



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:48 PM UTC

PDB ID : 6X1C / pdb_00006x1c
Title : Tubulin-RB3_SLD-TTL in complex with compound 5j
Authors : White, S.W.; Yun, M.
Deposited on : 2020-05-18
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

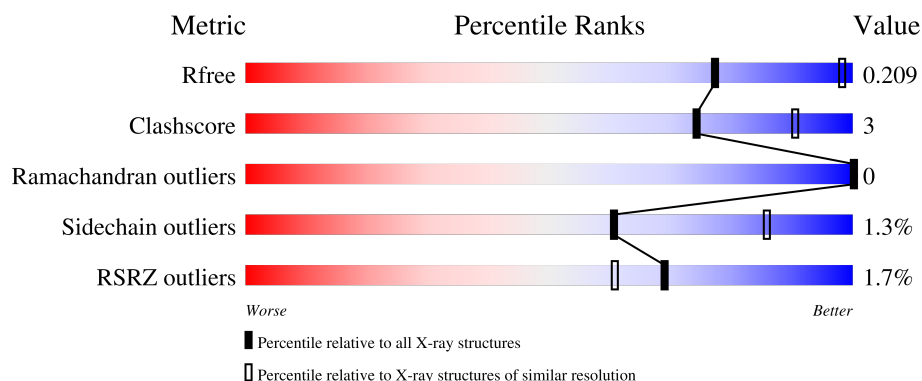
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

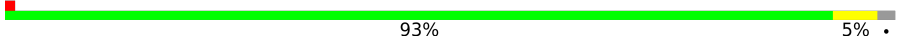
The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	450	
1	C	450	
2	B	445	
2	D	445	
3	E	143	

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Mol	Chain	Length	Quality of chain
4	F	384	5% 75% 9% 15%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17509 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3361	2110	576	649	26			
2	D	421	Total	C	N	O	S	0	0	0
			3305	2078	562	639	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	328	Total	C	N	O	S	0	0	0
			2654	1707	457	476	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

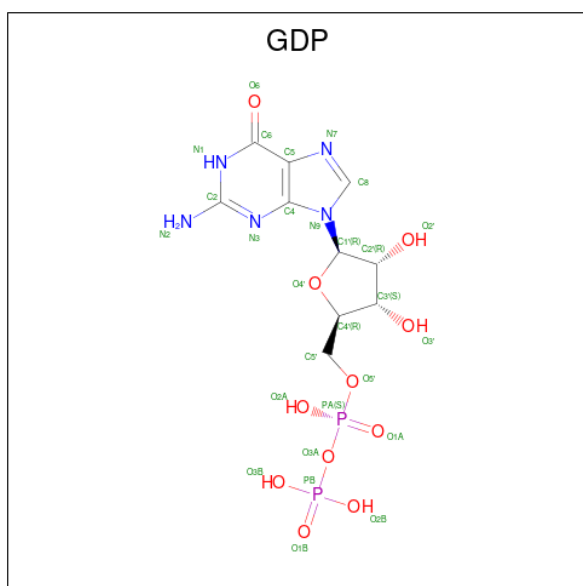
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0
7	F	1	Total Mg 1 1	0	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



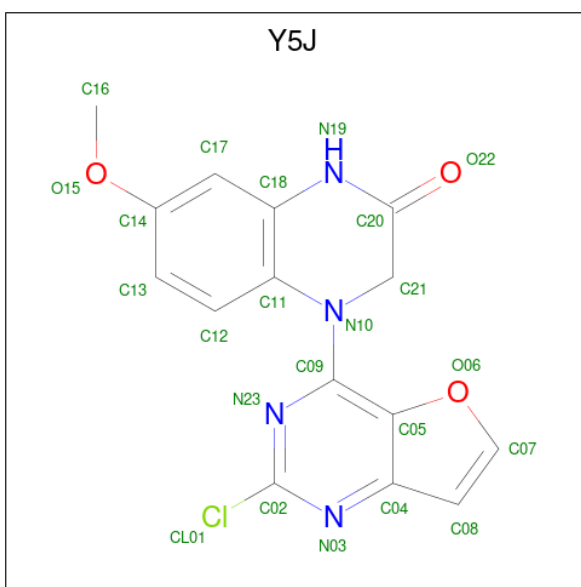
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 4-(2-chlorofuro[3,2-d]pyrimidin-4-yl)-7-methoxy-3,4-dihydroquinoxalin-2(1H)-one (CCD ID: Y5J) (formula: C₁₅H₁₁ClN₄O₃) (labeled as "Ligand of Interest" by depositor).



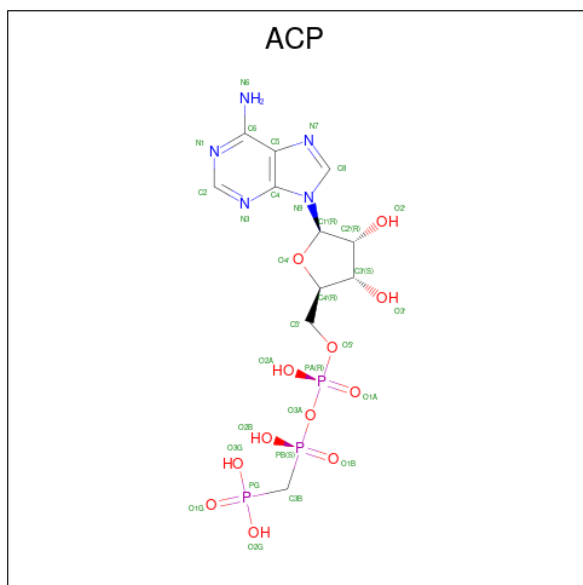
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	Cl	N	O	0	0
			23	15	1	4	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	Cl	N	O	0	0
			23	15	1	4	3		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



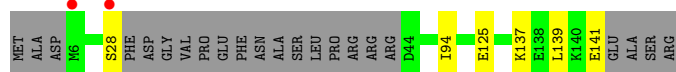
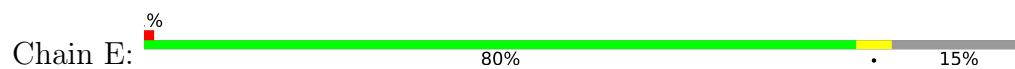
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 12 is water.

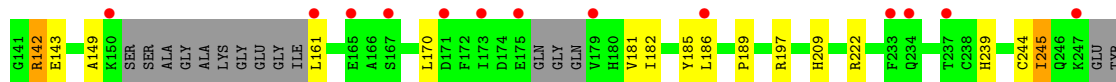
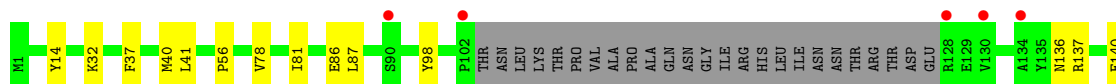
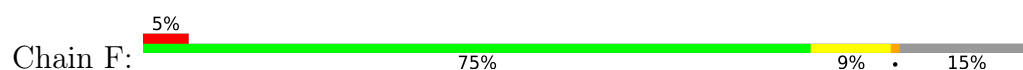
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	25	Total	O	0	0
			25	25		
12	B	23	Total	O	0	0
			23	23		
12	C	41	Total	O	0	0
			41	41		
12	D	5	Total	O	0	0
			5	5		
12	E	4	Total	O	0	0
			4	4		
12	F	6	Total	O	0	0
			6	6		



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.34Å 158.32Å 181.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 2.90 48.14 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.14-2.90) 95.2 (48.14-2.90)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.174 , 0.216 0.172 , 0.209	Depositor DCC
R_{free} test set	2000 reflections (2.90%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17509	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: MES, CA, Y5J, ACP, GTP, GDP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/3494	0.29	0/4743
1	C	0.11	0/3515	0.29	0/4772
2	B	0.11	0/3436	0.30	0/4654
2	D	0.10	0/3378	0.27	0/4577
3	E	0.09	0/1008	0.26	0/1337
4	F	0.11	0/2714	0.33	0/3669
All	All	0.11	0/17545	0.30	0/23752

There are no bond length outliers.

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	3416	0	3330	22	0
1	C	3437	0	3348	10	0
2	B	3361	0	3238	29	0
2	D	3305	0	3179	23	0
3	E	1000	0	1018	3	0
4	F	2654	0	2592	23	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	B	28	0	12	2	0
9	B	24	0	24	3	0
10	B	23	0	0	0	0
10	D	23	0	0	0	0
11	F	31	0	13	0	0
12	A	25	0	0	0	0
12	B	23	0	0	0	0
12	C	41	0	0	0	0
12	D	5	0	0	0	0
12	E	4	0	0	0	0
12	F	6	0	0	0	0
All	All	17509	0	16790	107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (107) 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:B:170:MET:HG3	2:B:377:LEU:HD21	1.77	0.67
2:D:375:GLN:HB2	2:D:419:VAL:HG13	1.77	0.65
2:D:170:MET:HE2	2:D:377:LEU:HD21	1.77	0.65
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.77	0.64
4:F:209:HIS:HB2	4:F:310:GLN:HG3	1.82	0.61
4:F:185:TYR:OH	4:F:239:HIS:ND1	2.32	0.59
2:D:10:GLY:O	2:D:14:ASN:ND2	2.27	0.58
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.85	0.58
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.87	0.57
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.37	0.56
4:F:222:ARG:NH1	4:F:318:ASP:OD2	2.38	0.56
1:A:345:ASP:HB3	3:E:28:SER:HB3	1.87	0.56
1:A:335:ILE:HG23	1:A:339:ARG:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:86:GLU:OE1	4:F:86:GLU:N	2.28	0.55
3:E:137:LYS:O	3:E:141:GLU:HG2	2.06	0.55
1:A:88:HIS:O	1:A:91:GLN:HG2	2.07	0.54
2:D:134:GLN:HA	2:D:165:ASN:O	2.07	0.54
2:B:174:LYS:HD2	2:B:205:GLU:HG3	1.90	0.54
2:B:219:THR:HG21	1:C:326:LYS:HA	1.89	0.53
4:F:137:ARG:HD2	4:F:140:GLU:HB3	1.92	0.52
2:B:35:SER:HG	2:B:58:LYS:HZ3	1.55	0.51
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.91	0.51
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.29	0.50
2:B:134:GLN:HA	2:B:165:ASN:O	2.10	0.50
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.93	0.50
2:B:15:GLN:NE2	8:B:501:GDP:O6	2.45	0.50
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.38	0.50
1:C:46:ASP:OD1	1:C:46:ASP:N	2.44	0.49
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.94	0.49
2:B:313:VAL:HB	2:B:349:VAL:HG22	1.92	0.49
1:A:166:LYS:HE2	1:A:197:HIS:O	2.13	0.48
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.53	0.48
4:F:98:TYR:HD2	4:F:182:ILE:HD11	1.78	0.48
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.94	0.48
1:A:399:TYR:O	1:A:402:ARG:NH1	2.46	0.48
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.25	0.48
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.95	0.48
2:B:67:ASP:HA	2:B:143:THR:HG21	1.95	0.47
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.32	0.47
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.97	0.47
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.46	0.47
2:D:74:ASP:OD1	2:D:74:ASP:N	2.47	0.47
4:F:142:ARG:HB2	4:F:142:ARG:HH11	1.79	0.47
4:F:78:VAL:HG21	4:F:181:VAL:HG11	1.96	0.47
9:B:503:MES:H51	9:B:503:MES:H81	1.71	0.46
2:D:72:THR:O	2:D:76:VAL:HG23	2.15	0.46
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.97	0.46
2:B:67:ASP:O	2:B:92:PHE:HA	2.15	0.46
1:A:88:HIS:CE1	1:A:90:GLU:HB2	2.52	0.45
2:B:173:PRO:HA	2:B:176:SER:HB2	1.97	0.45
1:A:176:GLN:NE2	4:F:56:PRO:HB3	2.32	0.45
2:B:333:VAL:HG13	9:B:503:MES:H22	1.97	0.45
2:D:202:ILE:HD13	2:D:229:VAL:HG13	1.98	0.45
2:B:295:ASP:HA	9:B:503:MES:O3S	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.25	0.45
2:B:44:LEU:HA	2:B:47:ILE:HB	1.98	0.44
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.52	0.44
2:B:145:SER:HG	2:B:188:SER:HG	1.63	0.44
1:C:165:SER:HA	1:C:199:ASP:OD2	2.17	0.44
2:B:2:ARG:C	2:B:131:GLN:HE21	2.24	0.44
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.99	0.44
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.53	0.44
2:D:247:ASN:O	2:D:252:LYS:HD2	2.17	0.44
4:F:149:ALA:HB2	4:F:182:ILE:HG22	1.99	0.44
2:B:65:LEU:HD22	2:B:90:PHE:CE2	2.53	0.44
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.00	0.44
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.53	0.44
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.53	0.44
1:A:147:SER:HB2	1:A:190:THR:HB	2.00	0.43
4:F:149:ALA:O	4:F:161:LEU:HB3	2.18	0.43
2:B:152:ILE:HG23	2:B:164:MET:HG2	2.00	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.53	0.43
2:D:44:LEU:HA	2:D:47:ILE:HB	1.99	0.43
2:B:141:GLY:HA3	8:B:501:GDP:O3A	2.19	0.43
2:B:203:ASP:OD2	2:B:380:ARG:NH1	2.47	0.43
2:B:267:MET:HG2	2:B:374:ILE:HD13	2.01	0.43
4:F:137:ARG:HD2	4:F:137:ARG:HA	1.76	0.43
2:B:261:PRO:O	2:B:264:HIS:ND1	2.49	0.43
4:F:81:ILE:HA	4:F:87:LEU:HD12	2.00	0.43
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.54	0.43
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.01	0.43
2:D:267:MET:HG2	2:D:301:ALA:HB3	1.99	0.43
1:A:69:ASP:O	1:A:94:THR:HA	2.19	0.42
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.53	0.42
2:D:104:GLY:O	2:D:109:GLY:HA3	2.19	0.42
2:B:246:LEU:HD12	2:B:246:LEU:HA	1.75	0.42
2:D:1:MET:HE3	2:D:128:ASP:HB2	2.01	0.42
1:A:88:HIS:ND1	1:A:90:GLU:HB2	2.35	0.42
1:A:291:ILE:HD13	1:A:373:ARG:HG3	2.02	0.42
2:B:296:SER:HA	2:B:299:MET:HG2	2.02	0.42
2:B:273:LEU:HD11	2:B:298:ASN:HA	2.01	0.42
4:F:189:PRO:HA	4:F:322:ASP:HA	2.01	0.42
2:B:68:LEU:HD12	2:B:97:ALA:HB2	2.02	0.42
2:D:396:HIS:CD2	2:D:397:TRP:HD1	2.37	0.41
2:D:301:ALA:O	2:D:303:CYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:32:LYS:HB3	4:F:32:LYS:HE2	1.86	0.41
4:F:186:LEU:HD12	4:F:320:MET:HG2	2.02	0.41
2:D:404:ASP:OD1	2:D:405:GLU:N	2.53	0.41
1:C:245:ASP:OD1	1:C:245:ASP:N	2.54	0.41
2:D:239:CYS:O	2:D:248:ALA:HB3	2.20	0.41
2:D:382:SER:HB2	2:D:415:MET:HE3	2.03	0.41
2:D:107:THR:OG1	2:D:108:GLU:N	2.53	0.41
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.86	0.41
4:F:244:CYS:SG	4:F:245:ILE:HD12	2.61	0.41
1:A:346:TRP:CD1	1:A:346:TRP:H	2.39	0.40
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.04	0.40
2:D:169:VAL:HA	2:D:202:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/450 (97%)	428 (98%)	7 (2%)	0	100	100
1	C	438/450 (97%)	431 (98%)	7 (2%)	0	100	100
2	B	425/445 (96%)	415 (98%)	10 (2%)	0	100	100
2	D	417/445 (94%)	407 (98%)	10 (2%)	0	100	100
3	E	117/143 (82%)	117 (100%)	0	0	100	100
4	F	316/384 (82%)	307 (97%)	9 (3%)	0	100	100
All	All	2148/2317 (93%)	2105 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/378 (97%)	364 (99%)	4 (1%)	65	88
1	C	371/378 (98%)	364 (98%)	7 (2%)	50	79
2	B	369/383 (96%)	368 (100%)	1 (0%)	86	96
2	D	362/383 (94%)	357 (99%)	5 (1%)	59	85
3	E	109/127 (86%)	107 (98%)	2 (2%)	51	80
4	F	284/342 (83%)	278 (98%)	6 (2%)	47	77
All	All	1863/1991 (94%)	1838 (99%)	25 (1%)	61	86

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	176	GLN
1	A	320	ARG
1	A	363	VAL
2	B	78	SER
1	C	2	ARG
1	C	71	GLU
1	C	177	VAL
1	C	198	SER
1	C	251	ASP
1	C	284	GLU
1	C	340	SER
2	D	215	LEU
2	D	246	LEU
2	D	284	LEU
2	D	343	GLU
2	D	350	LYS
3	E	125	GLU
3	E	139	LEU
4	F	136	ASN
4	F	142	ARG
4	F	143	GLU

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Mol	Chain	Res	Type
4	F	170	LEU
4	F	245	ILE
4	F	310	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	85	GLN
1	A	393	HIS
2	B	15	GLN
2	B	227	HIS
2	B	347	ASN
2	B	426	GLN
1	C	256	GLN
1	C	372	GLN
1	C	406	HIS
2	D	37	HIS
2	D	195	ASN
2	D	247	ASN
3	E	103	GLN
4	F	310	GLN
4	F	348	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 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
9	MES	B	502	-	12,12,12	2.16	1 (8%)	15,16,16	1.60	2 (13%)
8	GDP	B	501	7	29,30,30	1.18	2 (6%)	45,47,47	1.71	5 (11%)
5	GTP	C	501	7	33,34,34	0.91	1 (3%)	50,54,54	1.48	7 (14%)
10	Y5J	B	505	-	26,26,26	3.04	11 (42%)	30,38,38	3.04	12 (40%)
11	ACP	F	401	7	31,33,33	1.96	6 (19%)	47,52,52	1.73	8 (17%)
5	GTP	D	501	7	33,34,34	0.90	0	50,54,54	1.49	7 (14%)
10	Y5J	D	502	-	26,26,26	3.03	11 (42%)	30,38,38	3.07	12 (40%)
5	GTP	A	501	7	33,34,34	0.94	1 (3%)	50,54,54	1.49	8 (16%)
9	MES	B	503	-	12,12,12	2.15	1 (8%)	15,16,16	1.68	2 (13%)

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
9	MES	B	502	-	-	0/6/14/14	0/1/1/1
8	GDP	B	501	7	-	3/16/32/32	0/3/3/3
5	GTP	C	501	7	-	9/22/38/38	0/3/3/3
10	Y5J	B	505	-	-	4/6/18/18	0/4/4/4
11	ACP	F	401	7	-	5/19/38/38	0/3/3/3
5	GTP	D	501	7	-	2/22/38/38	0/3/3/3
10	Y5J	D	502	-	-	5/6/18/18	0/4/4/4
5	GTP	A	501	7	-	6/22/38/38	0/3/3/3
9	MES	B	503	-	-	0/6/14/14	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	Y5J	C20-N19	9.20	1.45	1.35
10	D	502	Y5J	C20-N19	9.01	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	MES	C8-S	-7.28	1.67	1.77
9	B	503	MES	C8-S	-7.24	1.67	1.77
11	F	401	ACP	PB-O3A	6.50	1.65	1.58
10	D	502	Y5J	C09-N10	5.98	1.45	1.37
10	B	505	Y5J	C09-N10	5.80	1.45	1.37
10	B	505	Y5J	C18-N19	5.59	1.49	1.39
10	D	502	Y5J	C18-N19	5.44	1.49	1.39
11	F	401	ACP	C6-N6	4.35	1.45	1.34
10	D	502	Y5J	O06-C07	-4.23	1.32	1.38
10	B	505	Y5J	O06-C07	-4.15	1.32	1.38
10	D	502	Y5J	C21-C20	3.60	1.55	1.51
10	B	505	Y5J	C21-C20	3.58	1.55	1.51
10	B	505	Y5J	C08-C07	3.55	1.39	1.33
10	D	502	Y5J	C08-C07	3.48	1.39	1.33
10	D	502	Y5J	C11-N10	3.37	1.46	1.40
10	B	505	Y5J	C11-N10	3.25	1.45	1.40
8	B	501	GDP	C5-C4	3.17	1.47	1.38
11	F	401	ACP	C5-C4	-2.86	1.34	1.39
11	F	401	ACP	O3'-C3'	-2.82	1.36	1.43
11	F	401	ACP	C5-N7	-2.55	1.34	1.39
8	B	501	GDP	C6-N1	-2.44	1.34	1.38
5	C	501	GTP	PA-O3A	2.36	1.62	1.59
10	D	502	Y5J	O22-C20	-2.27	1.18	1.23
10	B	505	Y5J	C21-N10	-2.27	1.42	1.46
11	F	401	ACP	C8-N9	-2.26	1.33	1.37
10	B	505	Y5J	O22-C20	-2.23	1.18	1.23
10	D	502	Y5J	C21-N10	-2.21	1.42	1.46
10	D	502	Y5J	C18-C11	-2.15	1.38	1.40
10	B	505	Y5J	C18-C11	-2.11	1.38	1.40
5	A	501	GTP	PB-O3A	2.01	1.61	1.59
10	D	502	Y5J	C04-C08	2.01	1.45	1.42
10	B	505	Y5J	C04-C08	2.01	1.45	1.42

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	Y5J	C05-O06-C07	10.14	111.49	105.31
10	B	505	Y5J	C05-O06-C07	10.05	111.43	105.31
10	D	502	Y5J	C04-N03-C02	6.19	120.40	114.58
10	D	502	Y5J	O06-C07-C08	-6.06	107.50	112.49
10	B	505	Y5J	O06-C07-C08	-6.02	107.54	112.49
10	B	505	Y5J	C04-N03-C02	6.00	120.22	114.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C5-C4-N3	-5.85	119.08	128.39
11	F	401	ACP	N3-C2-N1	-5.44	120.35	128.58
10	D	502	Y5J	O06-C05-C09	5.09	131.46	126.46
10	B	505	Y5J	O06-C05-C09	4.94	131.31	126.46
8	B	501	GDP	C2-N3-C4	4.93	120.78	112.30
11	F	401	ACP	C5-C4-N3	-4.85	120.04	126.72
5	D	501	GTP	C5-C4-N3	-4.85	120.67	128.39
5	A	501	GTP	C5-C4-N3	-4.62	121.04	128.39
5	C	501	GTP	C5-C4-N3	-4.62	121.04	128.39
9	B	502	MES	C5-N4-C3	4.47	118.47	108.84
5	D	501	GTP	C2-N3-C4	4.46	119.98	112.30
5	A	501	GTP	C2-N3-C4	4.42	119.91	112.30
5	C	501	GTP	C2-N3-C4	4.35	119.78	112.30
8	B	501	GDP	N9-C4-N3	4.19	134.32	125.95
9	B	503	MES	C5-N4-C3	4.16	117.79	108.84
11	F	401	ACP	N9-C8-N7	-3.98	108.29	113.94
10	D	502	Y5J	N23-C02-N03	-3.76	122.64	129.52
10	B	505	Y5J	N23-C02-N03	-3.66	122.84	129.52
8	B	501	GDP	C6-C5-N7	3.56	136.77	130.29
10	D	502	Y5J	C02-N23-C09	3.55	121.03	110.98
10	B	505	Y5J	C02-N23-C09	3.50	120.88	110.98
10	B	505	Y5J	C18-N19-C20	-3.35	120.44	124.45
11	F	401	ACP	C2-N3-C4	3.34	119.98	111.83
10	D	502	Y5J	C18-N19-C20	-3.20	120.62	124.45
5	D	501	GTP	N9-C4-N3	2.97	131.88	125.95
5	A	501	GTP	C2-N1-C6	-2.90	119.85	125.11
5	D	501	GTP	C2-N1-C6	-2.90	119.86	125.11
5	A	501	GTP	N9-C4-N3	2.90	131.74	125.95
11	F	401	ACP	N3-C4-N9	2.86	132.03	127.17
5	C	501	GTP	C2-N1-C6	-2.83	119.98	125.11
10	D	502	Y5J	C05-C09-N23	-2.78	117.84	123.81
5	C	501	GTP	N9-C4-N3	2.78	131.50	125.95
5	C	501	GTP	N9-C8-N7	-2.77	108.26	113.40
10	B	505	Y5J	C05-C09-N23	-2.76	117.88	123.81
11	F	401	ACP	C5-N7-C8	2.75	107.77	103.45
10	B	505	Y5J	CL01-C02-N03	2.74	119.03	115.17
8	B	501	GDP	C4-C5-N7	-2.71	106.37	110.67
5	A	501	GTP	N9-C8-N7	-2.71	108.38	113.40
5	D	501	GTP	N9-C8-N7	-2.70	108.39	113.40
10	D	502	Y5J	CL01-C02-N03	2.63	118.87	115.17
10	D	502	Y5J	C21-N10-C11	2.60	117.63	114.97
5	D	501	GTP	C8-N7-C5	2.58	108.86	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C8-N7-C5	2.53	108.78	104.26
5	A	501	GTP	C5-C6-N1	2.53	119.70	113.25
9	B	503	MES	O1S-S-C8	2.44	110.42	106.73
10	B	505	Y5J	C21-N10-C11	2.44	117.46	114.97
5	C	501	GTP	C5-C6-N1	2.42	119.42	113.25
5	D	501	GTP	C5-C6-N1	2.39	119.33	113.25
5	A	501	GTP	C8-N7-C5	2.37	108.48	104.26
10	D	502	Y5J	CL01-C02-N23	2.36	118.49	115.17
10	B	505	Y5J	C11-N10-C09	2.26	123.38	119.21
11	F	401	ACP	C4-C5-N7	-2.25	108.01	110.58
11	F	401	ACP	C4-N9-C8	2.14	107.99	105.74
10	D	502	Y5J	C11-N10-C09	2.12	123.12	119.21
10	B	505	Y5J	CL01-C02-N23	2.10	118.13	115.17
9	B	502	MES	O2S-S-C8	2.07	109.85	106.73
5	A	501	GTP	O6-C6-C5	-2.03	121.17	126.53

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
10	B	505	Y5J	C05-C09-N10-C11
10	D	502	Y5J	C05-C09-N10-C11
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PG-C3B-PB-O1B
5	D	501	GTP	O4'-C4'-C5'-O5'
10	D	502	Y5J	C17-C14-O15-C16
10	D	502	Y5J	C13-C14-O15-C16
5	D	501	GTP	C3'-C4'-C5'-O5'
10	D	502	Y5J	N23-C09-N10-C21
10	D	502	Y5J	C05-C09-N10-C21
10	B	505	Y5J	N23-C09-N10-C21
5	C	501	GTP	C3'-C4'-C5'-O5'

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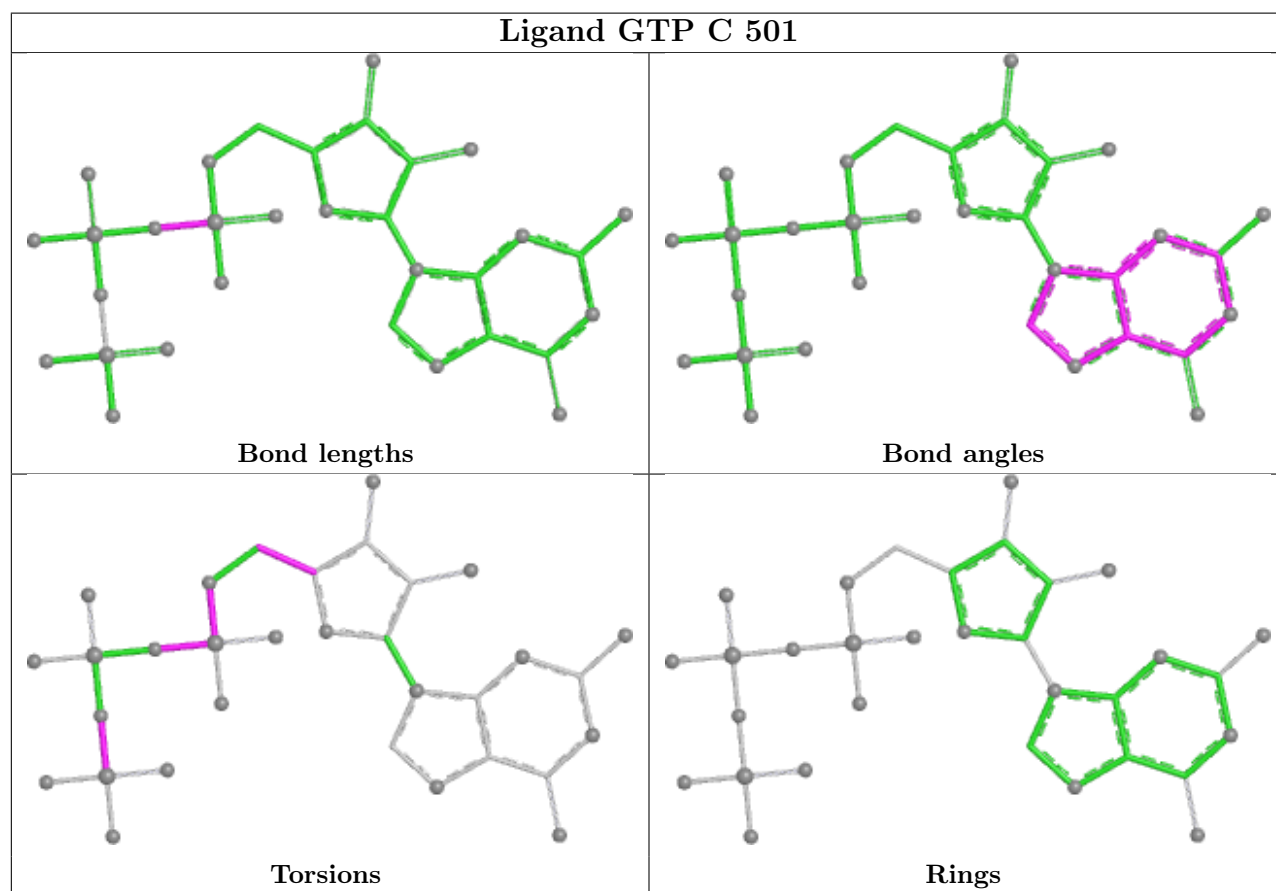
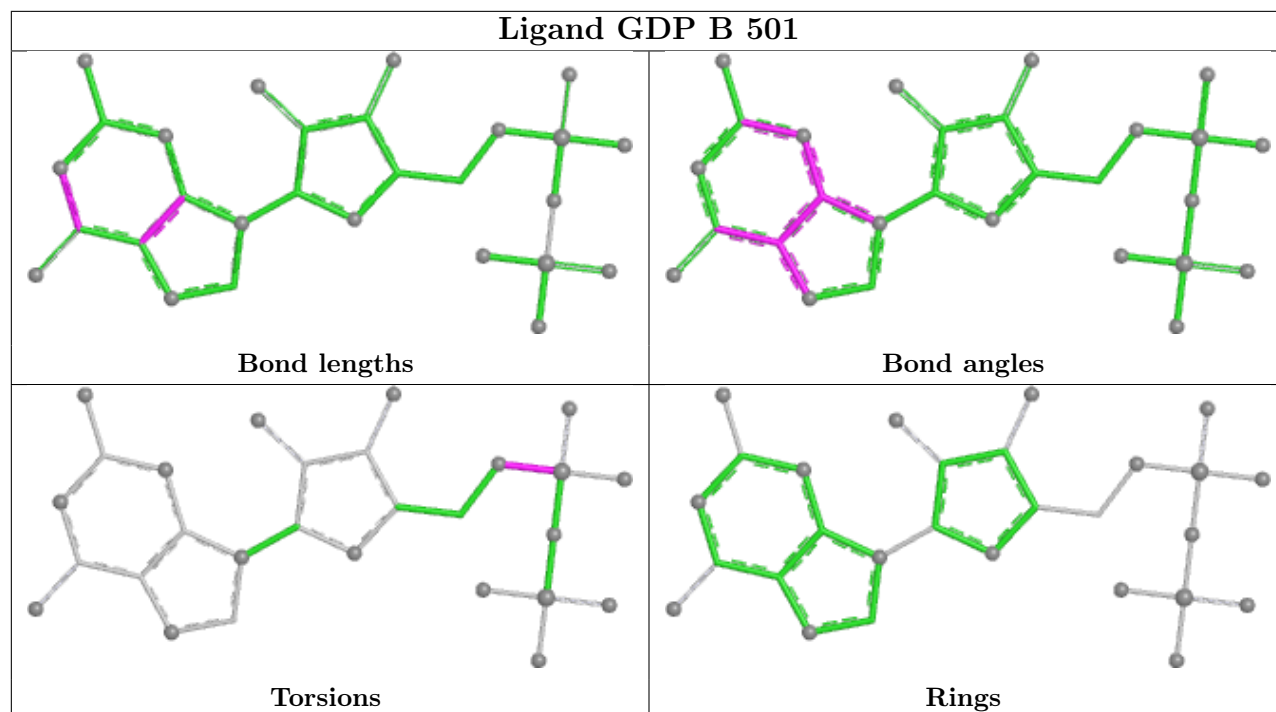
Mol	Chain	Res	Type	Atoms
10	B	505	Y5J	C17-C14-O15-C16
10	B	505	Y5J	C13-C14-O15-C16
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O2B
5	C	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3A-PA-O2A

There are no ring outliers.

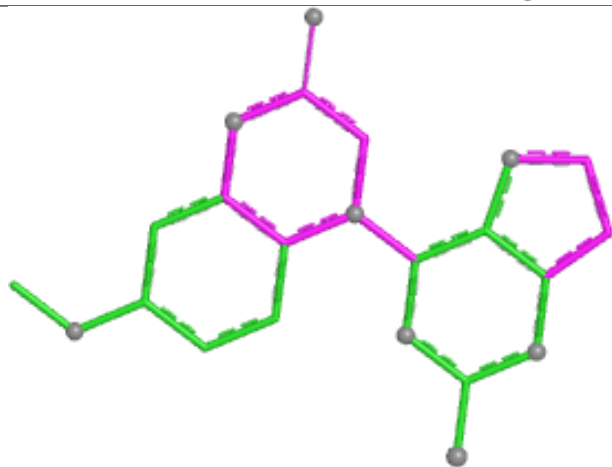
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	GDP	2	0
9	B	503	MES	3	0

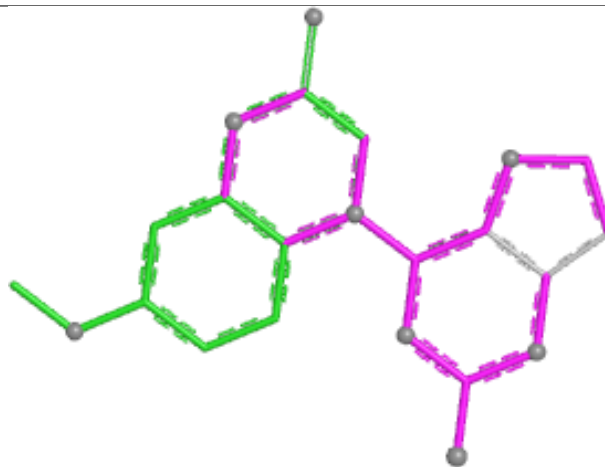
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



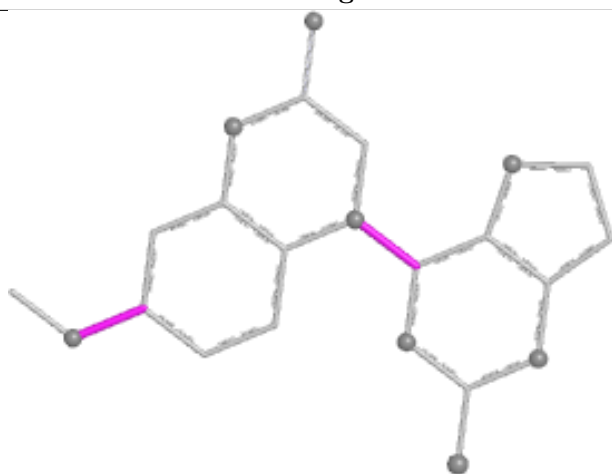
Ligand Y5J B 505



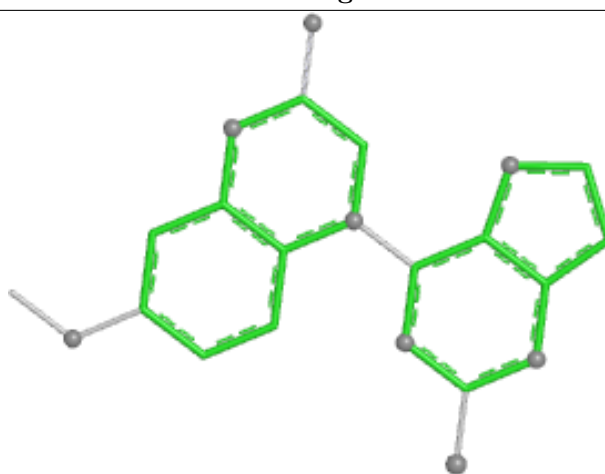
Bond lengths



Bond angles

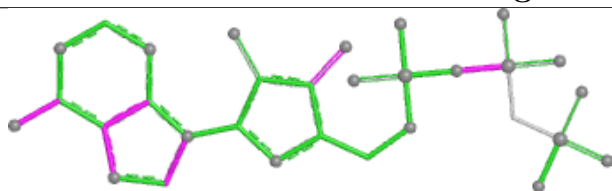


Torsions

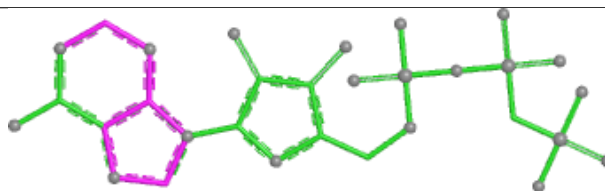


Rings

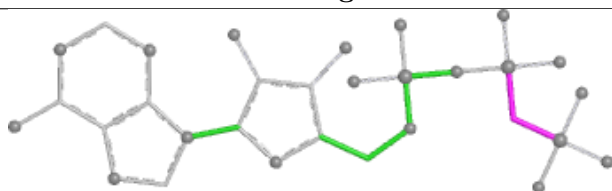
Ligand ACP F 401



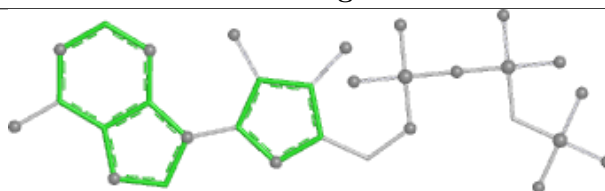
Bond lengths



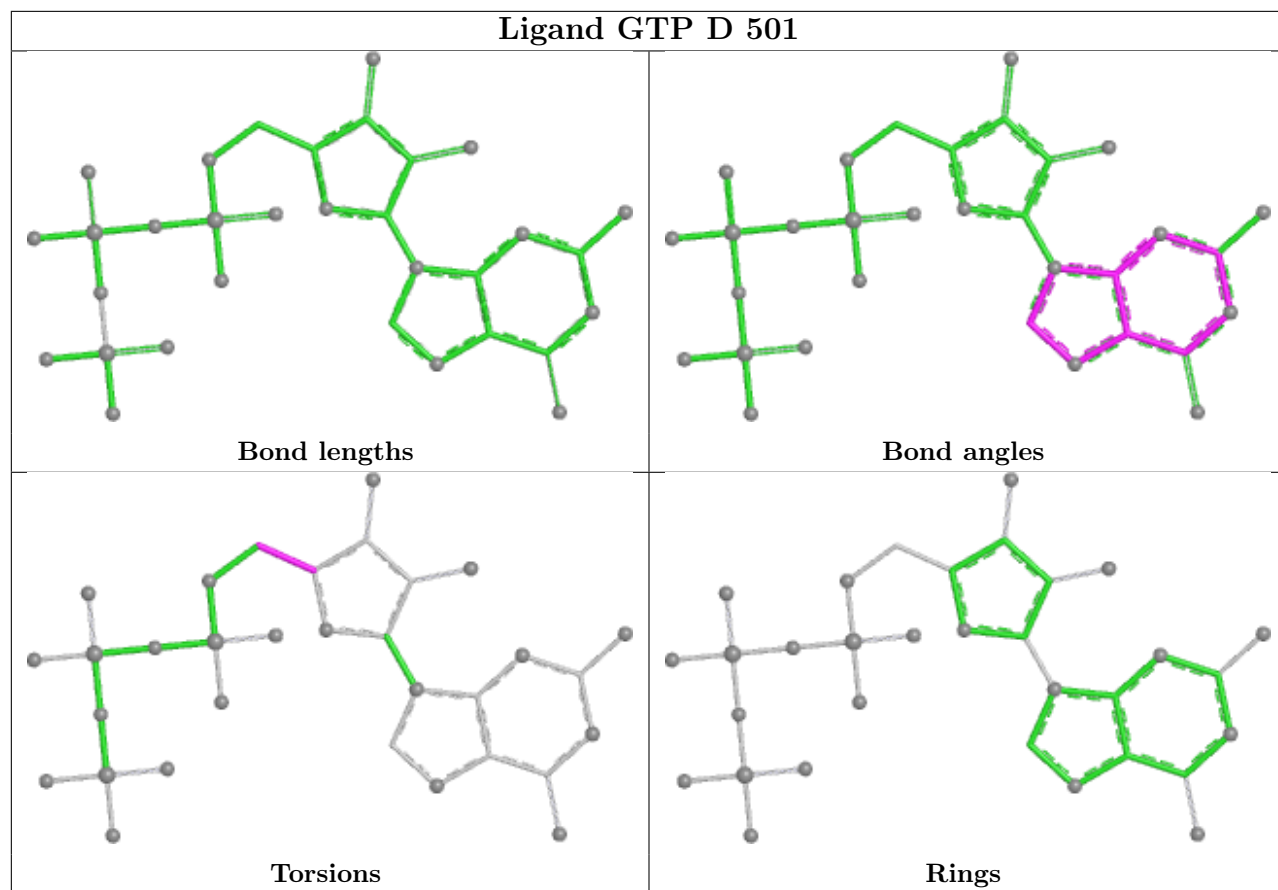
Bond angles



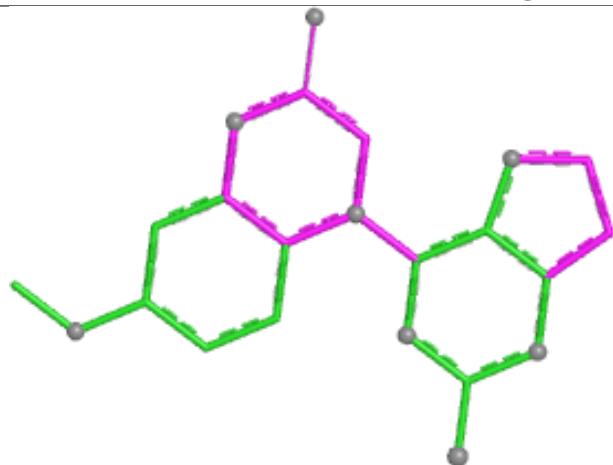
Torsions



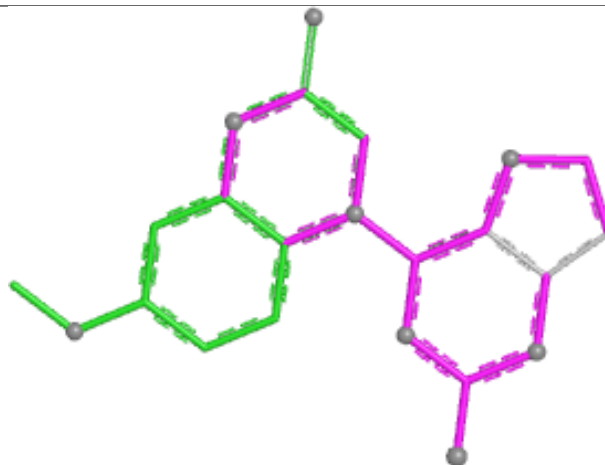
Rings



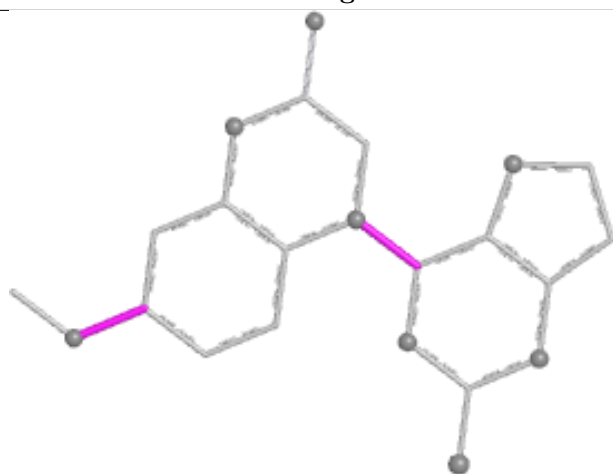
Ligand Y5J D 502



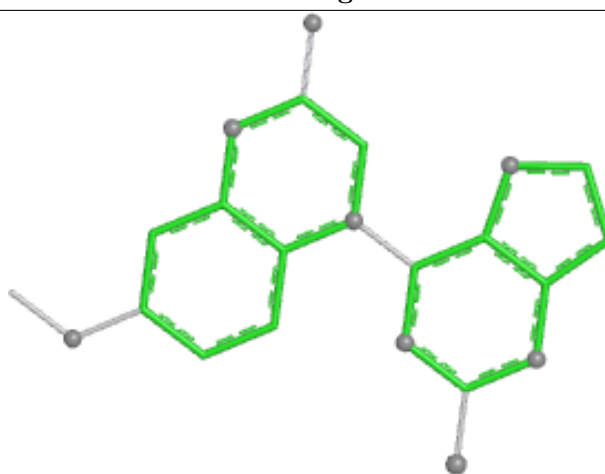
Bond lengths



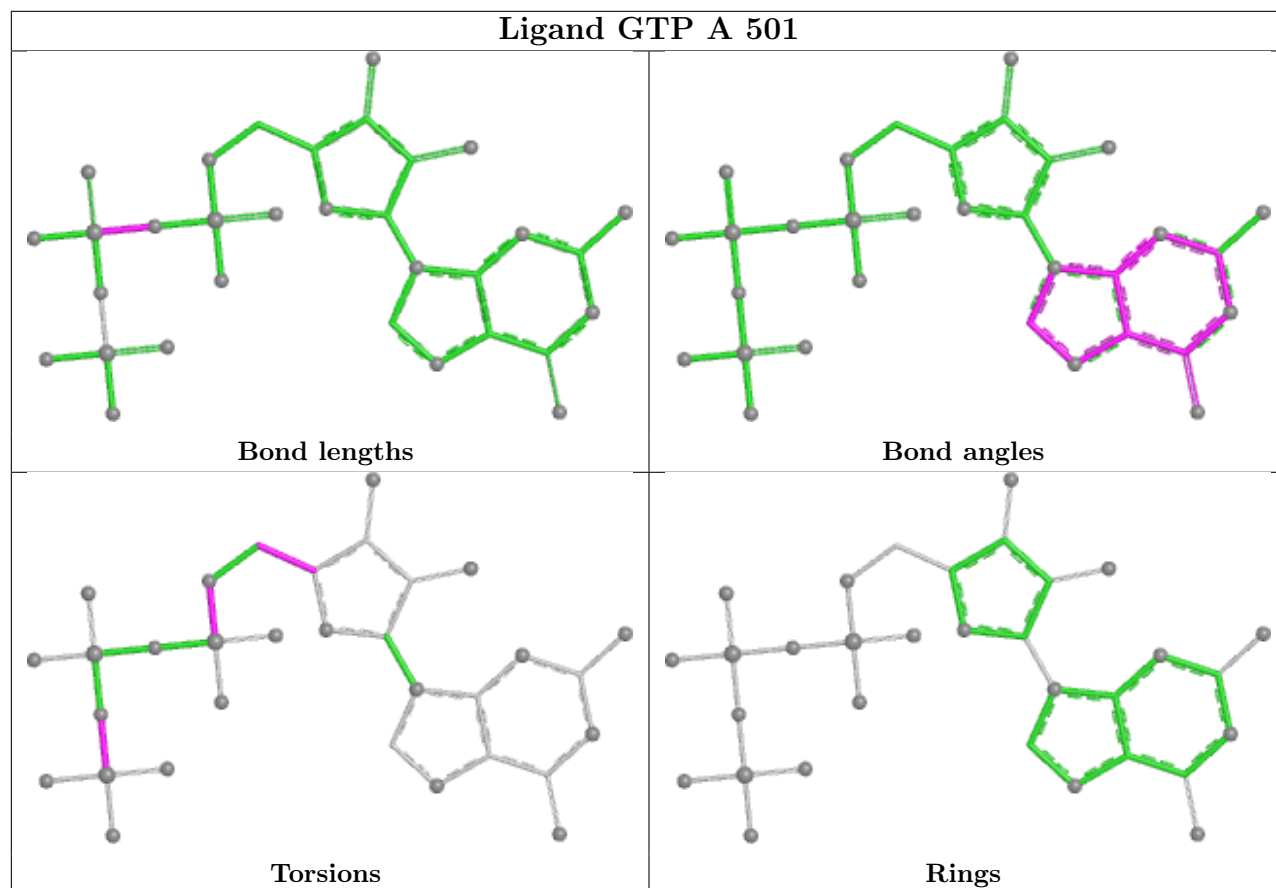
Bond angles



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	437/450 (97%)	-0.40	1 (0%) 91 89	24, 41, 74, 90	0
1	C	440/450 (97%)	-0.56	3 (0%) 84 79	18, 32, 62, 89	0
2	B	427/445 (95%)	-0.36	5 (1%) 76 69	19, 40, 84, 152	0
2	D	421/445 (94%)	0.01	6 (1%) 73 65	29, 61, 104, 133	0
3	E	121/143 (84%)	0.02	2 (1%) 69 61	33, 59, 102, 116	0
4	F	328/384 (85%)	0.25	20 (6%) 27 21	34, 69, 134, 146	0
All	All	2174/2317 (93%)	-0.22	37 (1%) 69 61	18, 47, 102, 152	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	5.4
2	D	1	MET	4.1
4	F	165	GLU	4.0
4	F	150	LYS	3.7
4	F	171	ASP	3.7
4	F	167	SER	3.6
1	C	440	VAL	3.5
4	F	175	GLU	3.5
2	D	247	ASN	3.4
2	D	219	THR	3.0
4	F	379	HIS	2.9
2	D	55	THR	2.8
4	F	134	ALA	2.8
4	F	102	PRO	2.7
4	F	90	SER	2.7
2	D	245	GLN	2.7
2	B	278	SER	2.6
4	F	247	LYS	2.6
2	D	95	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	245	ASP	2.5
4	F	186	LEU	2.5
4	F	173	ILE	2.4
1	C	1	MET	2.4
4	F	130	VAL	2.4
2	B	428	ALA	2.4
1	A	262	TYR	2.4
4	F	233	PHE	2.3
4	F	373	SER	2.3
4	F	128	ARG	2.2
4	F	179	VAL	2.2
4	F	237	THR	2.2
4	F	234	GLN	2.2
2	B	72	THR	2.2
2	B	323	MET	2.2
2	B	42	LEU	2.2
3	E	28	SER	2.2
3	E	6	MET	2.1

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
7	MG	F	402	1/1	0.64	0.12	101,101,101,101	0
11	ACP	F	401	31/31	0.86	0.11	61,85,116,121	0
7	MG	D	503	1/1	0.87	0.08	61,61,61,61	0
9	MES	B	503	12/12	0.92	0.13	53,69,80,81	0
5	GTP	D	501	32/32	0.93	0.09	44,56,106,109	0

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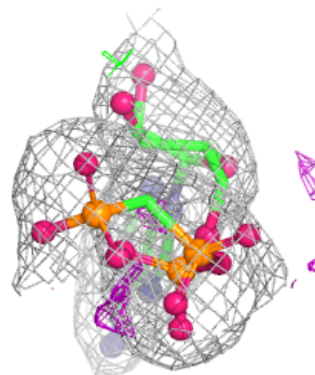
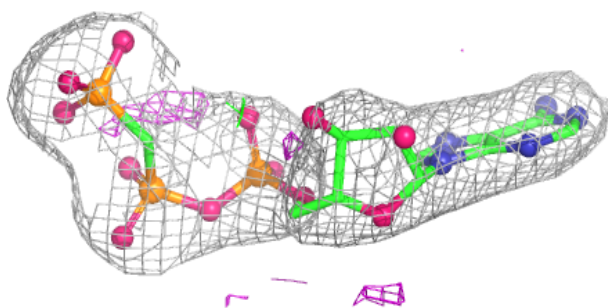
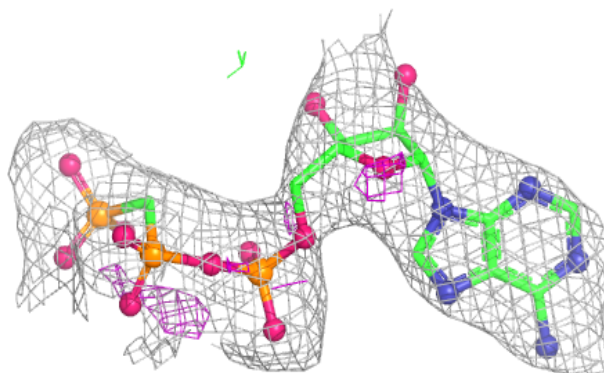
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	CA	A	502	1/1	0.94	0.07	65,65,65,65	0
9	MES	B	502	12/12	0.94	0.10	41,53,73,86	0
10	Y5J	D	502	23/23	0.95	0.09	32,38,57,78	0
10	Y5J	B	505	23/23	0.97	0.07	19,26,39,56	0
6	CA	C	502	1/1	0.98	0.04	43,43,43,43	0
7	MG	C	503	1/1	0.98	0.04	32,32,32,32	0
5	GTP	A	501	32/32	0.98	0.06	16,25,36,38	0
5	GTP	C	501	32/32	0.98	0.06	13,24,30,36	0
8	GDP	B	501	28/28	0.98	0.06	11,28,37,43	0
7	MG	A	503	1/1	0.99	0.04	32,32,32,32	0
7	MG	B	504	1/1	1.00	0.02	37,37,37,37	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.

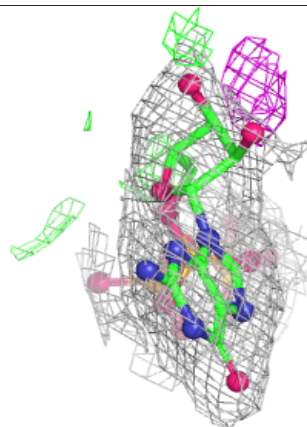
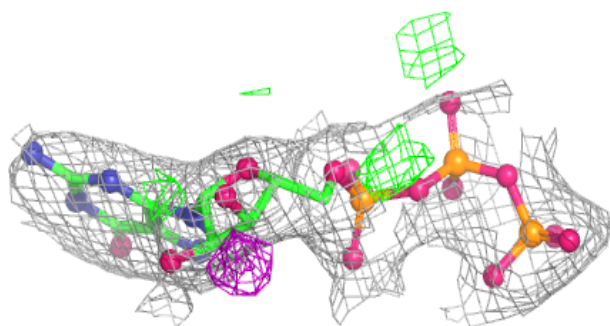
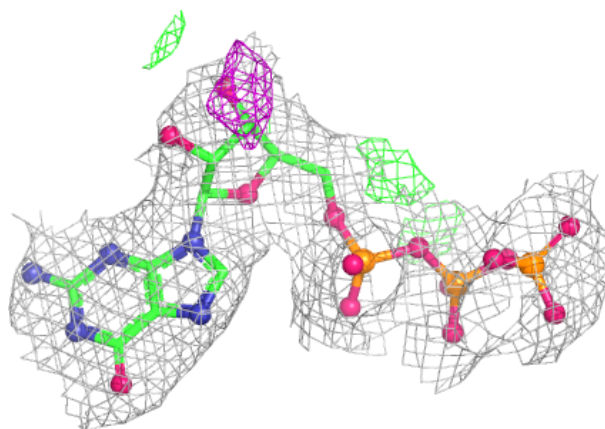
Electron density around ACP F 401:

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

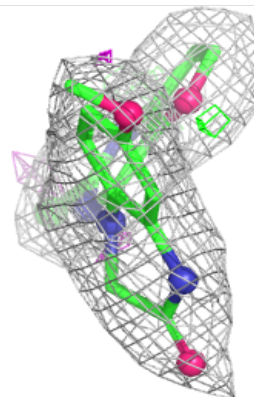
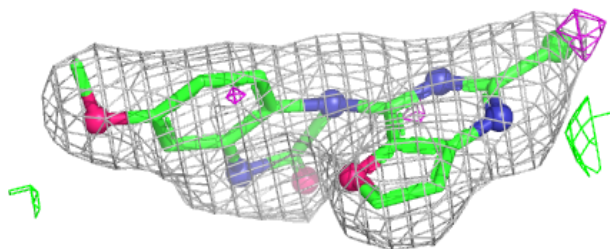
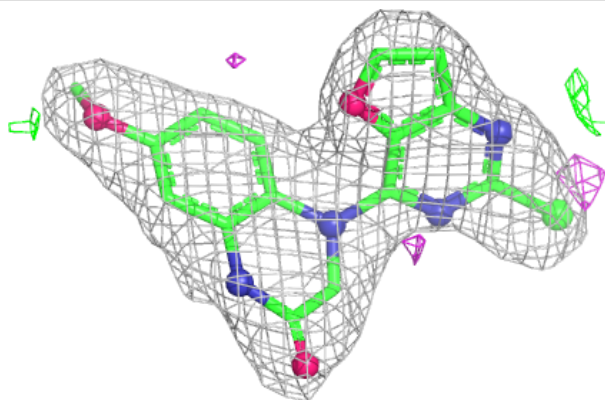


Electron density around GTP D 501:

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

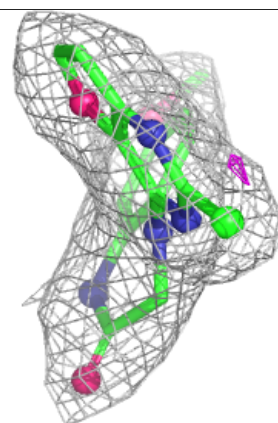
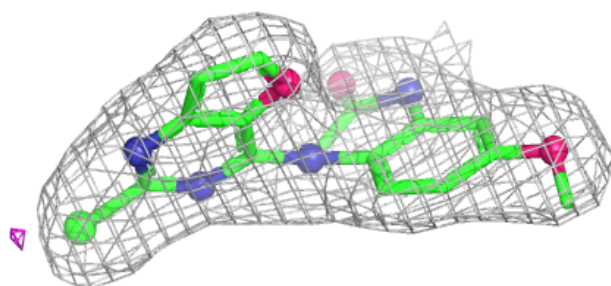
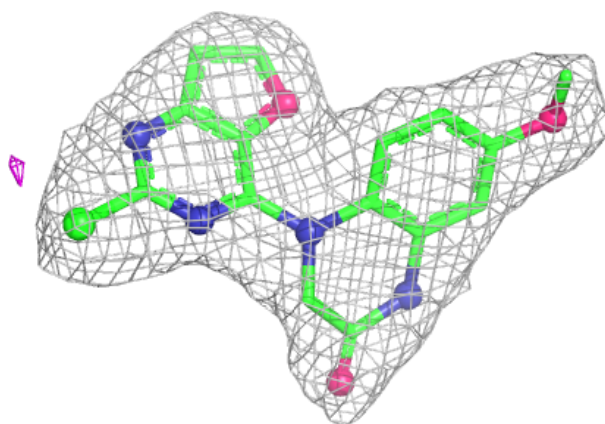
**Electron density around Y5J D 502:**

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

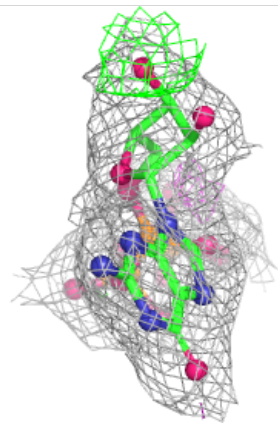
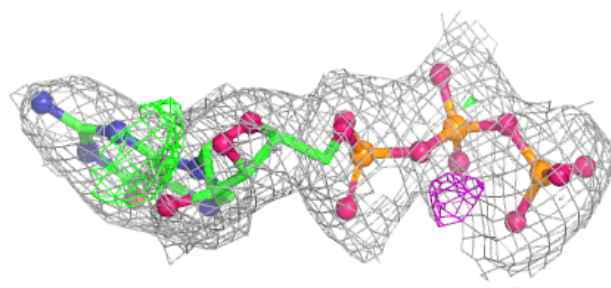
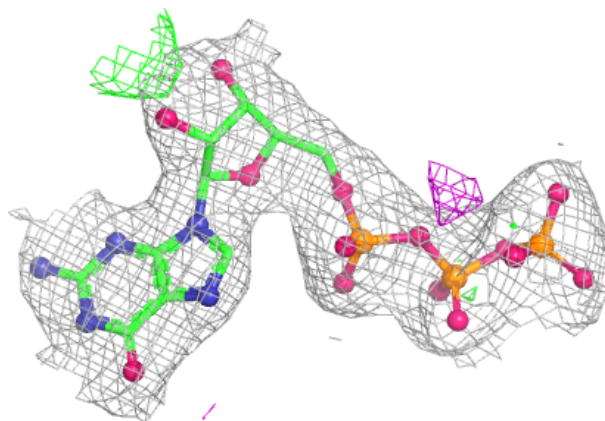


Electron density around Y5J B 505:

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

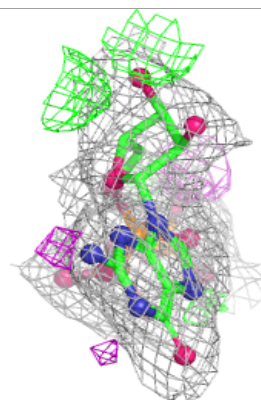
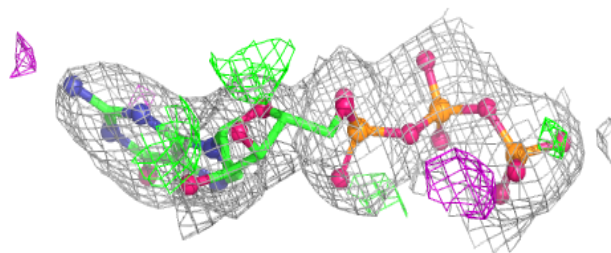
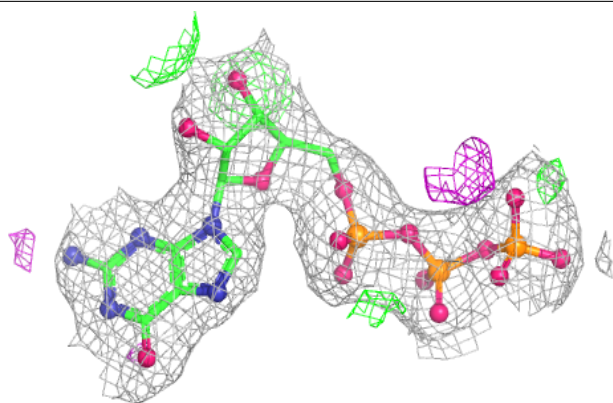
**Electron density around GTP A 501:**

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



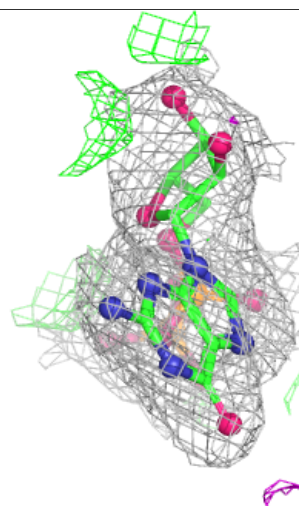
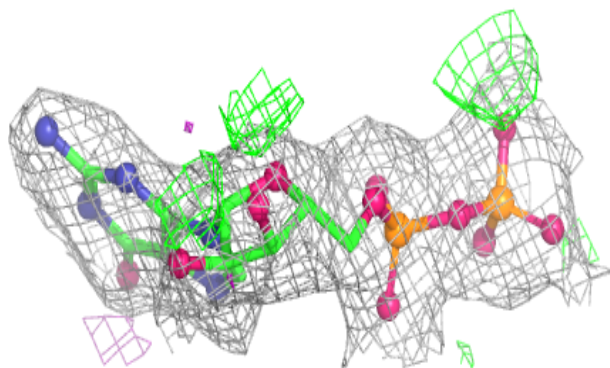
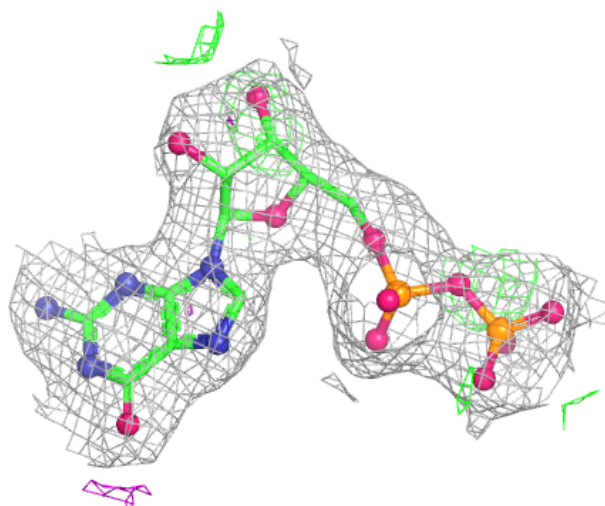
Electron density around GTP C 501:

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



Electron density around GDP B 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.