



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2021 – 03:09 PM EDT

PDB ID : 6X1F
Title : Tubulin-RB3_SLD-TTL in complex with compound 5m
Authors : White, S.W.; Yun, M.
Deposited on : 2020-05-18
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
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) : 2.23.1

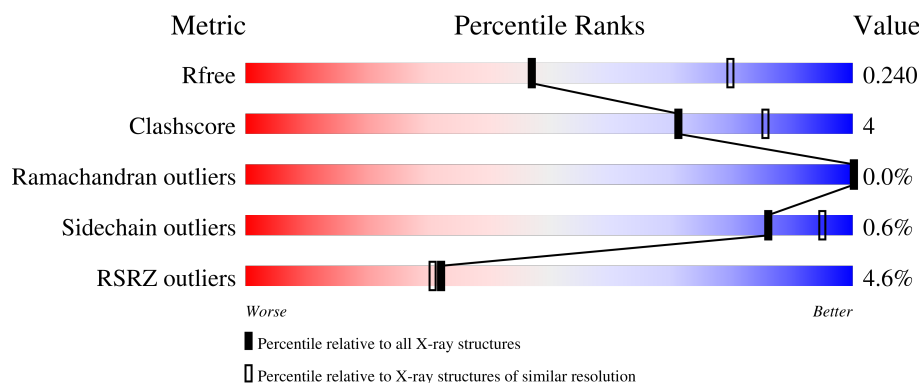
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





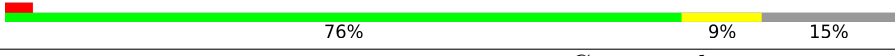
The reported resolution of this entry is 2.70 Å.

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div></div><div></div><div></div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17676 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	2	0
			3373	2119	578	650	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	1	0
			1007	622	183	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	324	Total	C	N	O	S	0	1	0
			2628	1689	451	473	15			

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 (three-letter code: 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		

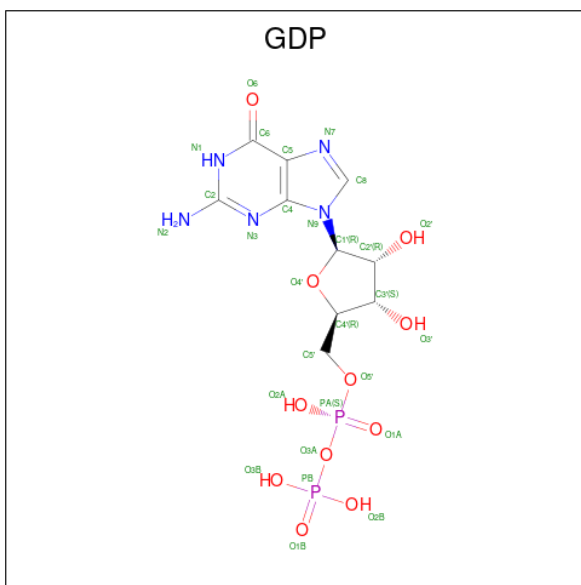
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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 (three-letter code: 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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



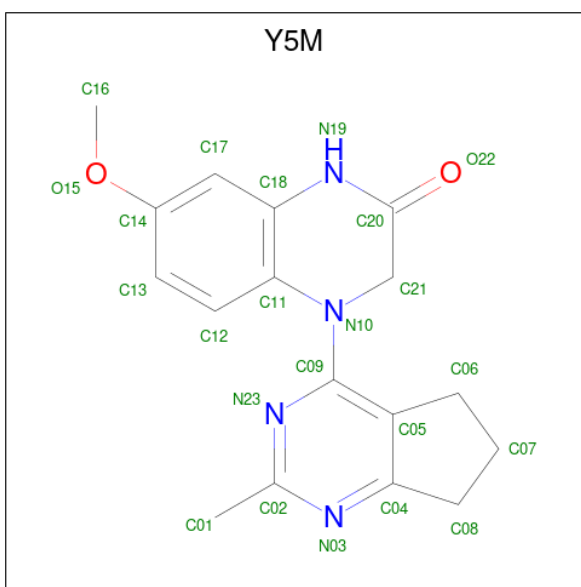
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: 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 7-methoxy-4-(2-methyl-6,7-dihydro-5H-cyclopenta[d]pyrimidin-4-yl)-3,4-dihydroquinoxalin-2(1H)-one (three-letter code: Y5M) (formula: C₁₇H₁₈N₄O₂) (labeled as "Ligand of Interest" by depositor).



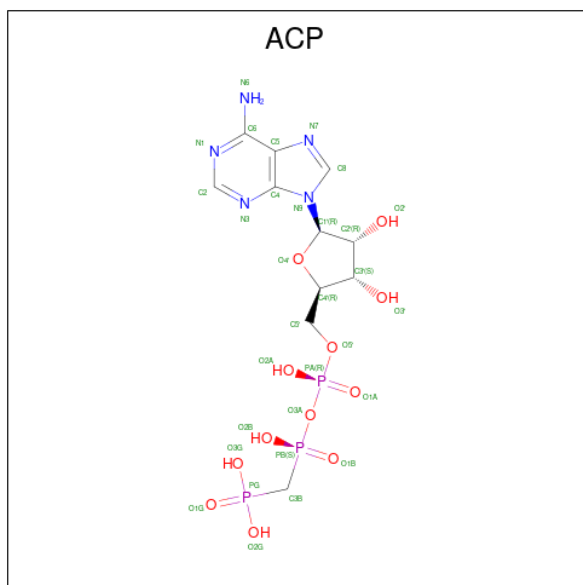
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O		0	0
			23	17	4	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			23	17	4	2		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: 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		

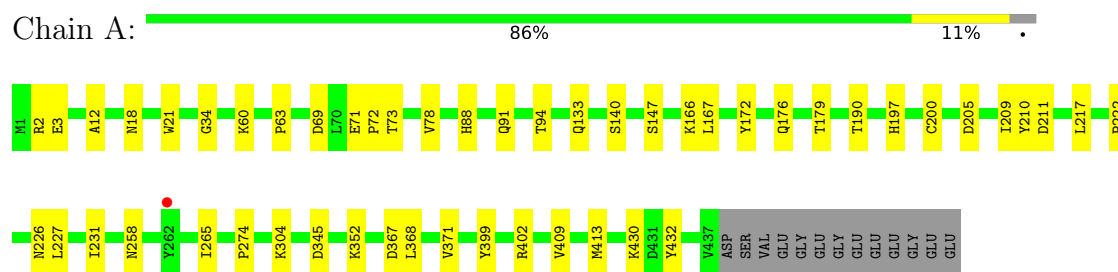
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	65	Total	O	0	0
			65	65		
12	B	63	Total	O	0	0
			63	63		
12	C	117	Total	O	0	0
			117	117		
12	D	21	Total	O	0	0
			21	21		
12	E	1	Total	O	0	0
			1	1		
12	F	13	Total	O	0	0
			13	13		

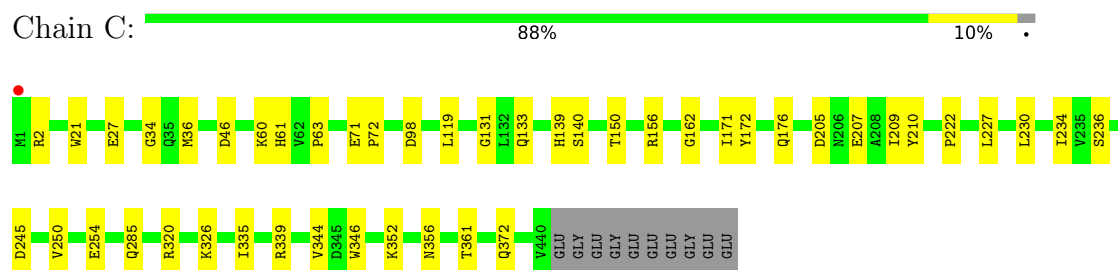
3 Residue-property plots

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.

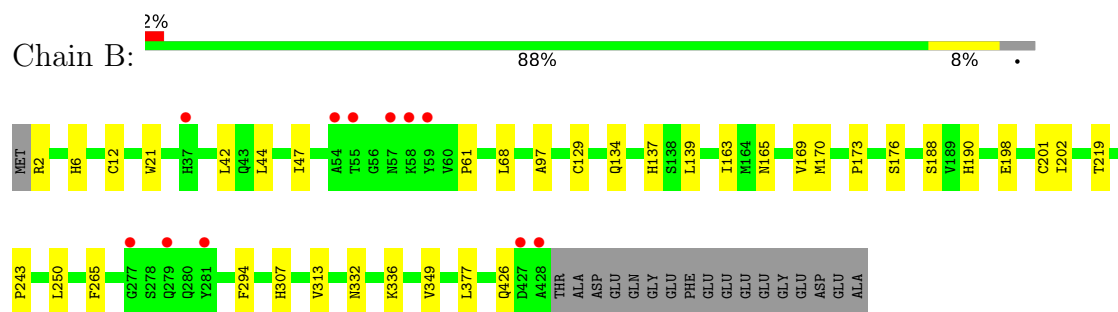
• Molecule 1: Tubulin alpha-1B chain



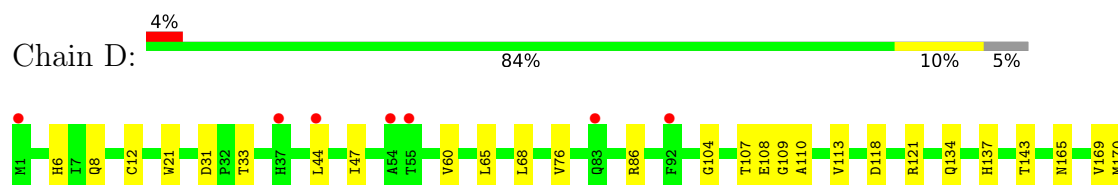
• Molecule 1: Tubulin alpha-1B chain

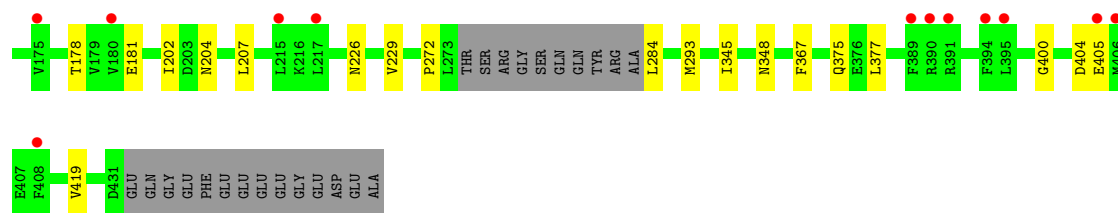


• Molecule 2: Tubulin beta-2B chain

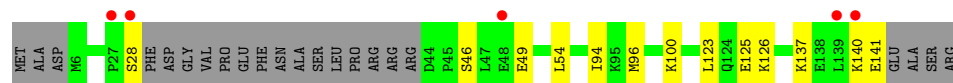
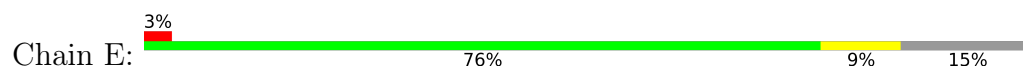


• Molecule 2: Tubulin beta-2B chain

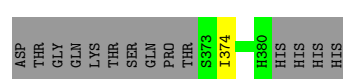
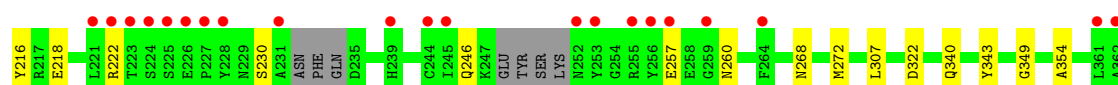
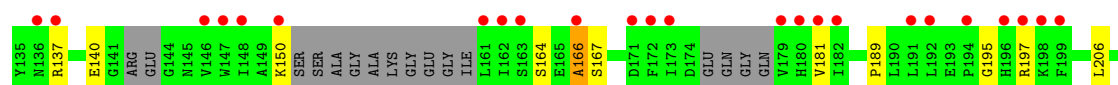
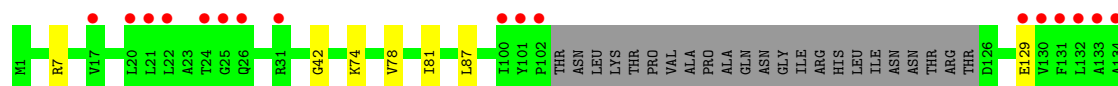
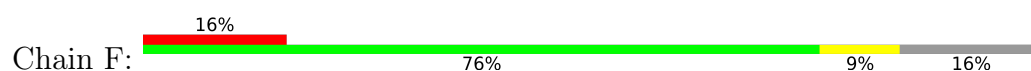




● Molecule 3: Stathmin-4



● 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	105.48Å 157.92Å 182.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.24 – 2.70 48.24 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.24-2.70) 90.7 (48.24-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.190 , 0.241 0.190 , 0.240	Depositor DCC
R_{free} test set	2000 reflections (2.47%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17676	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ACP, GTP, GDP, CA, Y5M, MES

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	0.24	0/3494	0.41	0/4743
1	C	0.25	0/3515	0.42	0/4772
2	B	0.25	0/3454	0.42	0/4677
2	D	0.24	0/3378	0.42	0/4577
3	E	0.23	0/1019	0.36	0/1352
4	F	0.25	0/2688	0.41	0/3629
All	All	0.25	0/17548	0.41	0/23750

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	28	0
1	C	3437	0	3348	26	0
2	B	3373	0	3259	20	0
2	D	3305	0	3179	25	0
3	E	1007	0	1025	8	0
4	F	2628	0	2572	16	0
5	A	32	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	32	0	12	2	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
8	B	28	0	12	1	0
9	B	24	0	24	2	0
10	B	23	0	0	1	0
10	D	23	0	0	0	0
11	F	31	0	13	0	0
12	A	65	0	0	0	0
12	B	63	0	0	0	0
12	C	117	0	0	0	0
12	D	21	0	0	0	0
12	E	1	0	0	0	0
12	F	13	0	0	0	0
All	All	17676	0	16798	120	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 4.

All (120) 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:D:60:VAL:HG11	2:D:86:ARG:HG3	1.66	0.76
2:D:400:GLY:HA2	3:E:140:LYS:HE2	1.73	0.71
2:D:375:GLN:HB2	2:D:419:VAL:HG13	1.75	0.69
2:B:173:PRO:HA	2:B:176:SER:HB2	1.77	0.66
2:B:170:MET:HG3	2:B:377:LEU:HD21	1.83	0.61
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.84	0.59
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.84	0.58
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.21	0.58
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.85	0.57
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.87	0.56
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.88	0.56
1:A:345:ASP:HB3	3:E:28:SER:HB3	1.88	0.55
1:C:2:ARG:HD2	1:C:133:GLN:HB2	1.90	0.54
2:D:404:ASP:OD1	2:D:405:GLU:N	2.42	0.53
1:A:88:HIS:O	1:A:91:GLN:HG2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:THR:HG21	1:C:326:LYS:HA	1.91	0.53
2:B:332:ASN:O	2:B:336:LYS:HB3	2.10	0.52
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.92	0.51
2:D:202:ILE:HD13	2:D:229:VAL:HG13	1.90	0.51
2:D:68:LEU:H	2:D:143:THR:HG21	1.75	0.51
2:B:165:ASN:HD22	2:B:198:GLU:HB2	1.74	0.51
2:B:134:GLN:HA	2:B:165:ASN:O	2.10	0.51
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.93	0.50
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.92	0.50
2:D:65:LEU:HD22	2:D:76:VAL:HG11	1.93	0.50
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.94	0.50
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.20	0.50
2:D:107:THR:OG1	2:D:108:GLU:N	2.44	0.50
4:F:164:SER:O	4:F:166:ALA:N	2.45	0.50
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.77	0.49
1:C:46:ASP:OD1	1:C:46:ASP:N	2.44	0.49
2:D:272:PRO:HB3	2:D:284:LEU:HD11	1.94	0.49
2:D:6:HIS:HE2	2:D:8:GLN:HG2	1.76	0.49
2:D:226:ASN:OD1	5:D:501:GTP:N1	2.32	0.49
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.46	0.49
1:A:399:TYR:O	1:A:402:ARG:NH1	2.45	0.48
1:C:176:GLN:HE22	1:C:207:GLU:HG3	1.78	0.48
1:C:320:ARG:HA	1:C:356:ASN:O	2.12	0.48
4:F:189:PRO:HA	4:F:322:ASP:HA	1.95	0.48
4:F:268:ASN:O	4:F:272:MET:HG3	2.13	0.48
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.94	0.48
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.96	0.47
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.49	0.47
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.54	0.47
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.96	0.47
2:B:42:LEU:HD22	2:B:243:PRO:HG2	1.95	0.47
1:A:147:SER:HB2	1:A:190:THR:HB	1.97	0.47
4:F:7:ARG:HB2	4:F:42:GLY:HA2	1.96	0.47
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.50	0.47
2:D:204:ASN:HA	2:D:207:LEU:HD12	1.97	0.46
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.50	0.46
2:B:2:ARG:HA	2:B:129:CYS:O	2.14	0.46
1:C:230:LEU:O	1:C:234:ILE:HD12	2.16	0.46
2:D:134:GLN:HA	2:D:165:ASN:O	2.16	0.46
1:C:245:ASP:N	1:C:245:ASP:OD1	2.49	0.46
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.97	0.45
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.52	0.45
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.99	0.45
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.99	0.45
1:A:258:ASN:OD1	1:A:352:LYS:NZ	2.46	0.45
1:A:409:VAL:HA	1:A:413:MET:O	2.17	0.45
2:B:307:HIS:O	2:B:426:GLN:NE2	2.49	0.45
1:A:209:ILE:HD12	1:A:227:LEU:HB3	1.98	0.45
3:E:137:LYS:O	3:E:141:GLU:HG2	2.17	0.45
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.48	0.45
1:A:274:PRO:HG2	1:A:371:VAL:HG11	1.98	0.44
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.00	0.44
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.99	0.44
3:E:123:LEU:HD23	3:E:126:LYS:HD3	2.00	0.44
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.34	0.44
4:F:206:LEU:HD21	4:F:354:ALA:HB2	1.99	0.44
2:B:313:VAL:HB	2:B:349:VAL:HG22	1.99	0.44
1:C:2:ARG:HA	1:C:131:GLY:O	2.17	0.44
4:F:74:LYS:HE3	4:F:150:LYS:HD2	2.00	0.44
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.51	0.43
2:B:68:LEU:HD12	2:B:97:ALA:HB2	2.00	0.43
4:F:78:VAL:HG21	4:F:181:VAL:HG11	2.00	0.43
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.37	0.43
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.53	0.43
1:A:69:ASP:O	1:A:94:THR:HA	2.18	0.43
1:A:430:LYS:HA	1:A:430:LYS:HD2	1.79	0.43
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.83	0.43
2:D:31:ASP:OD1	2:D:33:THR:OG1	2.28	0.43
1:A:2:ARG:HB3	1:A:133:GLN:HG2	2.01	0.43
1:C:285:GLN:NE2	1:C:372:GLN:OE1	2.52	0.43
4:F:195:GLY:HA3	4:F:197:ARG:HD2	2.00	0.42
2:D:12:CYS:HB2	5:D:501:GTP:C8	2.55	0.42
3:E:46:SER:HB3	3:E:49:GLU:HG3	2.01	0.42
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.54	0.42
2:D:104:GLY:O	2:D:109:GLY:HA3	2.19	0.42
2:B:139:LEU:HD22	2:B:188:SER:HB3	2.02	0.42
9:B:503:MES:H51	9:B:503:MES:H81	1.85	0.42
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.55	0.42
2:D:44:LEU:HA	2:D:47:ILE:HB	2.01	0.42
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.84	0.42
1:C:140:SER:HA	1:C:171:ILE:HB	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:ALA:O	2:D:113:VAL:HG12	2.20	0.41
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.55	0.41
1:A:179:THR:O	10:B:505:Y5M:N19	2.53	0.41
2:D:118:ASP:OD1	2:D:121:ARG:NH1	2.51	0.41
2:B:44:LEU:HA	2:B:47:ILE:HB	2.01	0.41
2:B:294:PHE:O	9:B:503:MES:H82	2.20	0.41
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.56	0.41
2:D:293:MET:CG	2:D:367:PHE:HB2	2.51	0.41
2:D:169:VAL:HA	2:D:202:ILE:O	2.21	0.41
4:F:81:ILE:HA	4:F:87:LEU:HD12	2.02	0.41
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.55	0.41
1:A:166:LYS:HE2	1:A:197:HIS:O	2.21	0.41
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.56	0.41
2:D:178:THR:O	2:D:181:GLU:HG3	2.20	0.41
1:A:3:GLU:O	1:A:133:GLN:HG3	2.21	0.41
1:A:209:ILE:HD13	1:A:231:ILE:HD11	2.02	0.41
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.57	0.40
1:A:34:GLY:HA3	1:A:60:LYS:HG3	2.04	0.40
2:B:169:VAL:HA	2:B:202:ILE:O	2.21	0.40
1:C:27:GLU:OE1	1:C:236:SER:OG	2.23	0.40
1:C:209:ILE:HG22	1:C:227:LEU:HD22	2.03	0.40
3:E:96:MET:O	3:E:100:LYS:HB2	2.21	0.40
3:E:54:LEU:HD23	3:E:54:LEU:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/450 (97%)	426 (98%)	9 (2%)	0	100	100
1	C	438/450 (97%)	426 (97%)	12 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	427/445 (96%)	419 (98%)	8 (2%)	0	100	100
2	D	417/445 (94%)	407 (98%)	10 (2%)	0	100	100
3	E	118/143 (82%)	118 (100%)	0	0	100	100
4	F	309/384 (80%)	301 (97%)	7 (2%)	1 (0%)	41	66
All	All	2144/2317 (92%)	2097 (98%)	46 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	166	ALA

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%)	367 (100%)	1 (0%)	92	98
1	C	371/378 (98%)	370 (100%)	1 (0%)	92	98
2	B	371/383 (97%)	369 (100%)	2 (0%)	88	96
2	D	362/383 (94%)	361 (100%)	1 (0%)	92	98
3	E	110/127 (87%)	109 (99%)	1 (1%)	78	92
4	F	283/342 (83%)	277 (98%)	6 (2%)	53	80
All	All	1865/1991 (94%)	1853 (99%)	12 (1%)	86	95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
2	B	137	HIS
2	B	190	HIS
1	C	361	THR
2	D	137	HIS
3	E	125	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	F	129	GLU
4	F	137	ARG
4	F	140	GLU
4	F	167	SER
4	F	222	ARG
4	F	230	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	18	ASN
1	A	176	GLN
2	B	165	ASN
1	C	31	GLN
1	C	285	GLN
1	C	406	HIS
2	D	8	GLN
2	D	99	ASN
2	D	291	GLN
3	E	91	ASN
3	E	124	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 5 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
5	GTP	D	501	-	26,34,34	0.99	1 (3%)	33,54,54	1.84	7 (21%)
8	GDP	B	501	7	24,30,30	1.21	2 (8%)	31,47,47	1.91	7 (22%)
10	Y5M	B	505	-	26,26,26	2.94	10 (38%)	33,38,38	2.21	11 (33%)
5	GTP	C	501	7	26,34,34	0.99	1 (3%)	33,54,54	1.76	6 (18%)
9	MES	B	502	-	12,12,12	2.27	1 (8%)	14,16,16	1.88	3 (21%)
10	Y5M	D	502	-	26,26,26	3.00	10 (38%)	33,38,38	2.13	10 (30%)
5	GTP	A	501	7	26,34,34	1.00	1 (3%)	33,54,54	1.74	6 (18%)
11	ACP	F	401	-	27,33,33	1.86	7 (25%)	32,52,52	1.38	2 (6%)
9	MES	B	503	-	12,12,12	2.32	1 (8%)	14,16,16	1.97	6 (42%)

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
5	GTP	D	501	-	-	8/18/38/38	0/3/3/3
8	GDP	B	501	7	-	3/12/32/32	0/3/3/3
10	Y5M	B	505	-	-	2/5/24/24	0/4/4/4
5	GTP	C	501	7	-	8/18/38/38	0/3/3/3
9	MES	B	502	-	-	4/6/14/14	0/1/1/1
10	Y5M	D	502	-	-	4/5/24/24	0/4/4/4
5	GTP	A	501	7	-	7/18/38/38	0/3/3/3
11	ACP	F	401	-	-	3/15/38/38	0/3/3/3
9	MES	B	503	-	-	4/6/14/14	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	Y5M	C20-N19	9.00	1.45	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	Y5M	C20-N19	8.78	1.44	1.35
9	B	503	MES	C8-S	-7.76	1.66	1.77
9	B	502	MES	C8-S	-7.59	1.66	1.77
11	F	401	ACP	PB-O3A	6.02	1.65	1.58
10	D	502	Y5M	C09-N10	5.97	1.45	1.37
10	B	505	Y5M	C09-N10	5.47	1.45	1.37
10	B	505	Y5M	C08-C04	5.18	1.54	1.50
10	D	502	Y5M	C18-N19	5.14	1.48	1.39
10	D	502	Y5M	C08-C04	5.10	1.54	1.50
10	B	505	Y5M	C18-N19	5.02	1.48	1.39
8	B	501	GDP	C6-C5	4.23	1.48	1.41
10	B	505	Y5M	C21-N10	-3.78	1.42	1.46
10	D	502	Y5M	C21-N10	-3.70	1.42	1.46
10	D	502	Y5M	C21-C20	3.52	1.55	1.51
10	B	505	Y5M	C21-C20	3.50	1.55	1.51
10	D	502	Y5M	C11-N10	3.26	1.45	1.40
5	D	501	GTP	C6-N1	3.18	1.38	1.33
5	A	501	GTP	C6-N1	3.13	1.38	1.33
11	F	401	ACP	O3'-C3'	-3.09	1.35	1.43
5	C	501	GTP	C6-N1	3.07	1.38	1.33
11	F	401	ACP	C6-N6	2.99	1.44	1.34
10	B	505	Y5M	C11-N10	2.95	1.45	1.40
11	F	401	ACP	C5-C4	-2.74	1.33	1.40
10	B	505	Y5M	C18-C11	-2.71	1.37	1.40
8	B	501	GDP	C5-C4	2.46	1.47	1.40
10	D	502	Y5M	O22-C20	-2.35	1.18	1.23
10	D	502	Y5M	C18-C11	-2.34	1.37	1.40
10	B	505	Y5M	O22-C20	-2.32	1.18	1.23
10	D	502	Y5M	C06-C05	2.32	1.55	1.51
10	B	505	Y5M	C06-C05	2.23	1.55	1.51
11	F	401	ACP	PB-O2B	-2.17	1.51	1.56
11	F	401	ACP	O4'-C4'	-2.04	1.40	1.45
11	F	401	ACP	C2-N3	2.04	1.35	1.32

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	Y5M	C07-C08-C04	6.13	108.39	103.93
10	D	502	Y5M	C07-C08-C04	5.88	108.21	103.93
5	C	501	GTP	N3-C2-N1	-5.33	120.12	127.22
5	D	501	GTP	N3-C2-N1	-5.27	120.19	127.22
5	A	501	GTP	N3-C2-N1	-5.25	120.22	127.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	N3-C2-N1	-5.24	120.49	128.68
8	B	501	GDP	C2-N3-C4	4.95	121.02	115.36
9	B	502	MES	C5-N4-C3	4.73	119.48	108.83
10	B	505	Y5M	C08-C04-N03	4.63	129.88	123.41
9	B	503	MES	C5-N4-C3	4.36	118.65	108.83
10	D	502	Y5M	C08-C04-N03	4.29	129.41	123.41
8	B	501	GDP	C6-N1-C2	4.19	122.59	115.93
5	D	501	GTP	C2-N3-C4	4.14	120.09	115.36
10	B	505	Y5M	C05-C04-N03	-4.14	121.26	125.80
8	B	501	GDP	C5-C6-N1	-4.06	117.88	123.43
5	C	501	GTP	C2-N3-C4	4.04	119.97	115.36
5	A	501	GTP	C2-N3-C4	4.00	119.93	115.36
10	D	502	Y5M	C05-C04-N03	-3.97	121.45	125.80
8	B	501	GDP	C6-C5-C4	-3.88	117.09	120.80
5	D	501	GTP	PB-O3B-PG	-3.78	119.84	132.83
10	D	502	Y5M	C18-N19-C20	-3.73	119.87	124.49
10	B	505	Y5M	C18-N19-C20	-3.72	119.89	124.49
8	B	501	GDP	N3-C2-N1	-3.43	122.64	127.22
10	D	502	Y5M	C07-C06-C05	3.28	107.85	103.52
5	C	501	GTP	PB-O3B-PG	-3.23	121.74	132.83
10	B	505	Y5M	C07-C06-C05	3.17	107.70	103.52
5	A	501	GTP	PB-O3B-PG	-3.12	122.12	132.83
10	B	505	Y5M	C08-C04-C05	-3.10	108.86	111.09
5	D	501	GTP	PA-O3A-PB	-3.08	122.27	132.83
11	F	401	ACP	C5-C6-N6	3.05	124.99	120.35
5	D	501	GTP	C5-C6-N1	-3.04	119.28	123.43
5	C	501	GTP	PA-O3A-PB	-2.86	123.00	132.83
5	A	501	GTP	C5-C6-N1	-2.86	119.52	123.43
5	C	501	GTP	C5-C6-N1	-2.85	119.54	123.43
5	A	501	GTP	PA-O3A-PB	-2.84	123.09	132.83
8	B	501	GDP	C4-C5-N7	-2.77	106.52	109.40
9	B	503	MES	C6-C5-N4	-2.77	105.91	110.10
10	D	502	Y5M	C08-C04-C05	-2.70	109.14	111.09
10	D	502	Y5M	C05-C09-N23	-2.62	118.58	122.61
8	B	501	GDP	PA-O3A-PB	-2.61	123.87	132.83
5	C	501	GTP	C6-N1-C2	2.61	120.07	115.93
5	D	501	GTP	C6-N1-C2	2.60	120.06	115.93
5	A	501	GTP	C6-N1-C2	2.54	119.97	115.93
10	B	505	Y5M	N23-C02-N03	-2.49	121.15	125.72
5	D	501	GTP	C3'-C2'-C1'	2.46	104.68	100.98
9	B	503	MES	O1S-S-C8	2.37	109.77	106.92
9	B	502	MES	O1S-S-C8	2.34	109.73	106.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	Y5M	N23-C02-N03	-2.31	121.47	125.72
9	B	502	MES	O2S-S-C8	2.29	109.67	106.92
10	B	505	Y5M	C05-C09-N23	-2.25	119.14	122.61
10	B	505	Y5M	N23-C09-N10	2.20	118.59	116.26
9	B	503	MES	O3S-S-C8	2.18	109.30	105.77
10	D	502	Y5M	C02-N23-C09	2.09	122.13	116.99
10	D	502	Y5M	C06-C05-C04	-2.07	108.52	110.96
10	B	505	Y5M	C02-N23-C09	2.04	122.01	116.99
9	B	503	MES	C7-N4-C3	2.04	116.45	111.23
10	B	505	Y5M	C16-O15-C14	-2.01	113.15	117.51
9	B	503	MES	O2S-S-C8	2.01	109.33	106.92

There are no chirality outliers.

All (43) 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-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	PB-O3B-PG-O3G
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
9	B	502	MES	C7-C8-S-O1S
9	B	502	MES	C7-C8-S-O2S
9	B	502	MES	C7-C8-S-O3S
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
9	B	503	MES	C7-C8-S-O3S
10	B	505	Y5M	N23-C09-N10-C21
10	D	502	Y5M	N23-C09-N10-C21
10	D	502	Y5M	C05-C09-N10-C21
5	D	501	GTP	O4'-C4'-C5'-O5'
5	D	501	GTP	C3'-C4'-C5'-O5'
10	B	505	Y5M	C05-C09-N10-C21
10	D	502	Y5M	C13-C14-O15-C16

Continued on next page...

Continued from previous page...

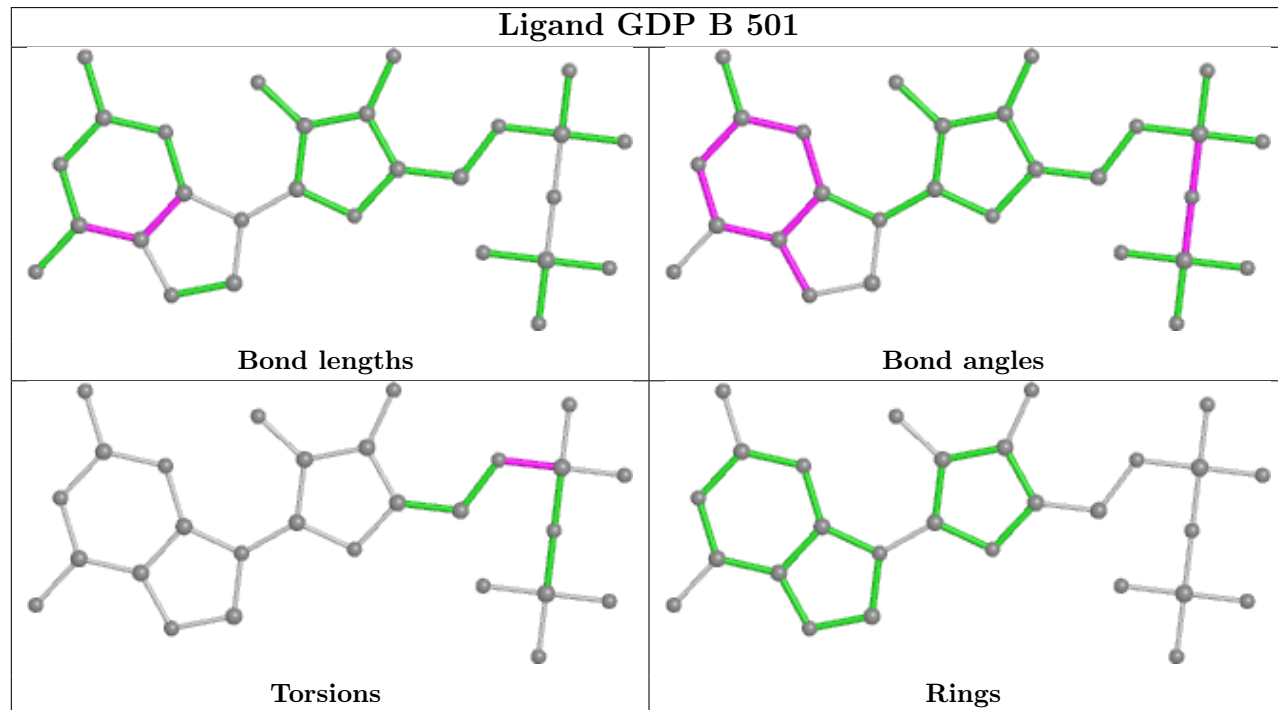
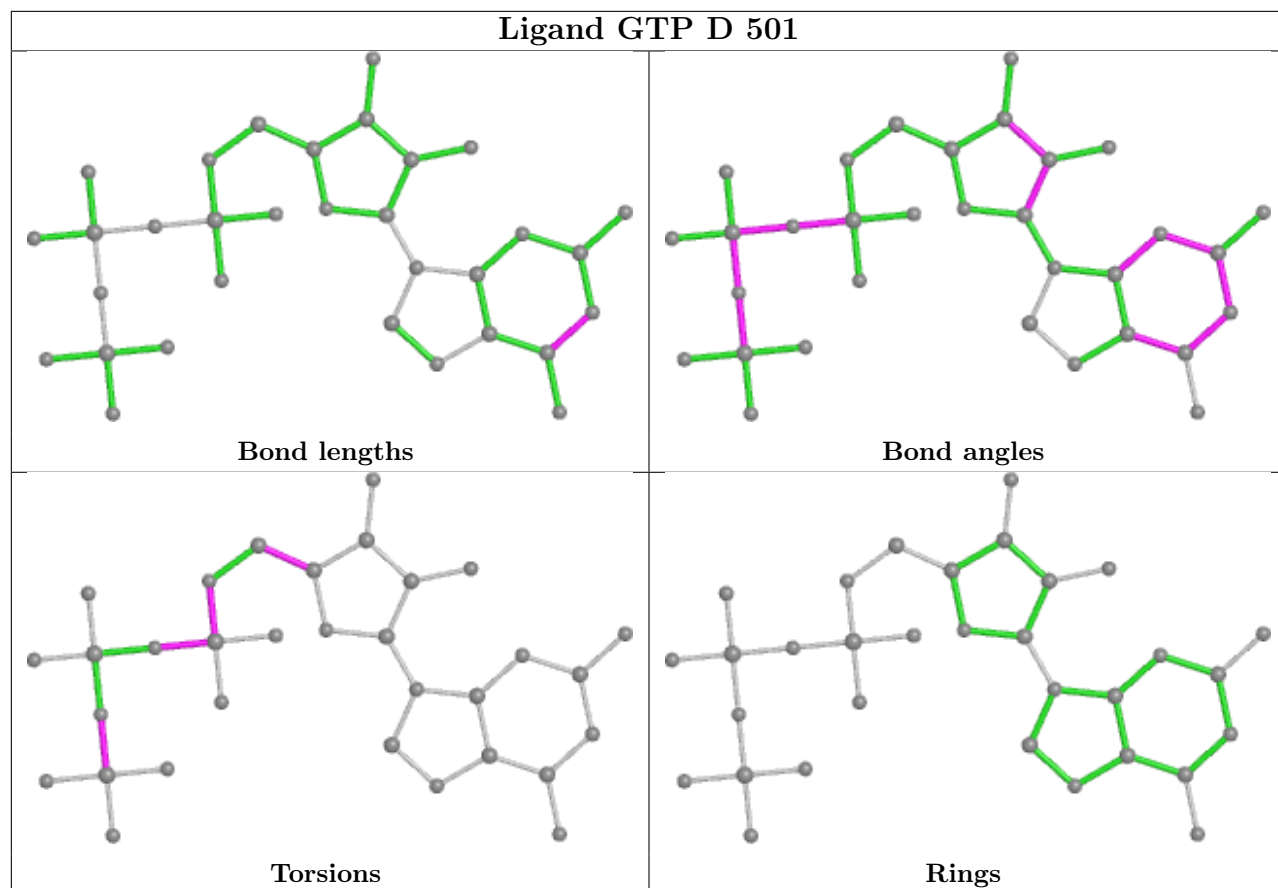
Mol	Chain	Res	Type	Atoms
10	D	502	Y5M	C17-C14-O15-C16
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
9	B	502	MES	C8-C7-N4-C3
9	B	503	MES	C8-C7-N4-C3
5	D	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
8	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA

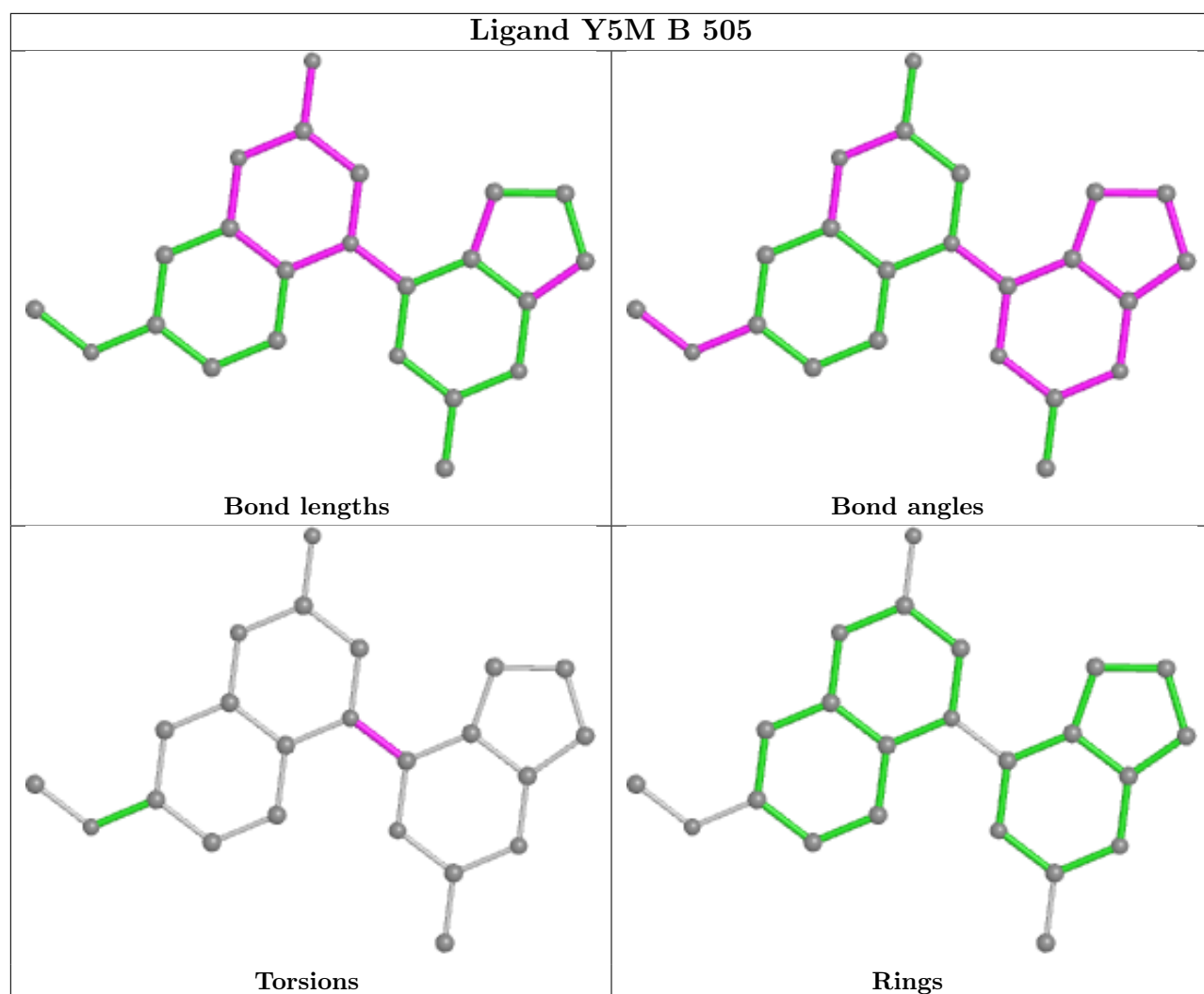
There are no ring outliers.

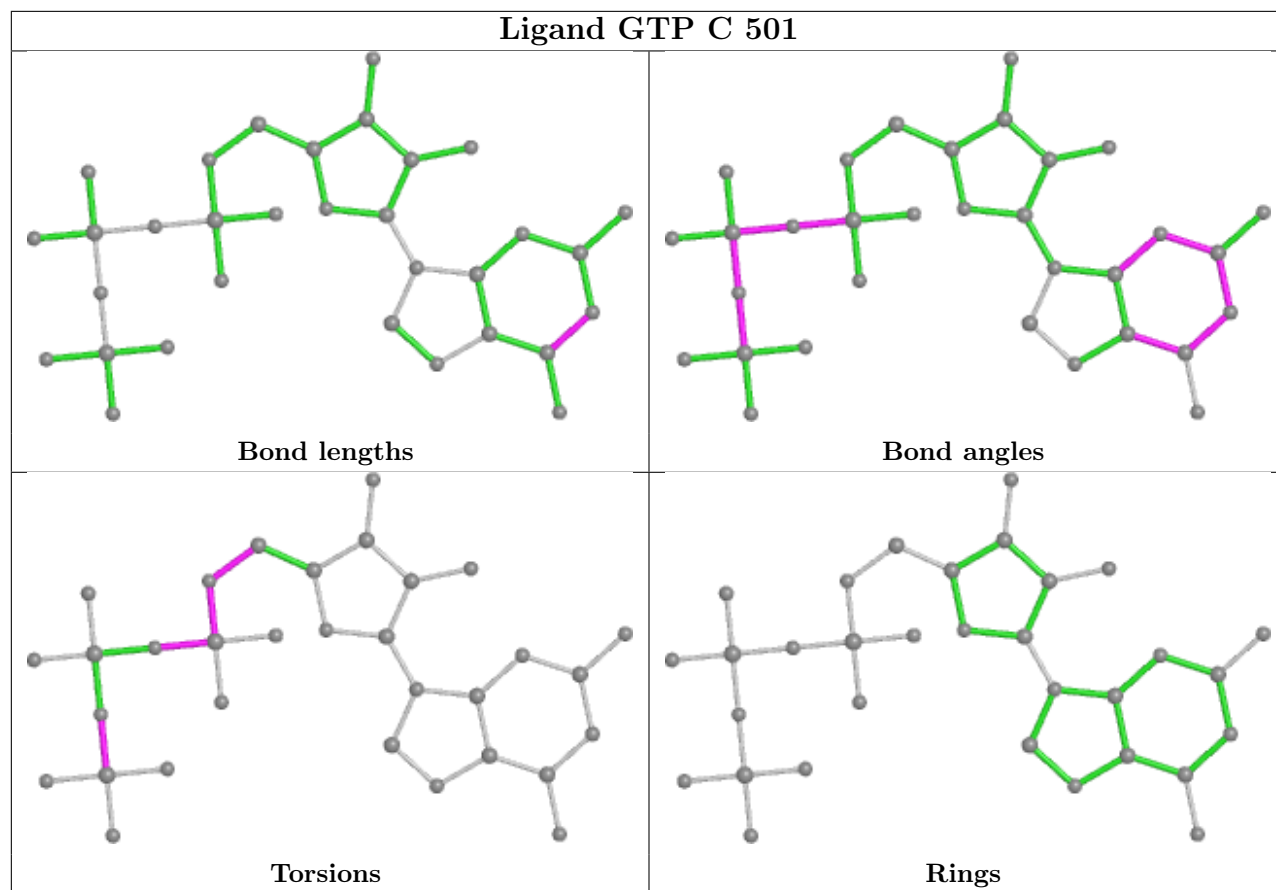
4 monomers are involved in 6 short contacts:

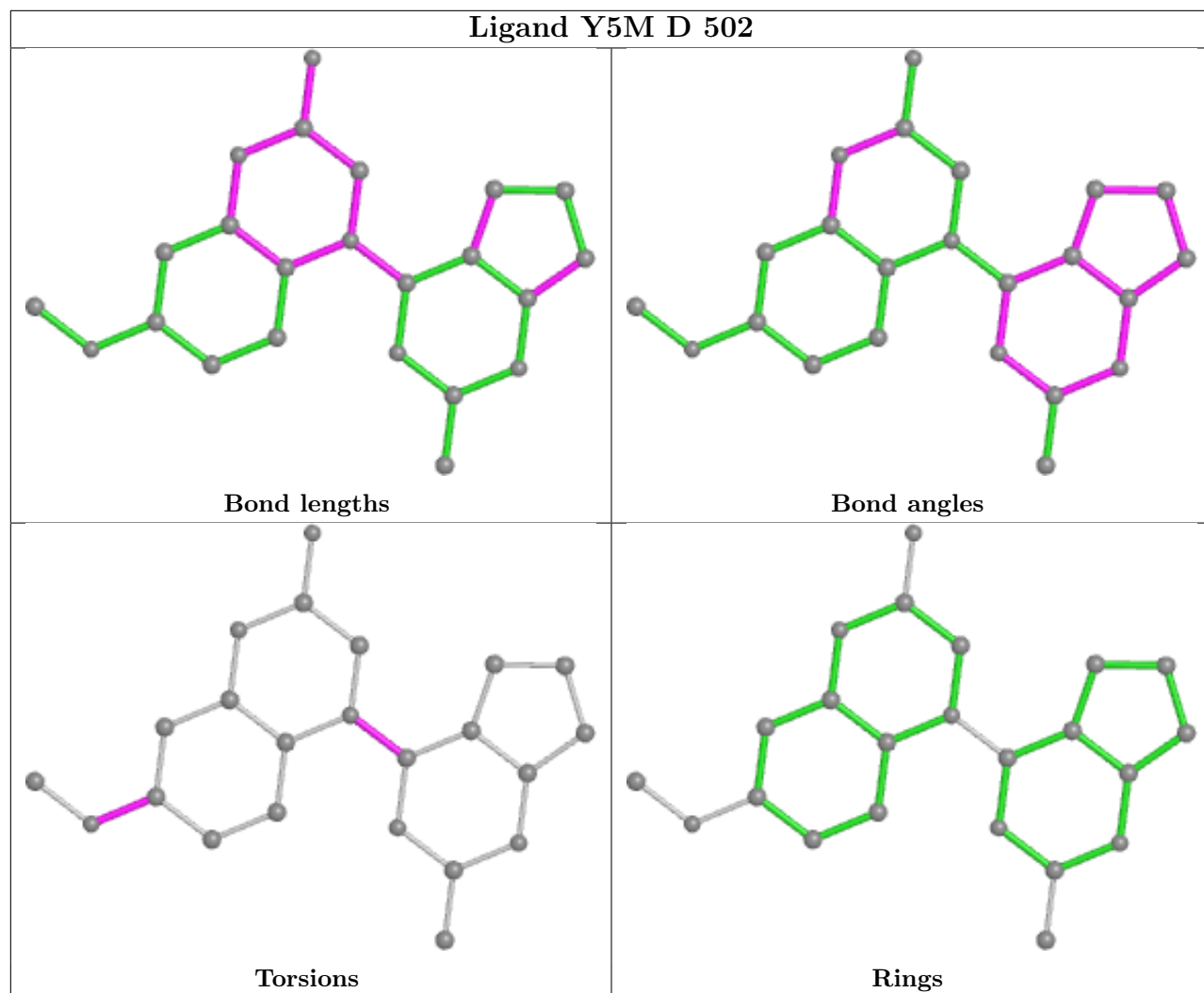
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	501	GTP	2	0
8	B	501	GDP	1	0
10	B	505	Y5M	1	0
9	B	503	MES	2	0

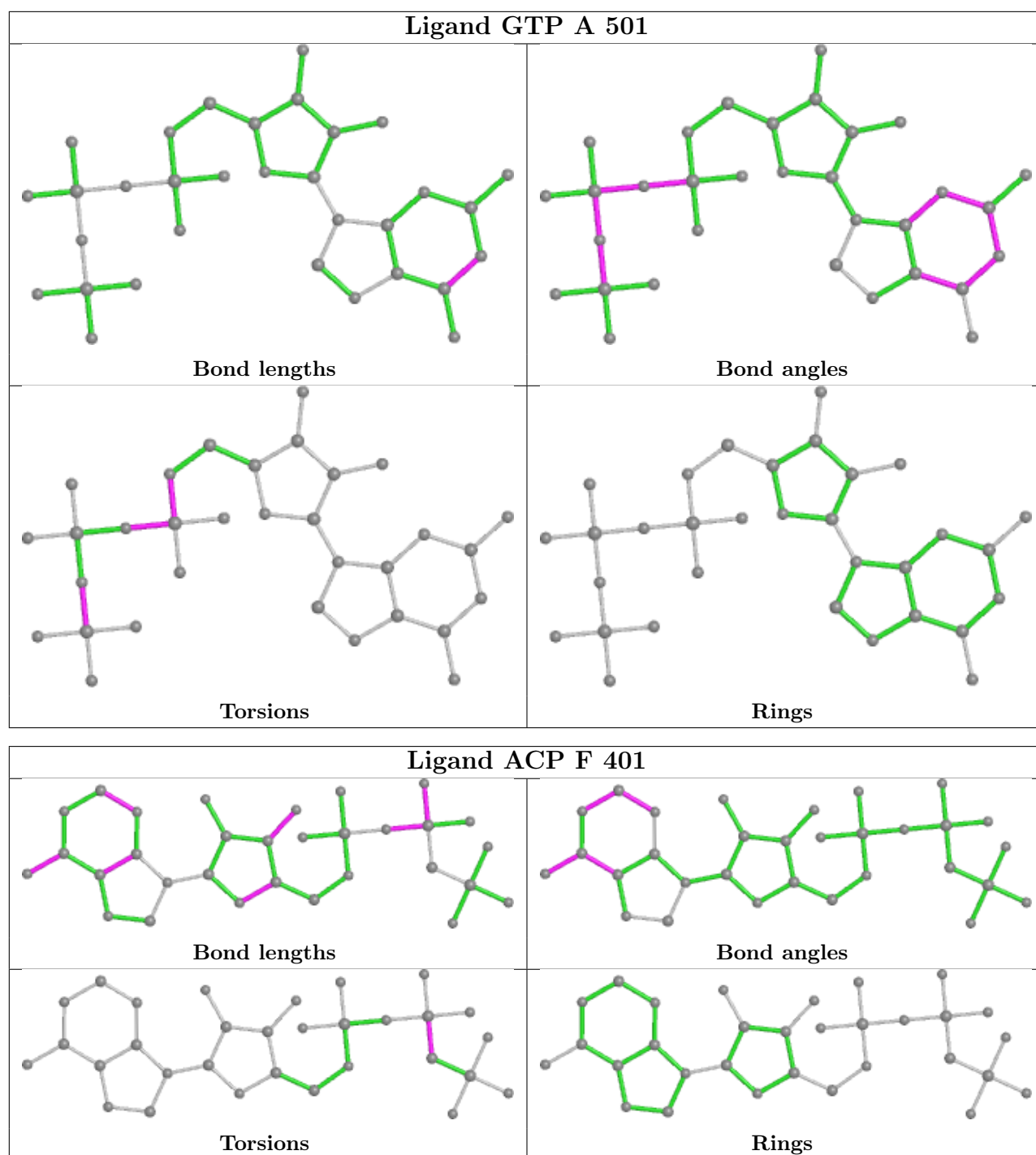
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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%)	-0.23	1 (0%) 95 96	22, 41, 70, 89	0
1	C	440/450 (97%)	-0.48	1 (0%) 95 96	17, 30, 59, 84	0
2	B	427/445 (95%)	-0.23	11 (2%) 56 57	17, 36, 78, 117	0
2	D	421/445 (94%)	0.11	19 (4%) 33 31	27, 63, 105, 127	0
3	E	121/143 (84%)	0.11	5 (4%) 37 36	31, 58, 96, 115	0
4	F	324/384 (84%)	0.68	62 (19%) 1 0	30, 69, 121, 146	0
All	All	2170/2317 (93%)	-0.06	99 (4%) 32 31	17, 46, 98, 146	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	277	GLY	4.7
2	B	55	THR	4.6
4	F	101	TYR	4.6
2	D	37	HIS	4.5
2	B	57	ASN	4.4
4	F	166	ALA	4.4
4	F	136	ASN	4.2
4	F	132	LEU	4.1
2	D	391	ARG	4.1
4	F	245	ILE	4.1
4	F	192	LEU	4.0
4	F	130	VAL	3.8
2	B	54	ALA	3.8
2	D	395	LEU	3.8
4	F	253	TYR	3.7
4	F	100	ILE	3.7
4	F	133	ALA	3.7
2	D	405	GLU	3.5
2	D	180	VAL	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	55	THR	3.4
4	F	194	PRO	3.3
2	B	58	LYS	3.3
4	F	256	TYR	3.3
4	F	172	PHE	3.3
2	B	279	GLN	3.3
4	F	180	HIS	3.2
4	F	163	SER	3.2
4	F	239	HIS	3.2
4	F	255	ARG	3.2
4	F	226	GLU	3.2
3	E	48	GLU	3.1
4	F	181	VAL	3.1
4	F	197	ARG	3.0
4	F	225	SER	3.0
3	E	27	PRO	3.0
4	F	162	ILE	3.0
2	D	394	PHE	2.9
2	D	390	ARG	2.9
3	E	140	LYS	2.9
3	E	28	SER	2.9
2	D	175	VAL	2.9
4	F	196	HIS	2.9
2	D	1	MET	2.8
2	B	59	TYR	2.8
4	F	21	LEU	2.8
2	B	428	ALA	2.8
2	D	83	GLN	2.8
4	F	24	THR	2.7
4	F	259	GLY	2.7
4	F	20	LEU	2.7
4	F	102	PRO	2.7
4	F	362	ALA	2.7
2	D	44	LEU	2.7
4	F	131	PHE	2.7
4	F	244	CYS	2.6
4	F	224	SER	2.6
2	D	217	LEU	2.5
4	F	146	VAL	2.5
4	F	227	PRO	2.5
4	F	257	GLU	2.5
4	F	137	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	22	LEU	2.4
4	F	223	THR	2.4
2	B	427	ASP	2.4
4	F	31	ARG	2.4
4	F	179	VAL	2.3
2	D	406	MET	2.3
4	F	228	TYR	2.3
4	F	17	VAL	2.3
4	F	264	PHE	2.3
2	D	215	LEU	2.3
2	D	92	PHE	2.3
2	D	389	PHE	2.3
3	E	139	LEU	2.3
2	B	37	HIS	2.2
4	F	252	ASN	2.2
4	F	129	GLU	2.2
1	A	262	TYR	2.2
2	B	281	TYR	2.2
4	F	171	ASP	2.2
1	C	1	MET	2.2
4	F	198	LYS	2.2
4	F	150	LYS	2.2
4	F	191	LEU	2.2
4	F	134	ALA	2.2
4	F	25	GLY	2.2
4	F	148	ILE	2.2
2	D	408	PHE	2.2
4	F	231	ALA	2.1
4	F	161	LEU	2.1
4	F	173	ILE	2.1
4	F	222	ARG	2.1
4	F	26	GLN	2.1
4	F	182	ILE	2.1
4	F	147	TRP	2.1
2	D	54	ALA	2.0
4	F	221	LEU	2.0
4	F	361	LEU	2.0
4	F	199	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

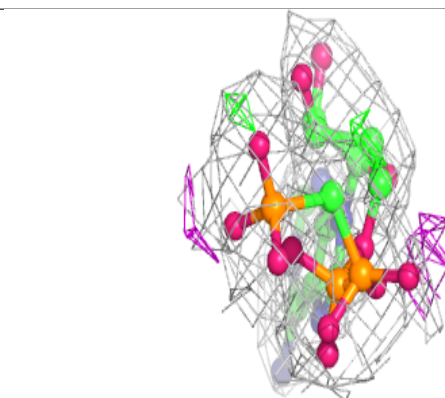
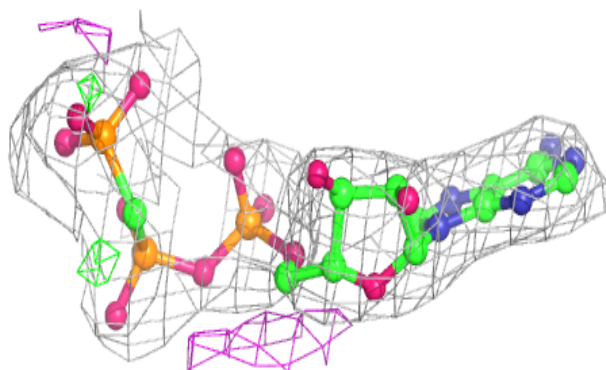
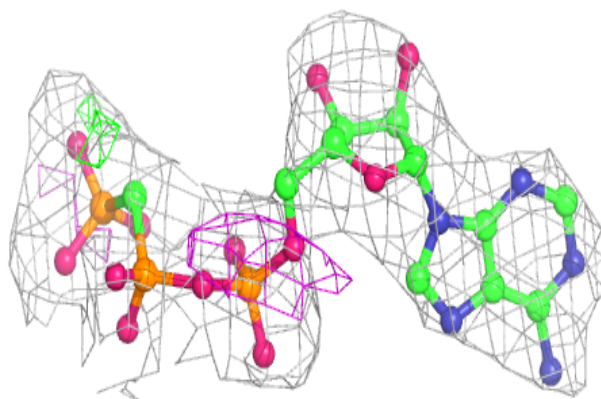
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	ACP	F	401	31/31	0.88	0.17	75,81,108,111	0
6	CA	C	502	1/1	0.91	0.06	49,49,49,49	0
6	CA	A	502	1/1	0.91	0.04	66,66,66,66	0
5	GTP	D	501	32/32	0.92	0.14	46,55,78,80	0
9	MES	B	502	12/12	0.93	0.18	34,52,82,84	0
9	MES	B	503	12/12	0.95	0.19	64,71,72,72	0
10	Y5M	D	502	23/23	0.96	0.16	28,39,51,53	0
10	Y5M	B	505	23/23	0.97	0.16	21,29,35,37	0
7	MG	B	504	1/1	0.97	0.18	41,41,41,41	0
7	MG	C	503	1/1	0.97	0.08	14,14,14,14	0
8	GDP	B	501	28/28	0.98	0.16	14,23,27,28	0
5	GTP	A	501	32/32	0.98	0.19	16,22,31,37	0
7	MG	A	503	1/1	0.98	0.16	24,24,24,24	0
5	GTP	C	501	32/32	0.99	0.14	16,20,23,25	0

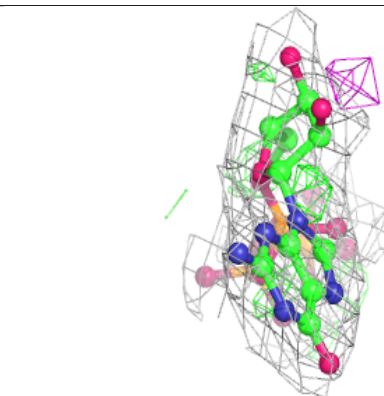
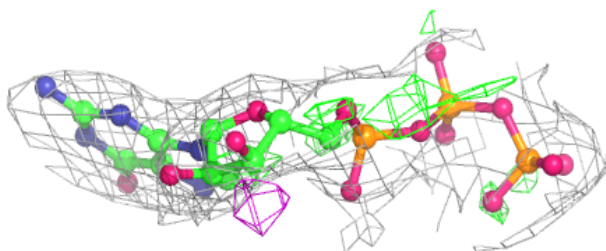
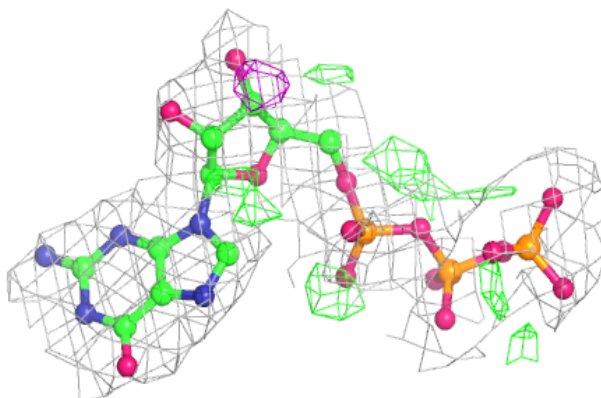
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

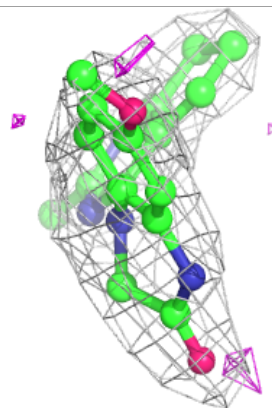
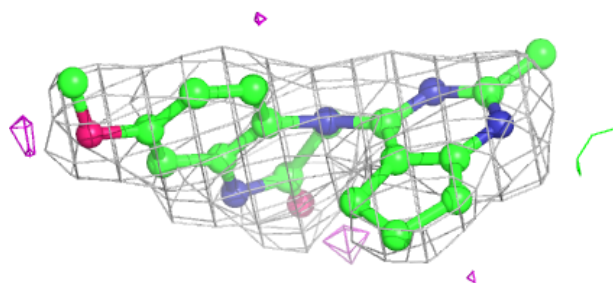
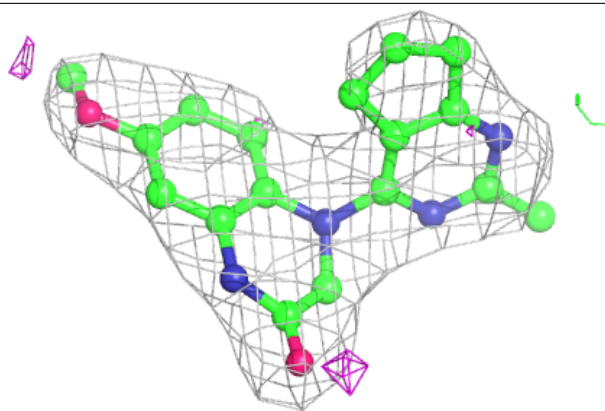
**Electron density around GTP D 501:**

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



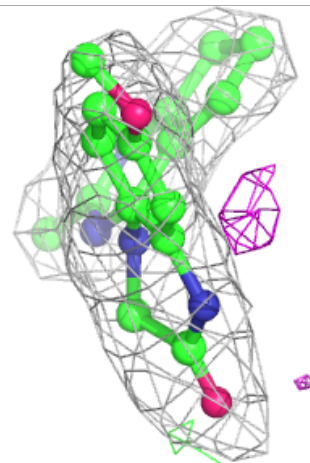
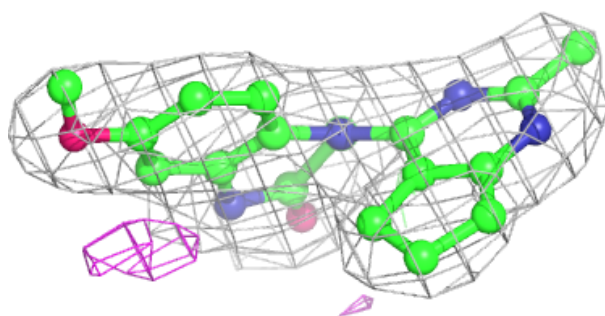
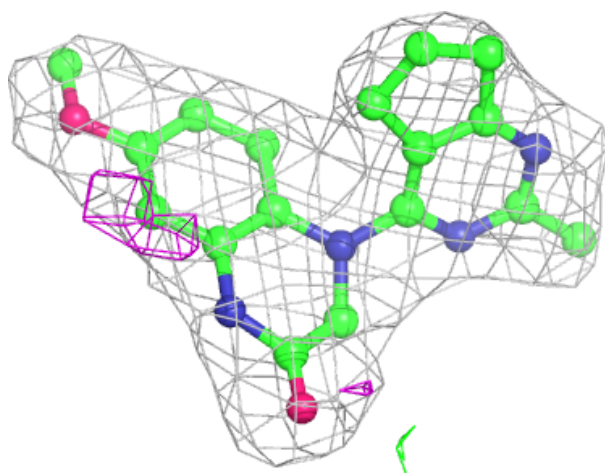
Electron density around Y5M D 502:

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



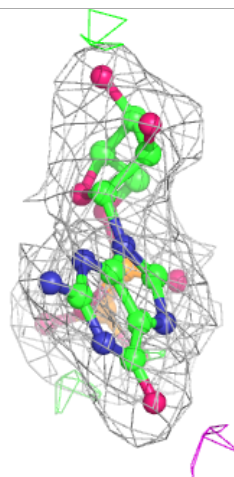
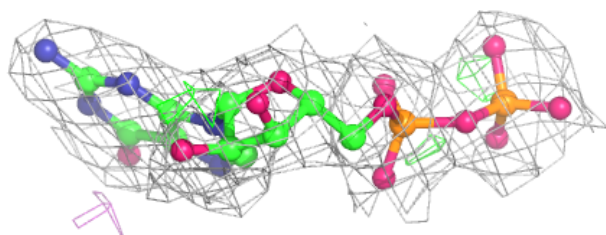
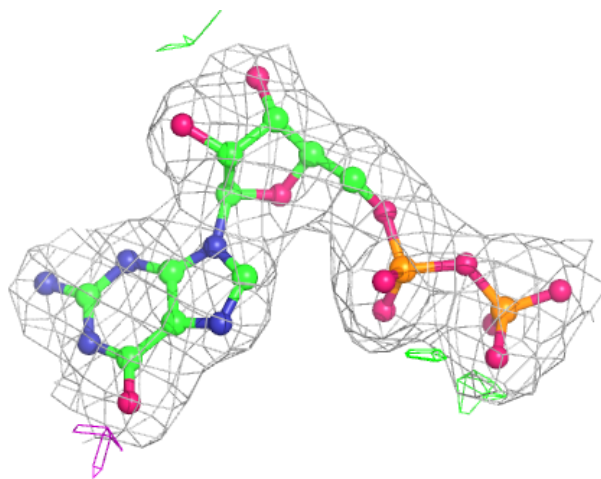
Electron density around Y5M B 505:

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



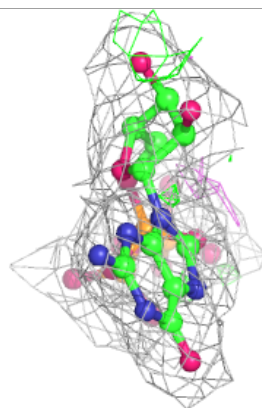
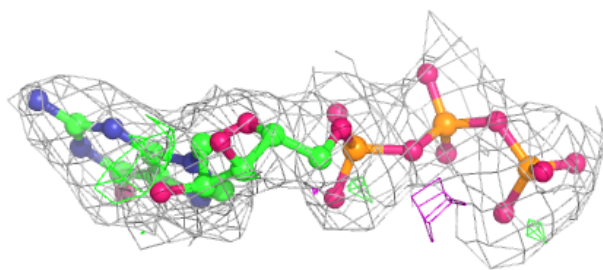
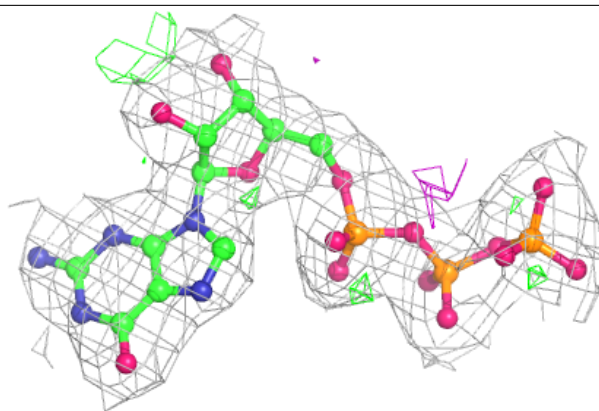
Electron density around GDP B 501:

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

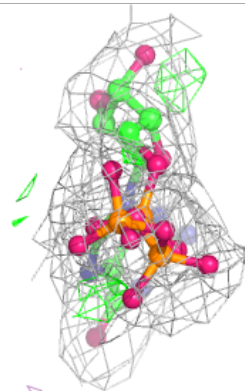
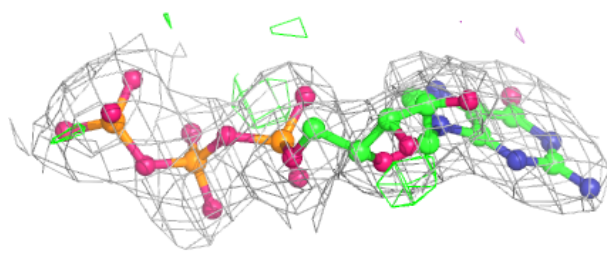
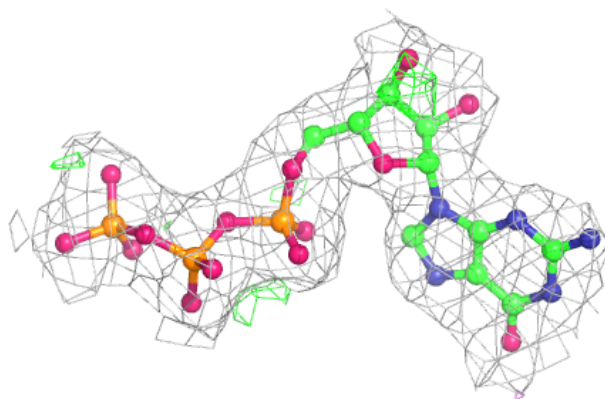


Electron density around GTP A 501:

$2mF_o - DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.