-PB-N3B	-3.16	107.12	111.77
2	B	500	GNP	C2-N3-C4	-3.04	111.88	115.36
2	C	500	GNP	N3-C2-N1	-3.01	123.21	127.22
2	C	500	GNP	O2G-PG-O3G	2.97	115.53	107.64
2	D	500	GNP	C4-C5-C6	-2.94	117.99	120.80
2	D	500	GNP	N3-C2-N1	-2.84	123.44	127.22
2	B	500	GNP	O2'-C2'-C3'	-2.74	102.96	111.82
2	D	500	GNP	O5'-PA-O1A	2.73	119.74	109.07
2	C	500	GNP	C4-C5-C6	-2.49	118.42	120.80
2	C	500	GNP	C2-N3-C4	-2.43	112.58	115.36
2	C	500	GNP	O5'-PA-O1A	2.35	118.23	109.07
2	D	500	GNP	O2G-PG-O1G	-2.25	107.78	113.45
2	B	500	GNP	N3-C2-N1	-2.23	124.25	127.22
2	D	500	GNP	C1'-N9-C4	-2.23	122.73	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	GNP	O2A-PA-O5'	2.20	117.98	107.75
2	B	500	GNP	O3'-C3'-C2'	-2.20	104.70	111.82
2	D	500	GNP	O1G-PG-N3B	-2.14	108.62	111.77
2	A	500	GNP	C4-C5-N7	2.11	111.60	109.40
2	C	500	GNP	O2'-C2'-C3'	-2.10	105.04	111.82
2	D	500	GNP	O3'-C3'-C2'	-2.09	105.06	111.82
2	D	500	GNP	O2B-PB-O3A	-2.04	97.84	104.64
2	A	500	GNP	C2-N3-C4	-2.01	113.06	115.36

There are no chirality outliers.

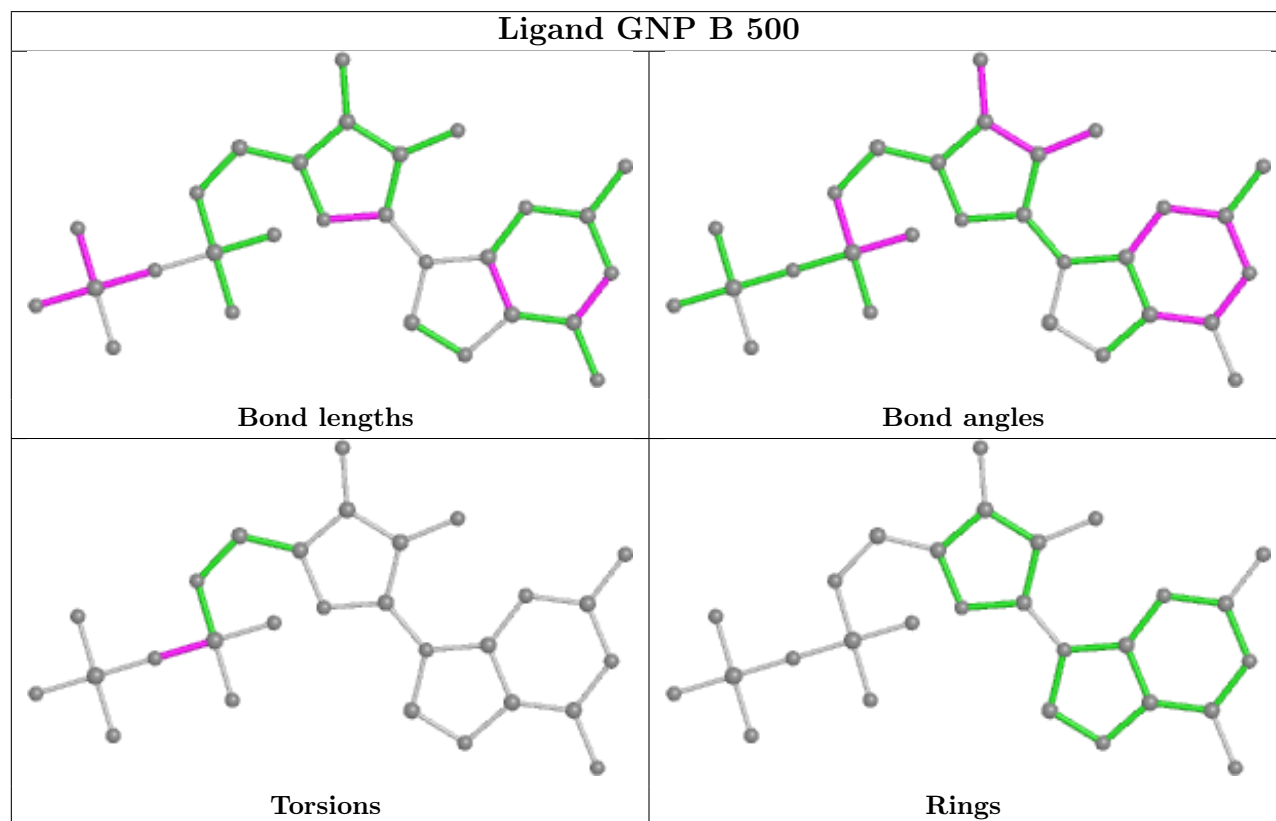
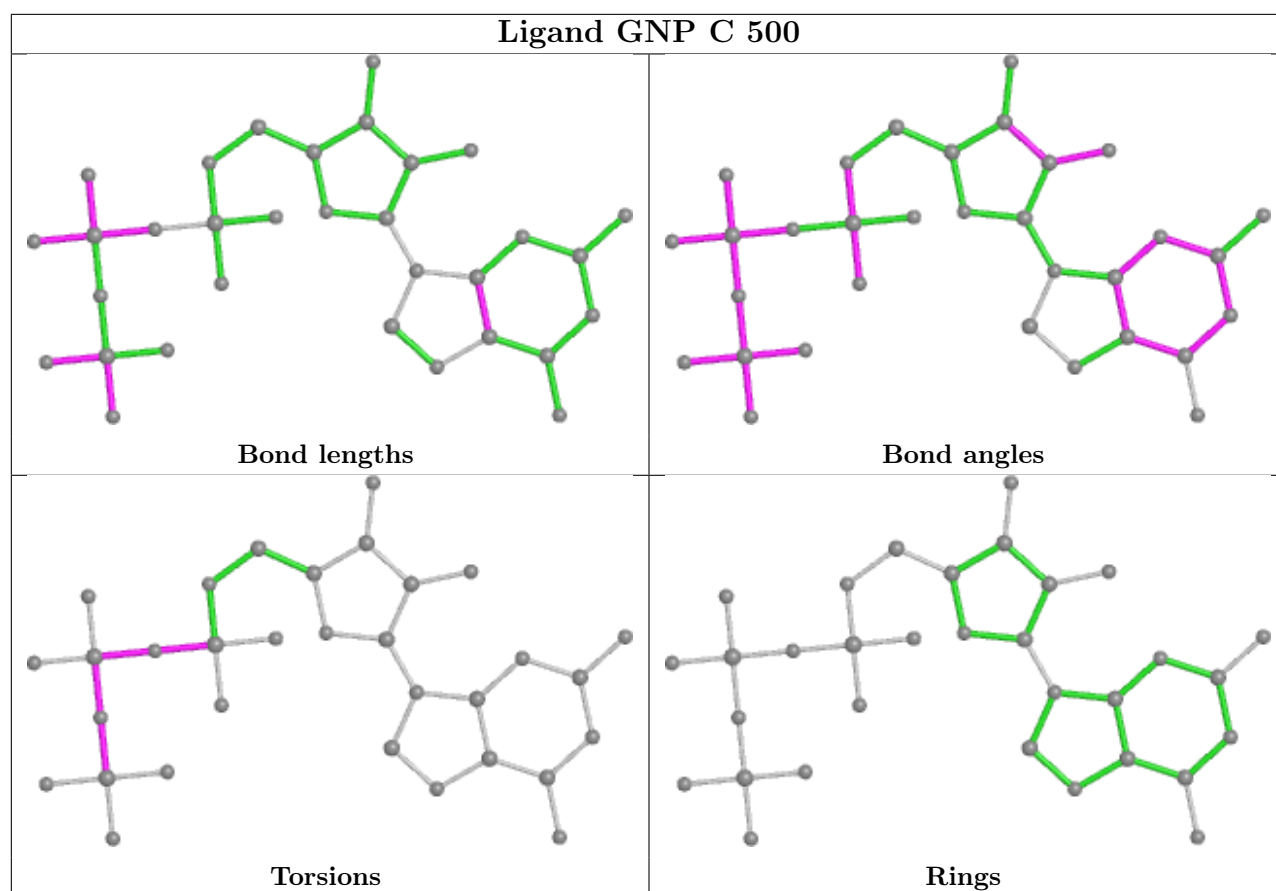
All (10) torsion outliers are listed below:

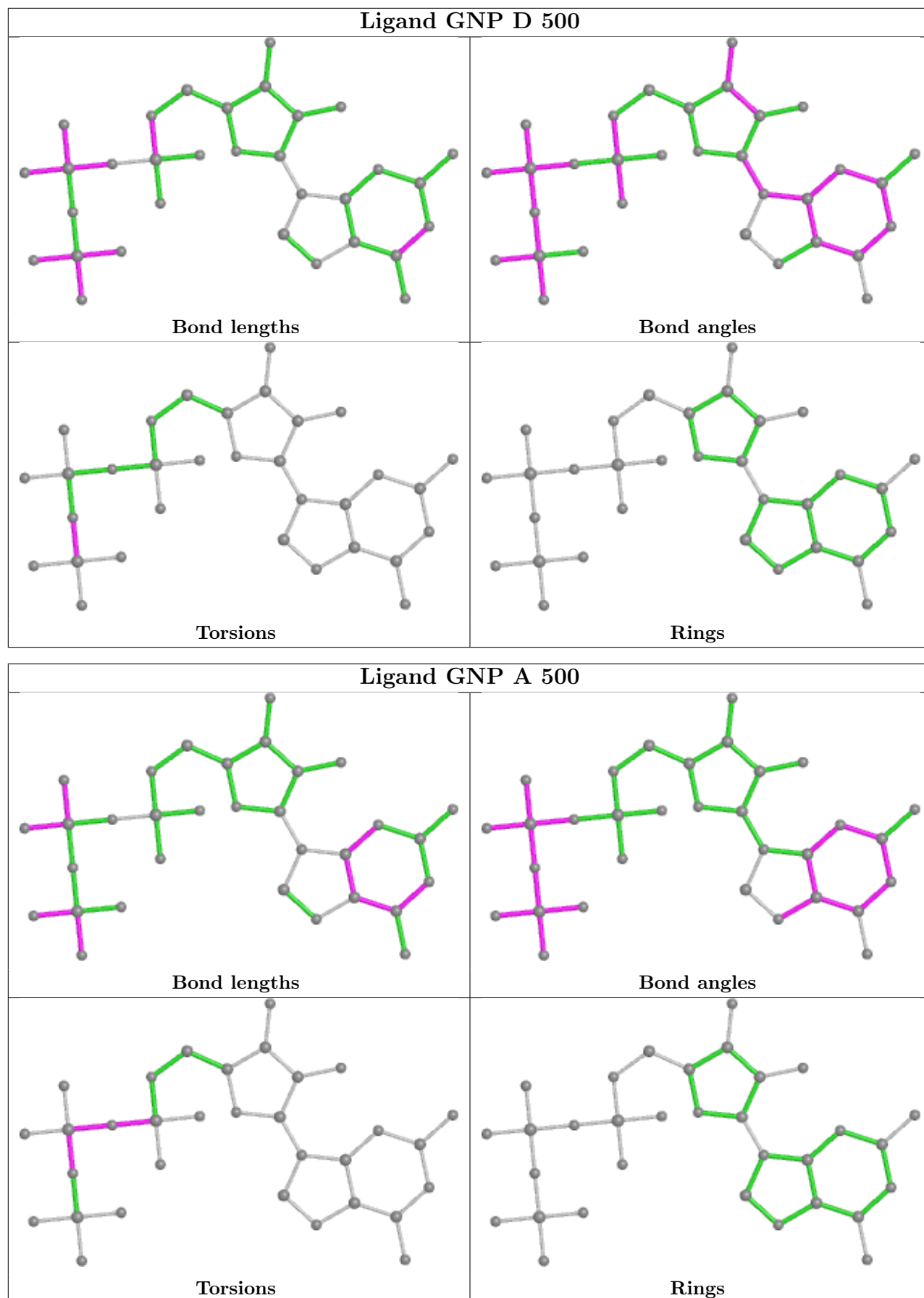
Mol	Chain	Res	Type	Atoms
2	A	500	GNP	PG-N3B-PB-O1B
2	A	500	GNP	PA-O3A-PB-O2B
2	C	500	GNP	PA-O3A-PB-O1B
2	C	500	GNP	PA-O3A-PB-O2B
2	D	500	GNP	PB-N3B-PG-O1G
2	B	500	GNP	PB-O3A-PA-O1A
2	A	500	GNP	PB-O3A-PA-O2A
2	C	500	GNP	PB-O3A-PA-O1A
2	C	500	GNP	PB-N3B-PG-O1G
2	C	500	GNP	PG-N3B-PB-O3A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	298/305 (97%)	0.05	6 (2%) 65 71	30, 48, 82, 101	0
1	B	297/305 (97%)	0.02	4 (1%) 77 81	32, 47, 79, 112	0
1	C	297/305 (97%)	0.09	8 (2%) 54 62	29, 48, 89, 111	0
1	D	282/305 (92%)	0.14	6 (2%) 63 70	40, 58, 88, 101	0
All	All	1174/1220 (96%)	0.07	24 (2%) 65 71	29, 50, 87, 112	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	179	TYR	8.0
1	A	212	TYR	5.3
1	A	231	THR	5.3
1	C	232	ASN	4.4
1	C	183	ALA	3.5
1	D	457	ILE	3.5
1	C	212	TYR	3.3
1	B	182	ASN	2.8
1	C	185	ASN	2.8
1	D	208	ILE	2.7
1	B	212	TYR	2.7
1	C	184	THR	2.6
1	A	236	GLY	2.6
1	D	185	ASN	2.5
1	D	229	PHE	2.2
1	D	215	VAL	2.2
1	D	455	TYR	2.2
1	A	213	ASP	2.1
1	C	186	VAL	2.1
1	B	213	ASP	2.1
1	A	479	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	479	ASP	2.0
1	C	208	ILE	2.0
1	A	254	ASN	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

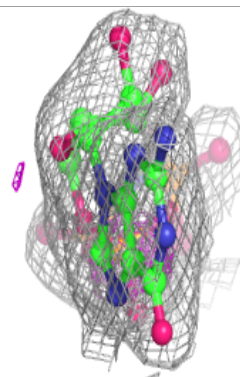
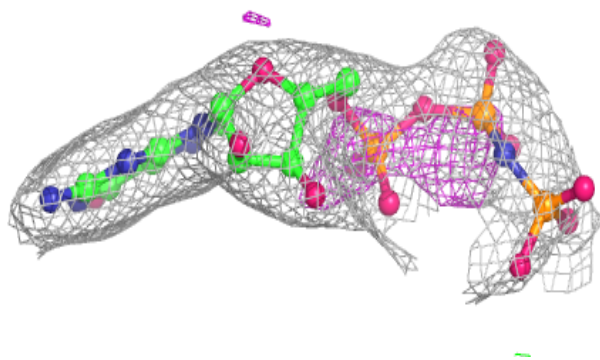
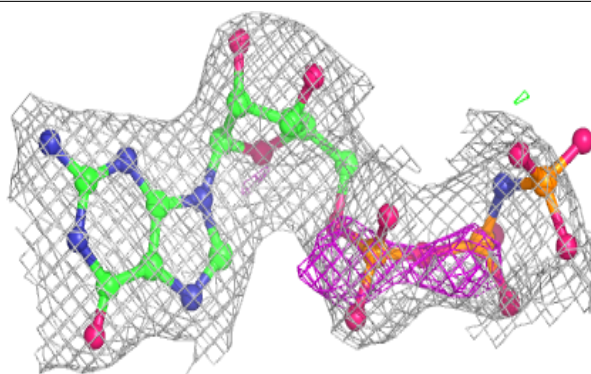
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	C	700	1/1	0.86	0.08	59,59,59,59	0
3	MG	B	700	1/1	0.88	0.10	62,62,62,62	0
3	MG	C	702	1/1	0.88	0.09	71,71,71,71	0
4	CL	C	802	1/1	0.89	0.10	70,70,70,70	0
3	MG	B	702	1/1	0.93	0.07	66,66,66,66	0
2	GNP	D	500	32/32	0.95	0.15	49,56,73,81	4
4	CL	A	802	1/1	0.95	0.16	79,79,79,79	0
4	CL	B	802	1/1	0.95	0.22	74,74,74,74	0
2	GNP	B	500	28/32	0.95	0.14	46,56,70,75	0
3	MG	A	702	1/1	0.96	0.05	66,66,66,66	0
2	GNP	C	500	32/32	0.96	0.13	47,56,67,67	4
3	MG	D	700	1/1	0.97	0.09	56,56,56,56	0
2	GNP	A	500	32/32	0.97	0.14	40,47,60,65	4
3	MG	A	700	1/1	0.98	0.12	46,46,46,46	0

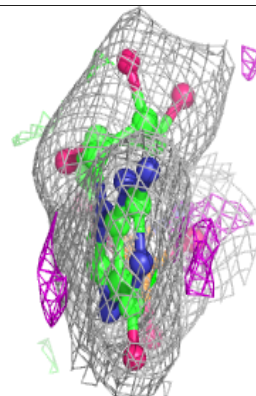
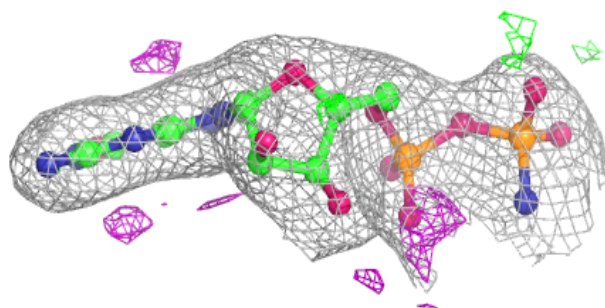
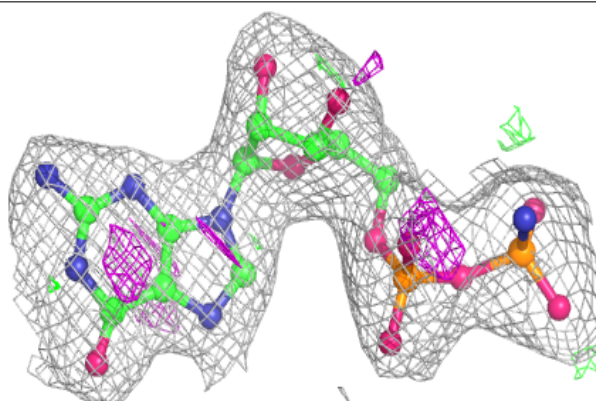
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 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:**

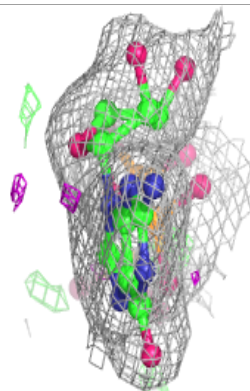
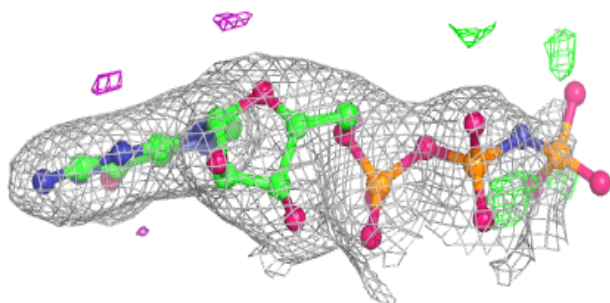
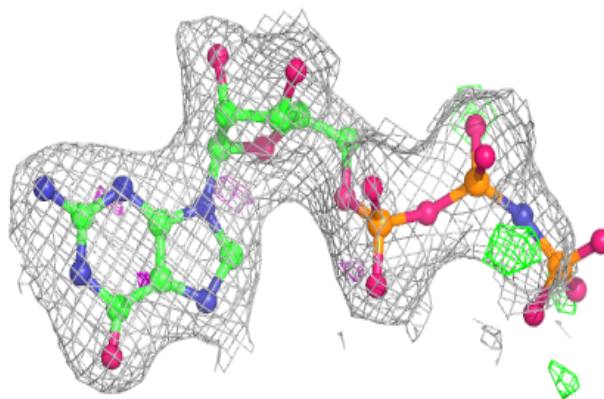
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



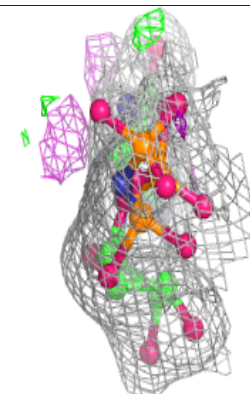
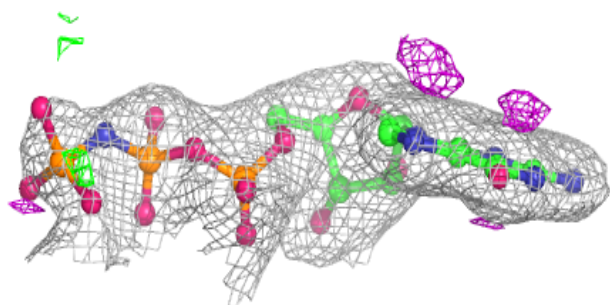
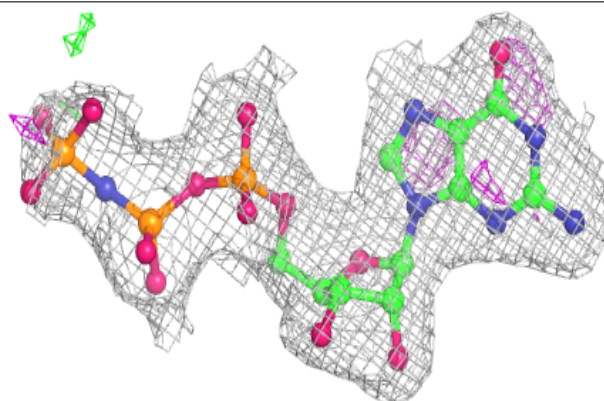


**Electron density around GNP C 500:**

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

**Electron density around GNP 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.