



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 6X1F / pdb_00006x1f
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 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

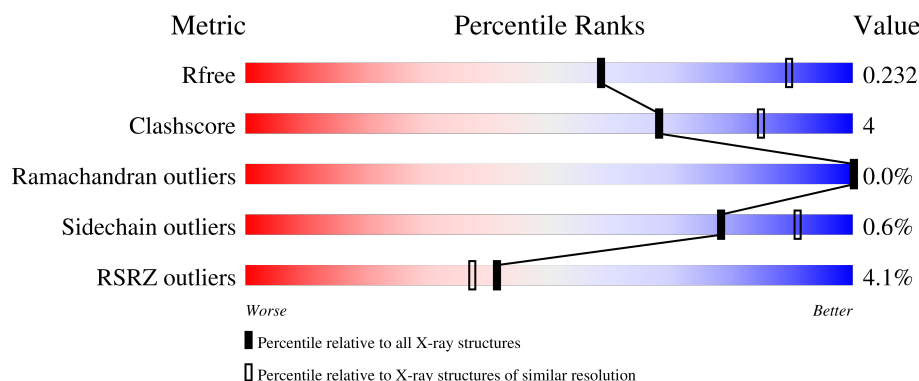
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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	11%75%9%16%

2 Entry composition [i](#)

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

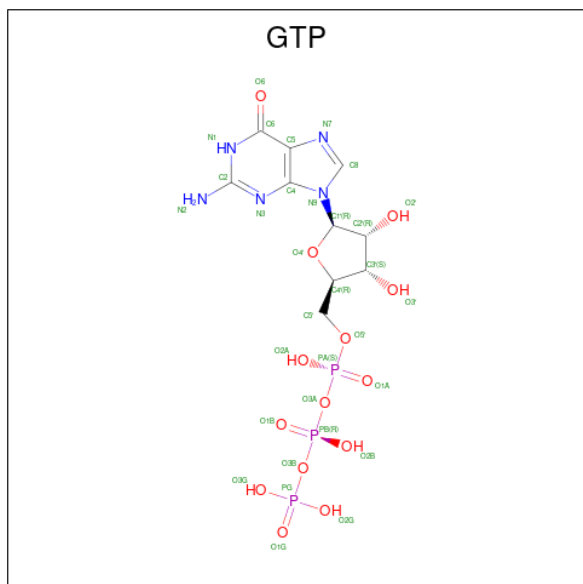
- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

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 (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		

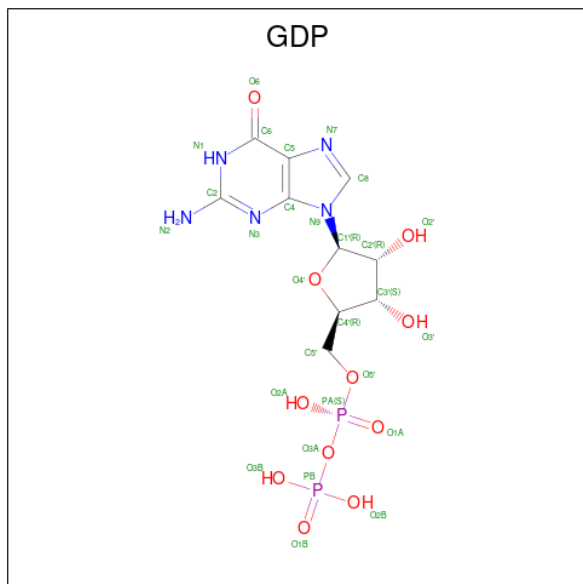
- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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).

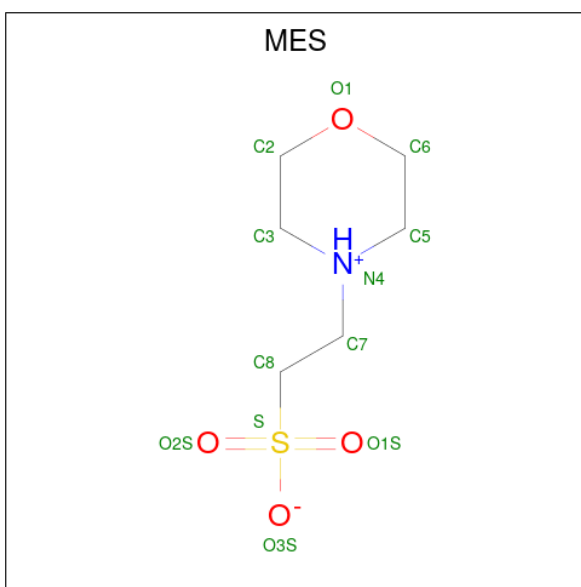
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		

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



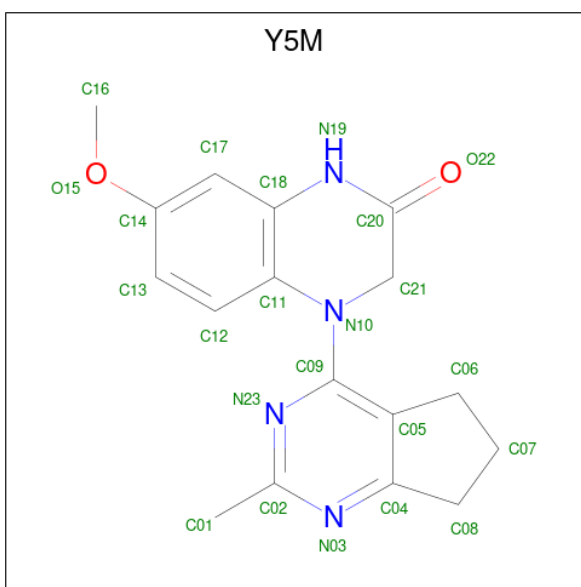
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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 (CCD ID: Y5M) (formula: C₁₇H₁₈N₄O₂) (labeled as "Ligand of Interest" by depositor).



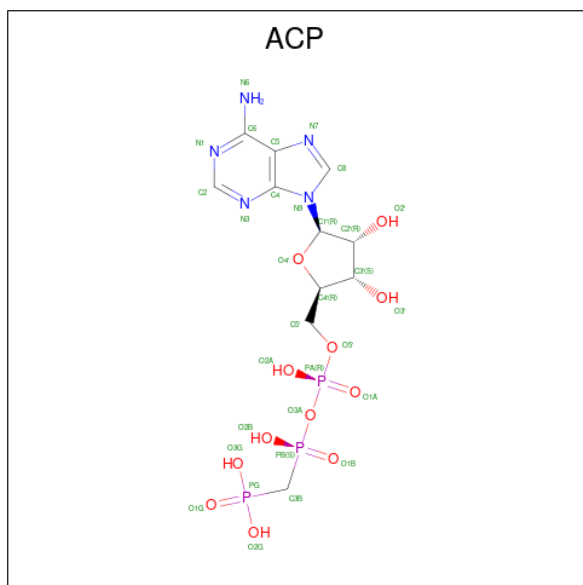
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			23	17	4	2		

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 (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		

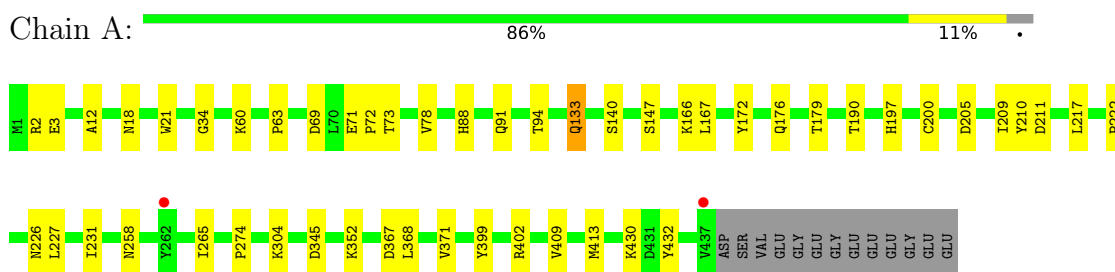
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	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		

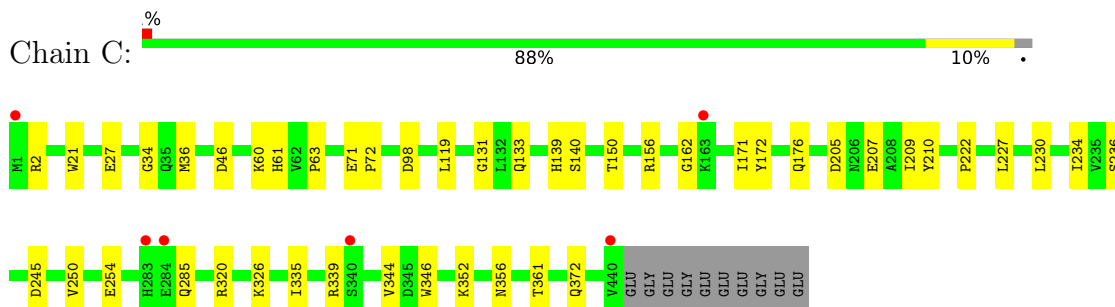
3 Residue-property plots

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.

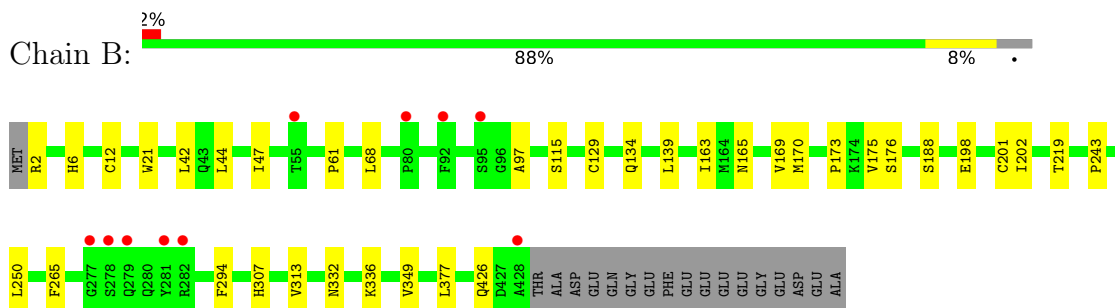
• Molecule 1: Tubulin alpha-1B chain



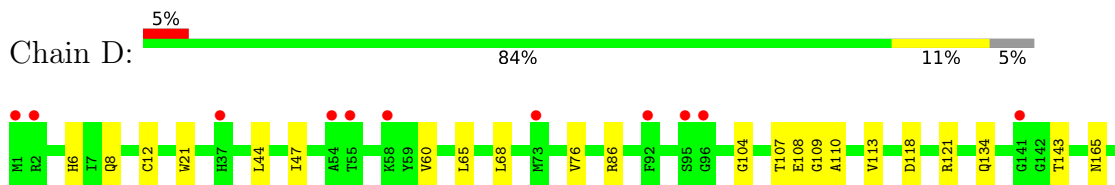
• Molecule 1: Tubulin alpha-1B chain

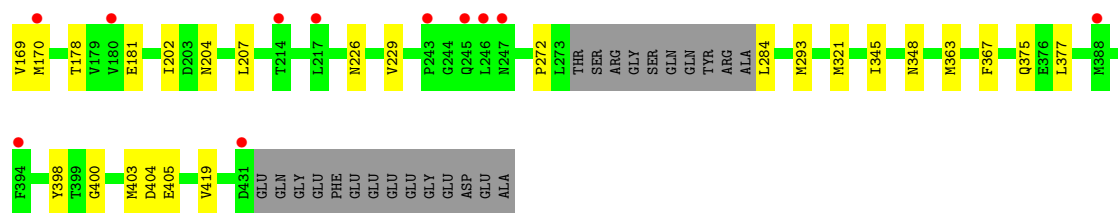


• Molecule 2: Tubulin beta-2B chain

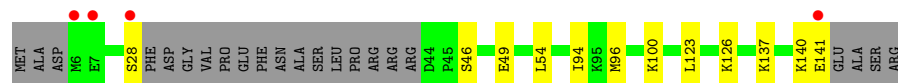
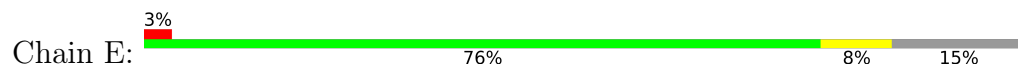


• Molecule 2: Tubulin beta-2B chain

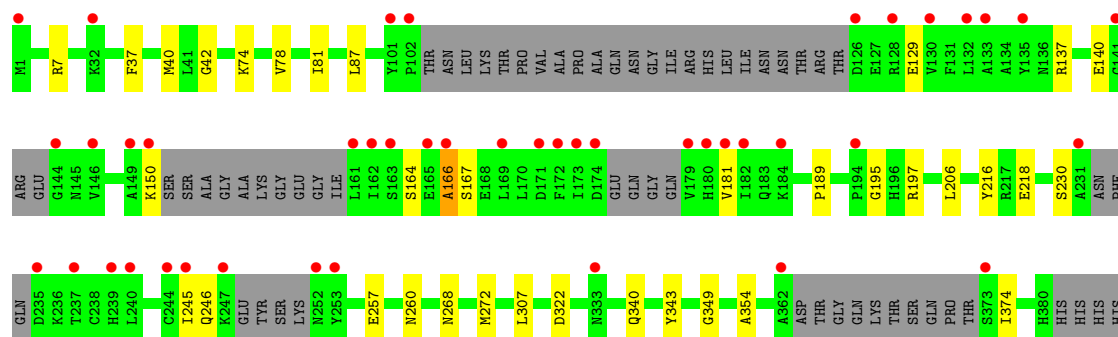
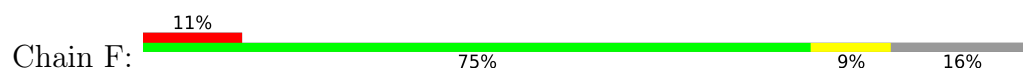




● Molecule 3: Stathmin-4



● 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 0.185 , 0.232	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 , 41.7	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: CA, Y5M, MES, GTP, ACP, 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	0.10	0/3494	0.29	0/4743
1	C	0.12	0/3515	0.31	0/4772
2	B	0.11	0/3454	0.30	0/4677
2	D	0.10	0/3378	0.29	0/4577
3	E	0.10	0/1019	0.27	0/1352
4	F	0.11	0/2688	0.34	0/3629
All	All	0.11	0/17548	0.30	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	27	0
3	E	1007	0	1025	8	0
4	F	2628	0	2572	18	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	124	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 (124) 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:170:MET:HE2	2:D:377:LEU:HD21	1.74	0.70
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
2:D:398:TYR:HB3	2:D:403:MET:HE3	1.87	0.55
1:C:2:ARG:HD2	1:C:133:GLN:HB2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:321:MET:HE2	2:D:363:MET:HE2	1.91	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
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:71:GLU:OE1	1:A:73:THR:OG1	2.20	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:A:258:ASN:OD1	1:A:352:LYS:NZ	2.46	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:37:PHE:CZ	4:F:40:MET:HE3	2.53	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:F:195:GLY:C	4:F:197:ARG:HG3	2.45	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 ⓘ

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%)	426 (98%)	9 (2%)	0	100	100
1	C	438/450 (97%)	426 (97%)	12 (3%)	0	100	100
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%)	36	60
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%)	366 (100%)	2 (0%)	81	92
1	C	371/378 (98%)	370 (100%)	1 (0%)	86	94
2	B	371/383 (97%)	369 (100%)	2 (0%)	81	92
2	D	362/383 (94%)	362 (100%)	0	100	100
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	283/342 (83%)	277 (98%)	6 (2%)	47	75
All	All	1865/1991 (94%)	1854 (99%)	11 (1%)	78	91

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	176	GLN
2	B	115	SER
2	B	175	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	361	THR
4	F	129	GLU
4	F	137	ARG
4	F	140	GLU
4	F	167	SER
4	F	230	SER
4	F	245	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	176	GLN
1	A	301	GLN
1	A	356	ASN
1	A	393	HIS
1	A	406	HIS
2	B	99	ASN
2	B	165	ASN
2	B	347	ASN
2	B	375	GLN
1	C	15	GLN
1	C	31	GLN
1	C	256	GLN
1	C	285	GLN
1	C	309	HIS
1	C	406	HIS
2	D	8	GLN
2	D	15	GLN
2	D	99	ASN
2	D	165	ASN
2	D	247	ASN
2	D	291	GLN
2	D	292	GLN
2	D	329	GLN
2	D	375	GLN
2	D	396	HIS
3	E	91	ASN
3	E	108	ASN
3	E	124	GLN
4	F	310	GLN
4	F	348	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
8	GDP	B	501	7	29,30,30	1.18	2 (6%)	45,47,47	1.72	6 (13%)
5	GTP	C	501	7	33,34,34	1.01	3 (9%)	50,54,54	1.52	8 (16%)
10	Y5M	B	505	-	26,26,26	2.84	11 (42%)	35,38,38	2.23	12 (34%)
10	Y5M	D	502	-	26,26,26	2.90	10 (38%)	35,38,38	2.17	10 (28%)
5	GTP	D	501	-	33,34,34	0.97	1 (3%)	50,54,54	1.58	8 (16%)
11	ACP	F	401	-	31,33,33	1.94	8 (25%)	47,52,52	1.69	8 (17%)
9	MES	B	503	-	12,12,12	2.37	1 (8%)	15,16,16	1.91	3 (20%)
9	MES	B	502	-	12,12,12	2.31	1 (8%)	15,16,16	1.79	1 (6%)
5	GTP	A	501	7	33,34,34	1.02	4 (12%)	50,54,54	1.53	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	B	501	7	-	3/16/32/32	0/3/3/3
5	GTP	C	501	7	-	8/22/38/38	0/3/3/3
10	Y5M	B	505	-	-	2/5/24/24	0/4/4/4
10	Y5M	D	502	-	-	4/5/24/24	0/4/4/4
5	GTP	D	501	-	-	9/22/38/38	0/3/3/3
11	ACP	F	401	-	-	3/19/38/38	0/3/3/3
9	MES	B	503	-	-	4/6/14/14	0/1/1/1
9	MES	B	502	-	-	4/6/14/14	0/1/1/1
5	GTP	A	501	7	-	7/22/38/38	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	502	Y5M	C20-N19	8.67	1.45	1.35
10	B	505	Y5M	C20-N19	8.46	1.44	1.35
9	B	503	MES	C8-S	-7.93	1.66	1.77
9	B	502	MES	C8-S	-7.75	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	D	502	Y5M	C18-N19	5.17	1.48	1.39
10	B	505	Y5M	C18-N19	5.05	1.48	1.39
10	B	505	Y5M	C08-C04	4.90	1.54	1.50
10	D	502	Y5M	C08-C04	4.83	1.54	1.50
11	F	401	ACP	C6-N6	4.20	1.44	1.34
10	D	502	Y5M	C21-C20	3.44	1.55	1.51
10	B	505	Y5M	C21-C20	3.42	1.55	1.51
8	B	501	GDP	C5-C4	3.16	1.47	1.38
10	D	502	Y5M	C11-N10	3.14	1.45	1.40
11	F	401	ACP	C5-C4	-3.03	1.33	1.39
11	F	401	ACP	O3'-C3'	-2.93	1.35	1.43
10	B	505	Y5M	C11-N10	2.84	1.45	1.40
10	B	505	Y5M	C18-C11	-2.76	1.37	1.40
11	F	401	ACP	C5-N7	-2.75	1.34	1.39
10	B	505	Y5M	C21-N10	-2.48	1.42	1.46
10	D	502	Y5M	C06-C05	2.46	1.55	1.51
10	D	502	Y5M	C21-N10	-2.42	1.42	1.46
10	D	502	Y5M	O22-C20	-2.40	1.18	1.23
8	B	501	GDP	C6-N1	-2.40	1.34	1.38
10	D	502	Y5M	C18-C11	-2.38	1.37	1.40
10	B	505	Y5M	O22-C20	-2.37	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	Y5M	C06-C05	2.36	1.55	1.51
5	C	501	GTP	PA-O3A	2.27	1.62	1.59
11	F	401	ACP	C8-N9	-2.24	1.33	1.37
5	D	501	GTP	C2-N3	2.22	1.38	1.33
5	A	501	GTP	PA-O3A	2.21	1.61	1.59
5	A	501	GTP	PB-O3A	2.13	1.61	1.59
5	C	501	GTP	C2-N3	2.11	1.38	1.33
11	F	401	ACP	PB-O2B	-2.09	1.51	1.56
5	A	501	GTP	PB-O3B	2.09	1.61	1.59
11	F	401	ACP	O4'-C4'	-2.05	1.40	1.45
5	A	501	GTP	C2-N3	2.05	1.38	1.33
5	C	501	GTP	PB-O3A	2.04	1.61	1.59
10	B	505	Y5M	C12-C11	2.02	1.42	1.39

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	Y5M	C07-C08-C04	6.40	108.39	103.84
10	D	502	Y5M	C07-C08-C04	6.15	108.21	103.84
8	B	501	GDP	C5-C4-N3	-6.04	118.78	128.39
11	F	401	ACP	N3-C2-N1	-5.35	120.48	128.58
10	B	505	Y5M	C08-C04-N03	5.10	129.87	123.41
8	B	501	GDP	C2-N3-C4	5.06	121.02	112.30
11	F	401	ACP	C5-C4-N3	-5.06	119.75	126.72
5	D	501	GTP	C5-C4-N3	-4.94	120.52	128.39
9	B	502	MES	C5-N4-C3	4.94	119.48	108.84
10	D	502	Y5M	C08-C04-N03	4.73	129.41	123.41
5	C	501	GTP	C5-C4-N3	-4.72	120.88	128.39
5	A	501	GTP	C5-C4-N3	-4.64	121.01	128.39
9	B	503	MES	C5-N4-C3	4.55	118.65	108.84
5	D	501	GTP	C2-N3-C4	4.52	120.09	112.30
5	C	501	GTP	C2-N3-C4	4.45	119.97	112.30
5	A	501	GTP	C2-N3-C4	4.43	119.93	112.30
8	B	501	GDP	N9-C4-N3	4.40	134.74	125.95
10	D	502	Y5M	C18-N19-C20	-3.83	119.87	124.45
10	B	505	Y5M	C18-N19-C20	-3.81	119.89	124.45
10	B	505	Y5M	C05-C04-N03	-3.73	121.27	125.50
11	F	401	ACP	N9-C8-N7	-3.71	108.67	113.94
10	D	502	Y5M	C05-C04-N03	-3.57	121.45	125.50
10	D	502	Y5M	C07-C06-C05	3.40	107.85	103.57
11	F	401	ACP	C2-N3-C4	3.36	120.03	111.83
8	B	501	GDP	C6-C5-N7	3.36	136.40	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	Y5M	C07-C06-C05	3.29	107.70	103.57
5	D	501	GTP	N9-C4-N3	3.14	132.24	125.95
10	D	502	Y5M	C11-N10-C09	3.09	124.91	119.21
5	C	501	GTP	N9-C4-N3	3.01	131.98	125.95
10	B	505	Y5M	C08-C04-C05	-2.96	108.86	111.25
5	A	501	GTP	N9-C4-N3	2.94	131.82	125.95
11	F	401	ACP	N3-C4-N9	2.88	132.07	127.17
5	D	501	GTP	N9-C8-N7	-2.88	108.06	113.40
5	A	501	GTP	N9-C8-N7	-2.86	108.09	113.40
5	A	501	GTP	C2-N1-C6	-2.83	119.97	125.11
5	D	501	GTP	C2-N1-C6	-2.79	120.06	125.11
5	C	501	GTP	C2-N1-C6	-2.78	120.07	125.11
9	B	503	MES	C6-C5-N4	-2.77	105.91	110.12
5	D	501	GTP	C8-N7-C5	2.73	109.11	104.26
10	B	505	Y5M	C11-N10-C09	2.70	124.19	119.21
5	C	501	GTP	N9-C8-N7	-2.69	108.41	113.40
10	D	502	Y5M	C05-C09-N23	-2.64	118.58	122.60
8	B	501	GDP	C4-C5-N7	-2.62	106.52	110.67
10	B	505	Y5M	N23-C02-N03	-2.62	121.15	125.77
10	D	502	Y5M	C08-C04-C05	-2.61	109.14	111.25
5	A	501	GTP	C8-N7-C5	2.52	108.75	104.26
11	F	401	ACP	C5-N7-C8	2.47	107.33	103.45
5	C	501	GTP	C5-C6-N1	2.47	119.54	113.25
5	D	501	GTP	O6-C6-C5	-2.47	120.02	126.53
5	C	501	GTP	O6-C6-C5	-2.47	120.03	126.53
5	A	501	GTP	C5-C6-N1	2.46	119.52	113.25
10	D	502	Y5M	N23-C02-N03	-2.44	121.47	125.77
5	A	501	GTP	O6-C6-C5	-2.42	120.15	126.53
5	C	501	GTP	C8-N7-C5	2.40	108.54	104.26
5	D	501	GTP	C5-C6-N1	2.37	119.28	113.25
10	B	505	Y5M	C21-N10-C11	2.32	117.34	114.97
10	B	505	Y5M	C05-C09-N23	-2.27	119.14	122.60
11	F	401	ACP	C5-C4-N9	2.17	108.18	105.81
10	D	502	Y5M	C02-N23-C09	2.08	122.13	115.02
8	B	501	GDP	O6-C6-C5	-2.07	121.07	126.53
10	B	505	Y5M	C02-N23-C09	2.04	122.01	115.02
10	B	505	Y5M	C16-O15-C14	-2.03	113.15	117.50
11	F	401	ACP	C4-C5-N7	-2.02	108.27	110.58
9	B	503	MES	O1S-S-C8	2.01	109.77	106.73

There are no chirality outliers.

All (44) 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-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
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-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	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
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
10	B	505	Y5M	C05-C09-N10-C21
5	D	501	GTP	O4'-C4'-C5'-O5'
5	D	501	GTP	C3'-C4'-C5'-O5'
9	B	503	MES	C7-C8-S-O1S
9	B	503	MES	C7-C8-S-O2S
10	D	502	Y5M	C13-C14-O15-C16
10	D	502	Y5M	C17-C14-O15-C16
5	C	501	GTP	PB-O3B-PG-O2G
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
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA

Continued on next page...

Continued from previous page...

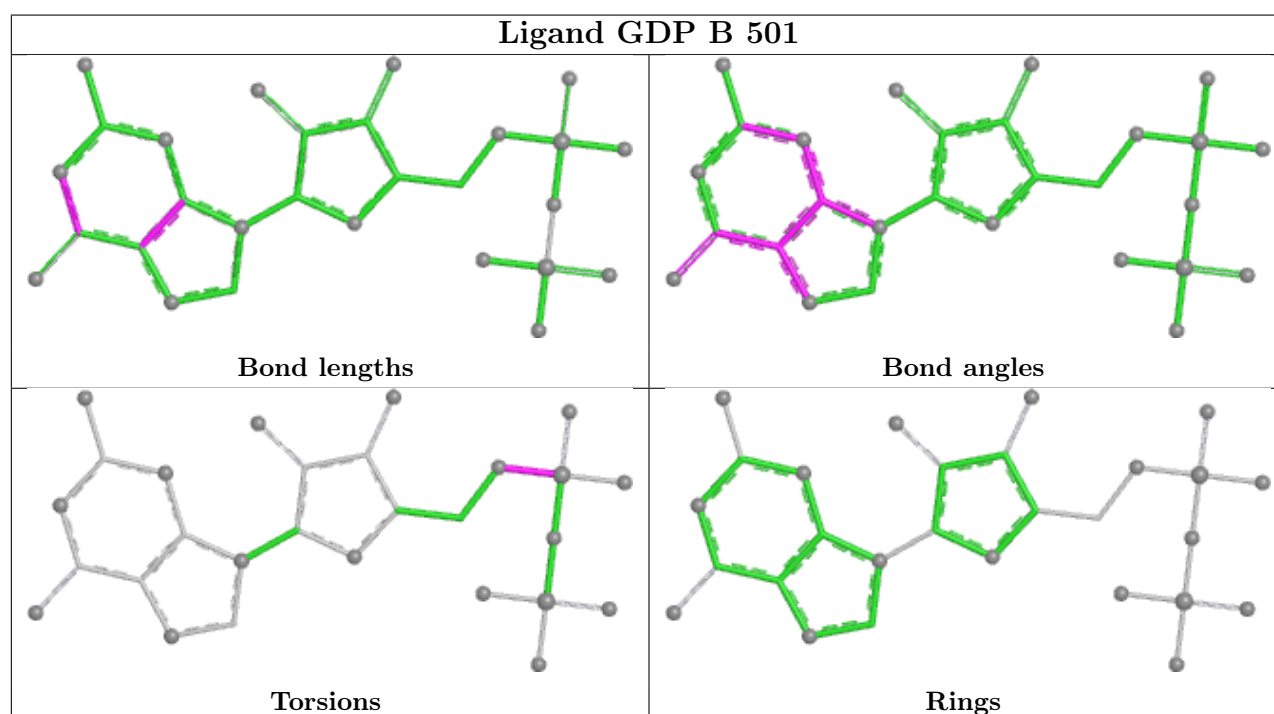
Mol	Chain	Res	Type	Atoms
5	D	501	GTP	PB-O3A-PA-O2A

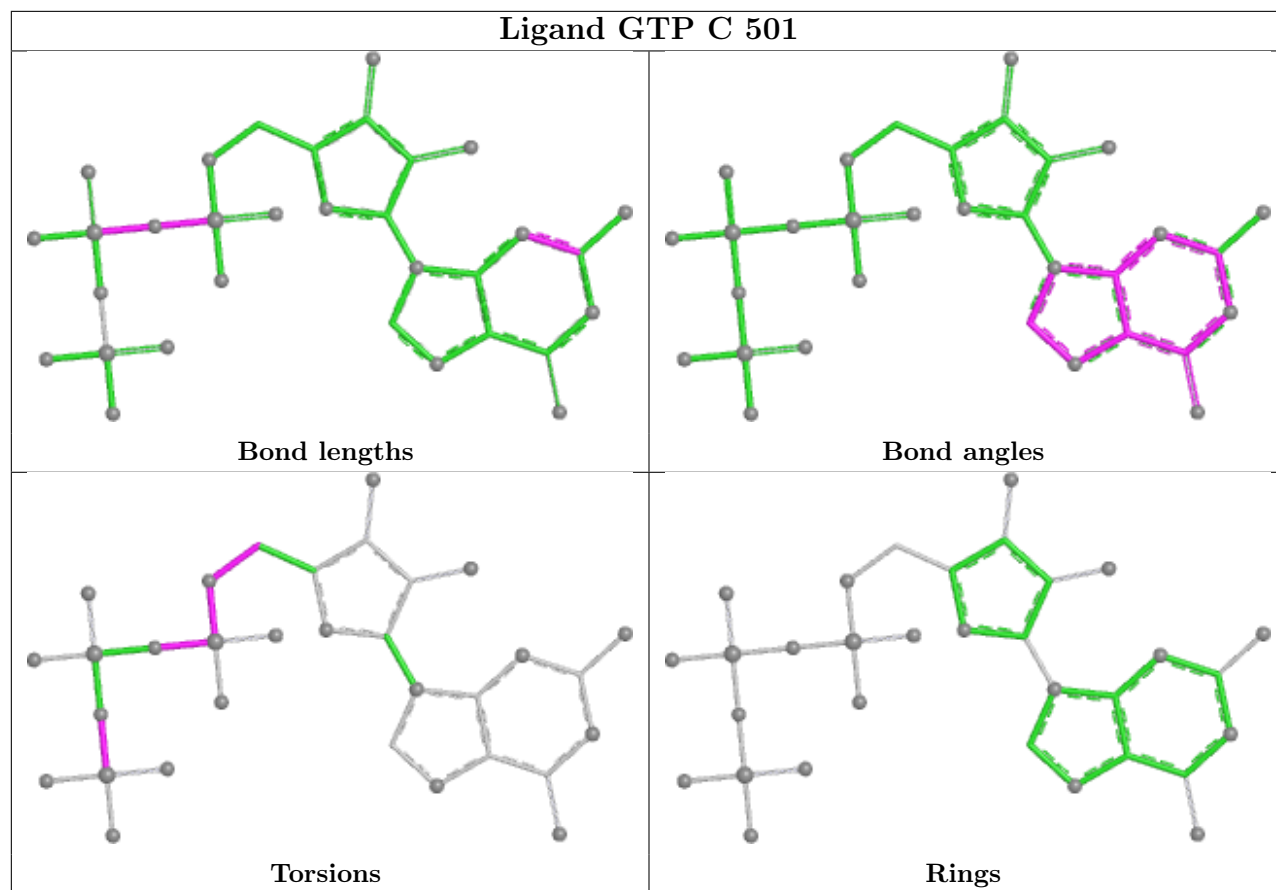
There are no ring outliers.

4 monomers are involved in 6 short contacts:

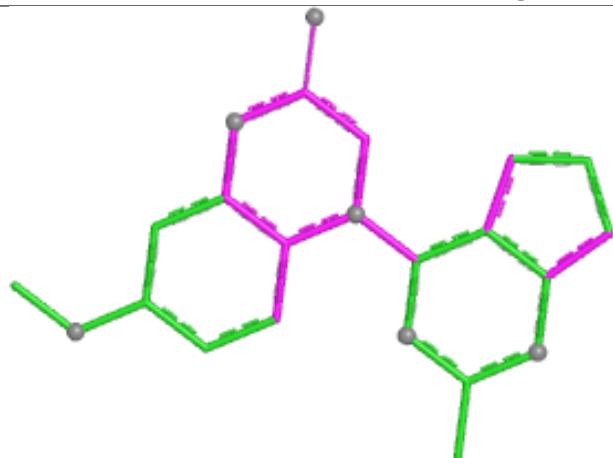
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	GDP	1	0
10	B	505	Y5M	1	0
5	D	501	GTP	2	0
9	B	503	MES	2	0

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.

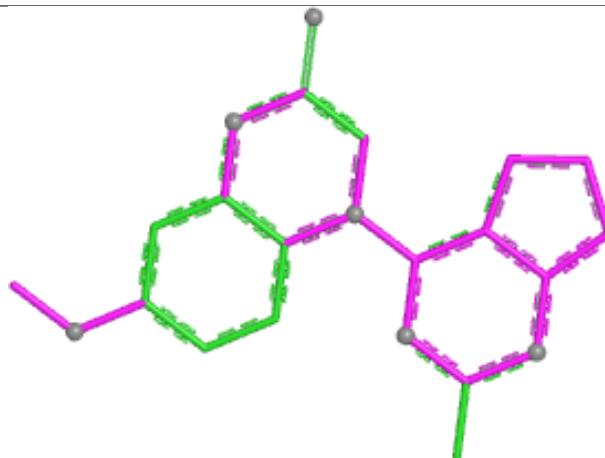




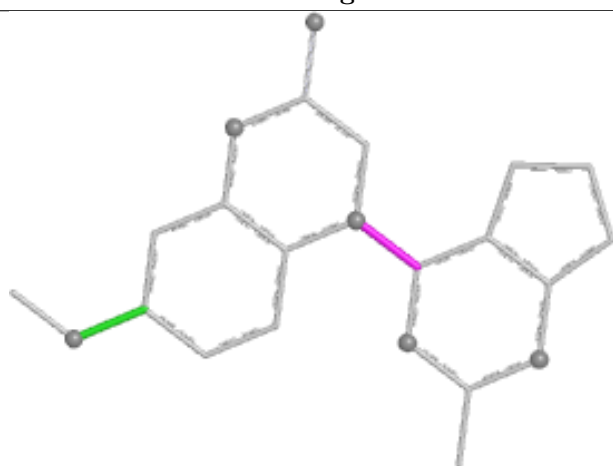
Ligand Y5M B 505



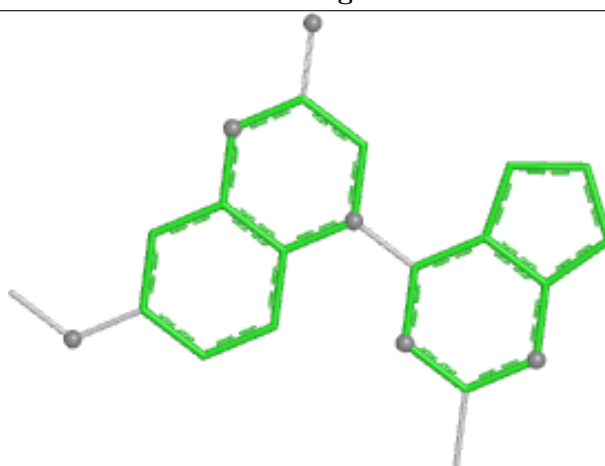
Bond lengths



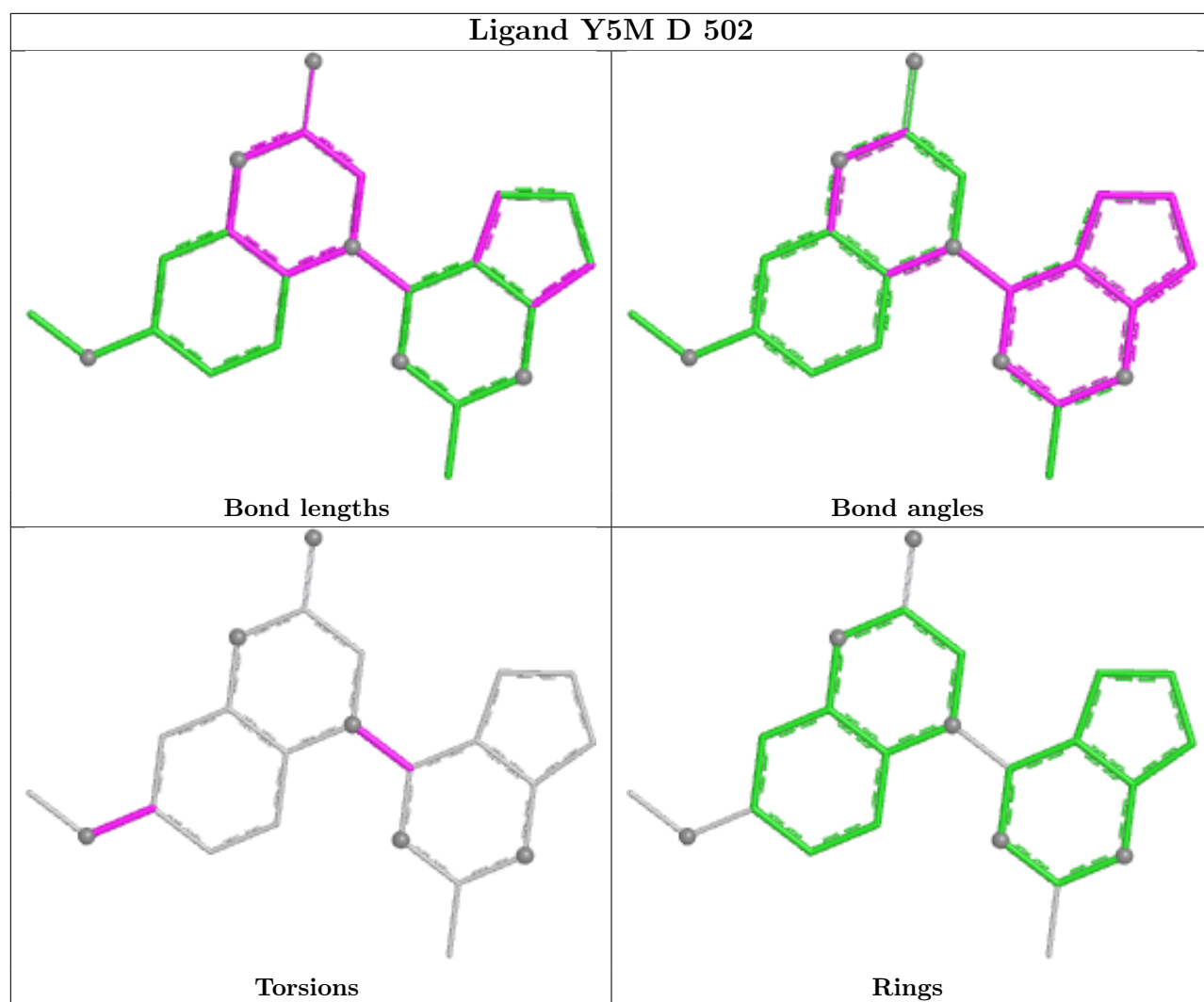
Bond angles

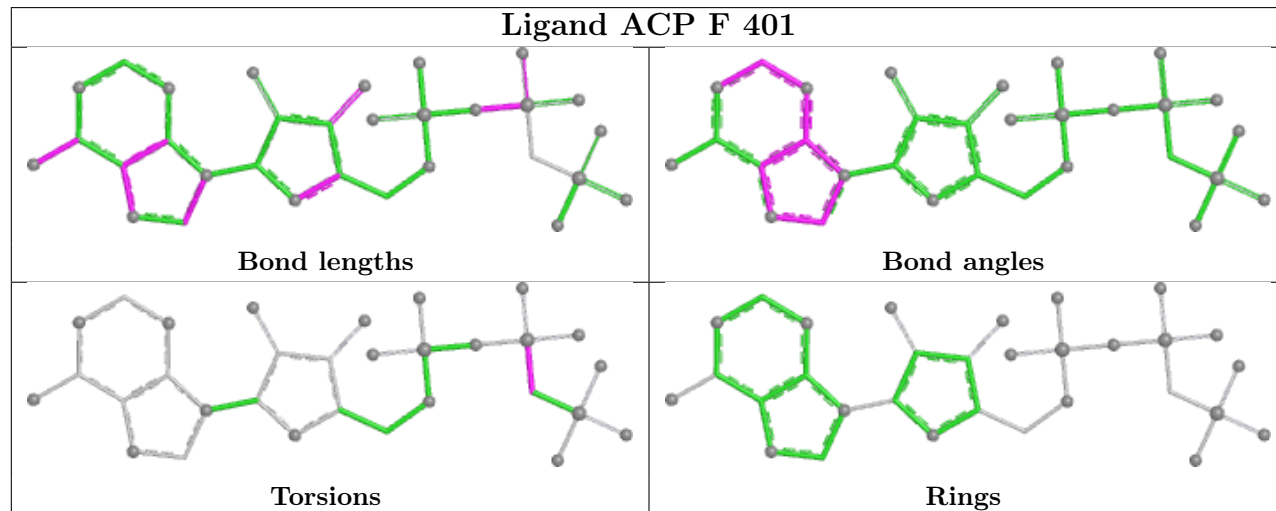
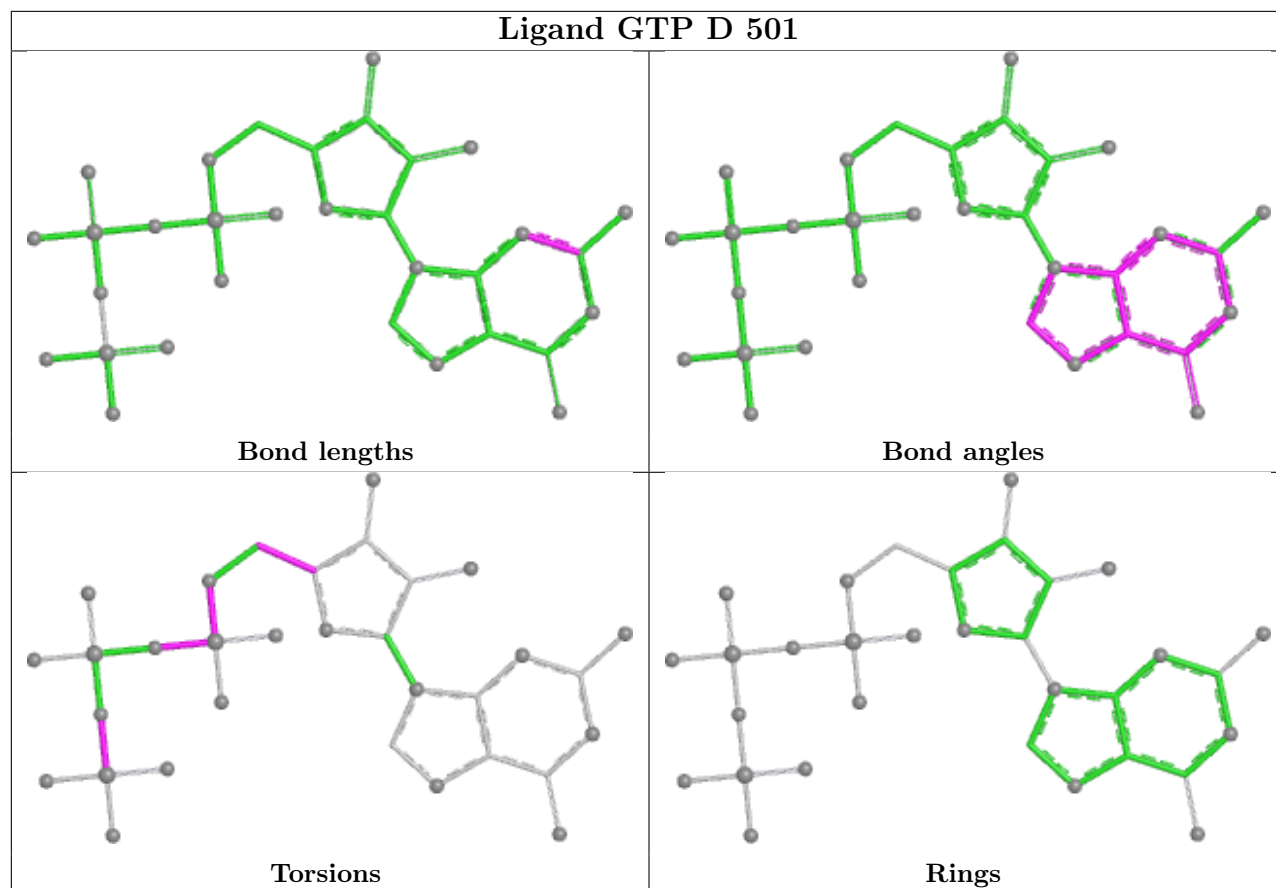


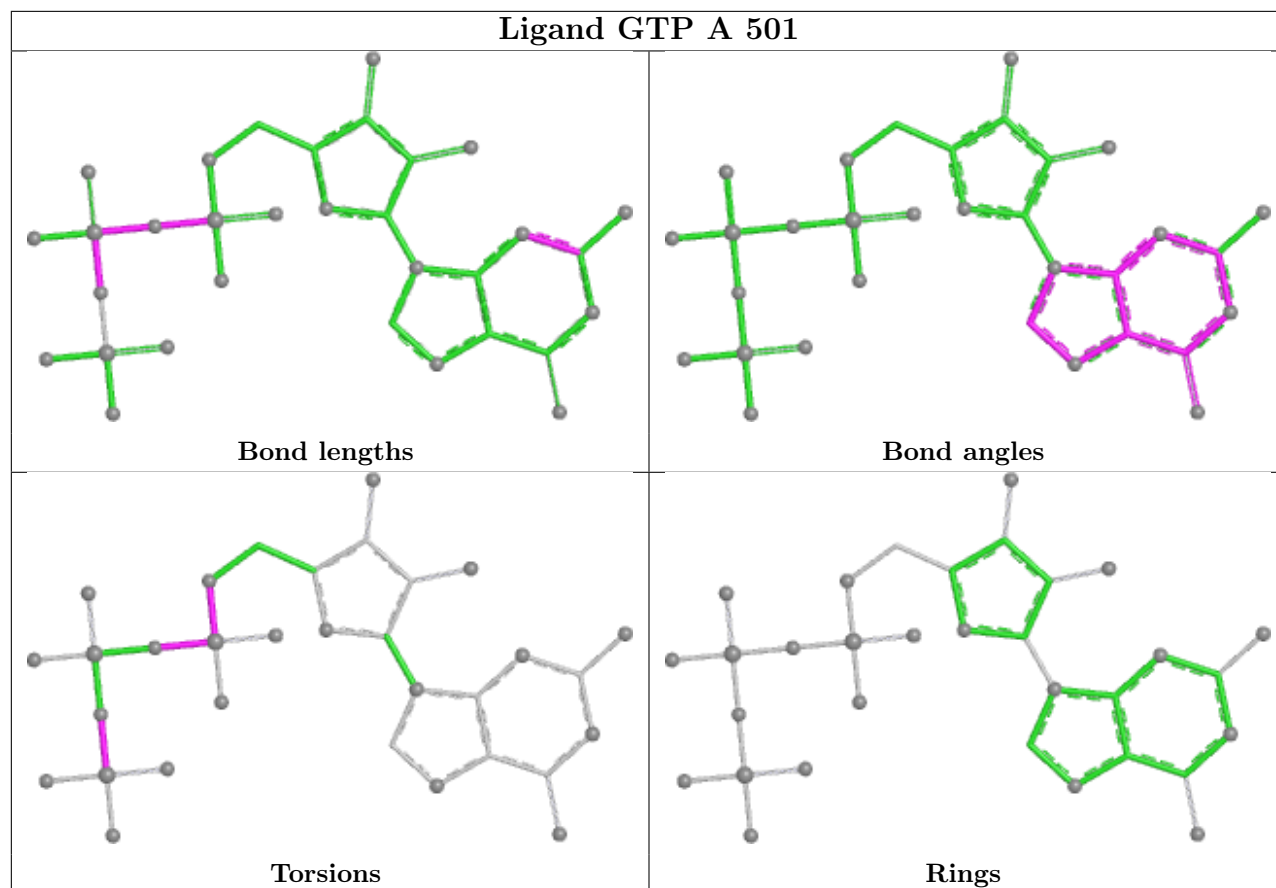
Torsions



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%)	-0.22	2 (0%) 87 86	22, 41, 70, 89	0
1	C	440/450 (97%)	-0.38	6 (1%) 73 72	17, 30, 59, 84	0
2	B	427/445 (95%)	-0.19	10 (2%) 61 58	17, 36, 78, 117	2 (0%)
2	D	421/445 (94%)	0.37	22 (5%) 33 29	27, 63, 105, 127	0
3	E	121/143 (84%)	0.32	4 (3%) 49 45	26, 58, 96, 115	1 (0%)
4	F	324/384 (84%)	0.65	44 (13%) 7 6	24, 69, 121, 146	1 (0%)
All	All	2170/2317 (93%)	0.03	88 (4%) 41 37	17, 46, 98, 146	4 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	5.0
4	F	141	GLY	4.6
1	C	440	VAL	4.6
4	F	252	ASN	4.5
4	F	182	ILE	4.5
4	F	165	GLU	4.5
4	F	247	LYS	4.4
4	F	102	PRO	4.0
4	F	126	ASP	4.0
4	F	179	VAL	4.0
2	D	1	MET	4.0
2	B	277	GLY	3.9
4	F	150	LYS	3.9
1	A	437	VAL	3.9
4	F	135	TYR	3.4
4	F	231	ALA	3.3
4	F	132	LEU	3.3
2	B	55	THR	3.2
2	B	95	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	3.1
4	F	166	ALA	3.1
2	D	394	PHE	3.1
4	F	245	ILE	3.0
2	D	431	ASP	3.0
4	F	101	TYR	3.0
2	D	73	MET	3.0
2	D	141	GLY	2.9
2	D	37	HIS	2.9
2	D	55	THR	2.9
2	D	58	LYS	2.9
2	D	92	PHE	2.9
4	F	181	VAL	2.9
2	D	245	GLN	2.8
4	F	174	ASP	2.8
4	F	149	ALA	2.8
4	F	144	GLY	2.8
4	F	235	ASP	2.8
2	B	428	ALA	2.8
1	C	1	MET	2.7
2	B	281	TYR	2.7
4	F	253	TYR	2.7
4	F	373	SER	2.5
2	D	246	LEU	2.5
4	F	180	HIS	2.5
2	D	214	THR	2.5
4	F	237	THR	2.5
4	F	362	ALA	2.5
4	F	162	ILE	2.5
4	F	172	PHE	2.5
4	F	128	ARG	2.4
4	F	194	PRO	2.4
4	F	184	LYS	2.4
2	D	95	SER	2.4
4	F	239	HIS	2.4
2	D	243	PRO	2.4
2	B	282	ARG	2.4
4	F	244	CYS	2.4
4	F	173	ILE	2.3
2	D	180	VAL	2.3
4	F	133	ALA	2.3
4	F	333	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	28	SER	2.3
1	C	163	LYS	2.3
2	D	170	MET	2.3
2	D	247	ASN	2.3
2	D	2	ARG	2.3
3	E	6	MET	2.3
1	C	284	GLU	2.3
2	B	279	GLN	2.2
4	F	171	ASP	2.2
3	E	141	GLU	2.2
4	F	240	LEU	2.2
4	F	130	VAL	2.2
2	D	54	ALA	2.1
3	E	7	GLU	2.1
4	F	32	LYS	2.1
2	D	217	LEU	2.1
1	C	340	SER	2.1
2	D	388	MET	2.1
4	F	169	LEU	2.1
1	C	283	HIS	2.1
2	B	92	PHE	2.1
4	F	163	SER	2.1
4	F	146	VAL	2.1
2	D	96	GLY	2.0
2	B	278	SER	2.0
4	F	1	MET	2.0
2	B	80	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

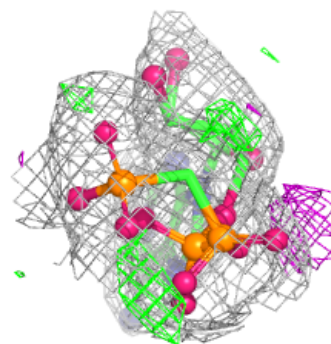
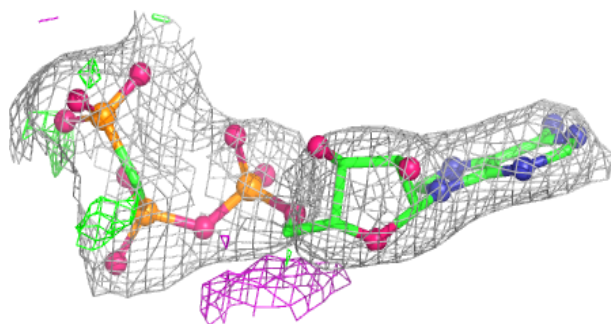
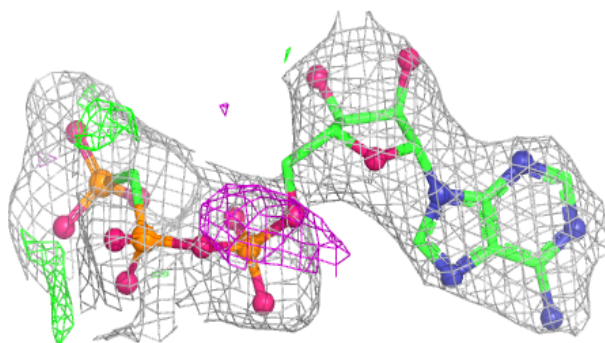
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	ACP	F	401	31/31	0.79	0.13	75,81,108,111	0
5	GTP	D	501	32/32	0.90	0.12	46,55,78,80	0
9	MES	B	503	12/12	0.91	0.14	64,71,72,72	0
9	MES	B	502	12/12	0.91	0.14	34,52,82,84	0
10	Y5M	D	502	23/23	0.95	0.09	28,39,51,53	0
10	Y5M	B	505	23/23	0.96	0.08	21,29,35,37	0
5	GTP	A	501	32/32	0.97	0.06	16,22,31,37	0
6	CA	C	502	1/1	0.98	0.04	49,49,49,49	0
7	MG	B	504	1/1	0.98	0.04	41,41,41,41	0
8	GDP	B	501	28/28	0.98	0.06	14,23,27,28	0
5	GTP	C	501	32/32	0.98	0.05	16,20,23,25	0
7	MG	A	503	1/1	0.99	0.02	24,24,24,24	0
6	CA	A	502	1/1	0.99	0.04	66,66,66,66	0
7	MG	C	503	1/1	0.99	0.05	14,14,14,14	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.

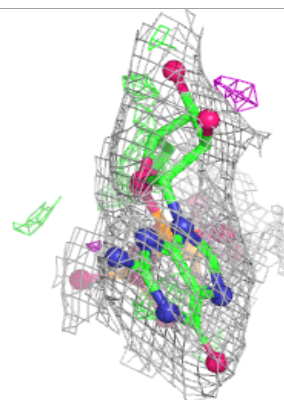
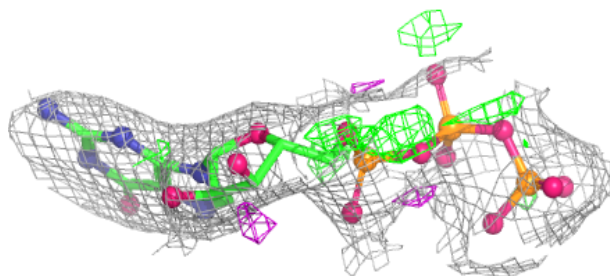
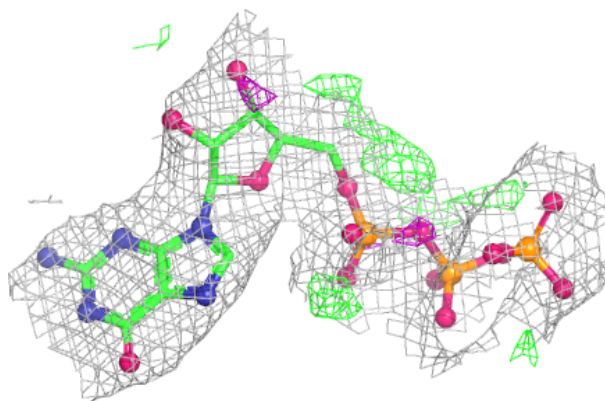
Electron density around ACP F 401:

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

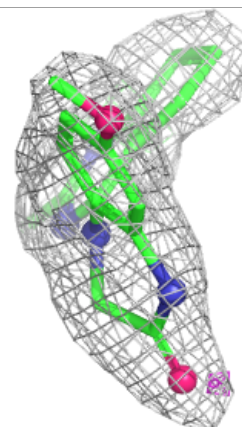
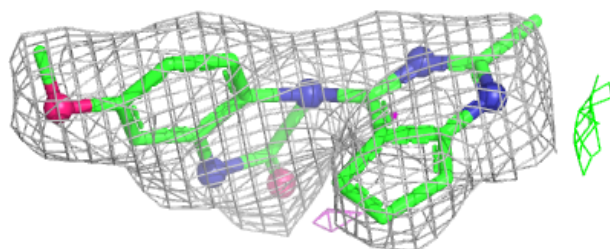
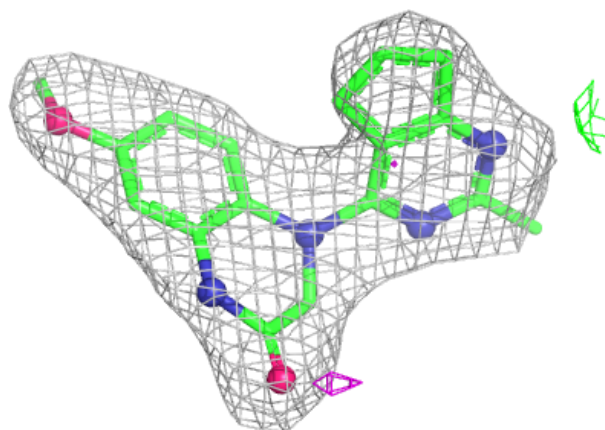


Electron density around GTP D 501:

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

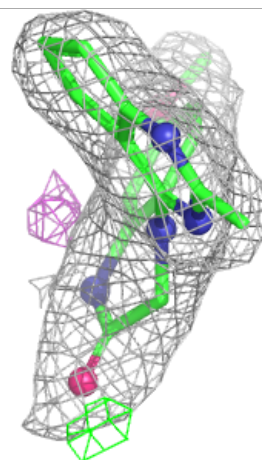
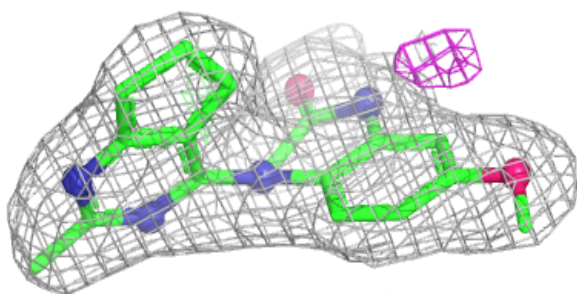
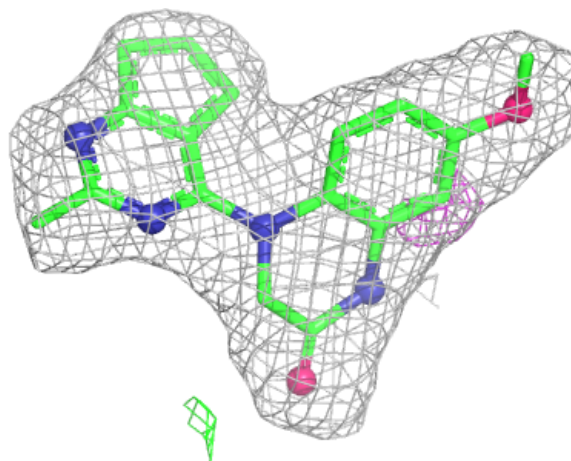
**Electron density around Y5M D 502:**

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



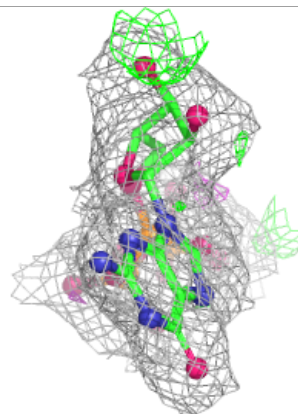
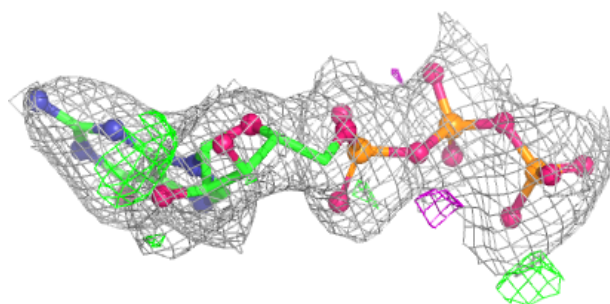
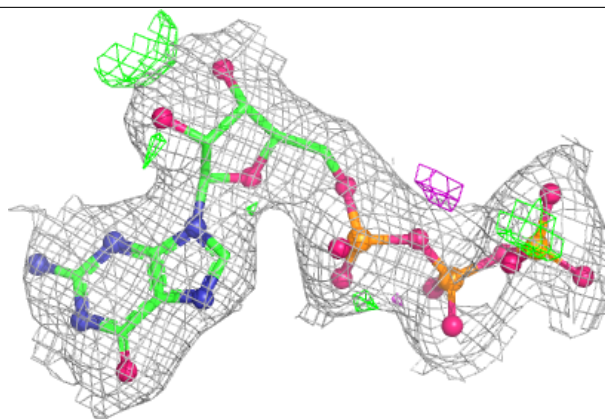
Electron density around Y5M B 505:

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



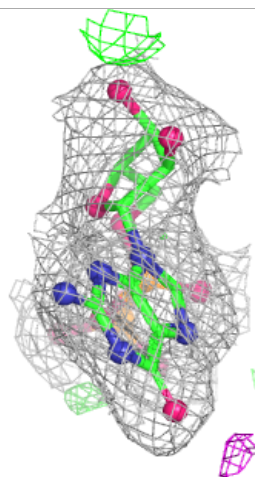
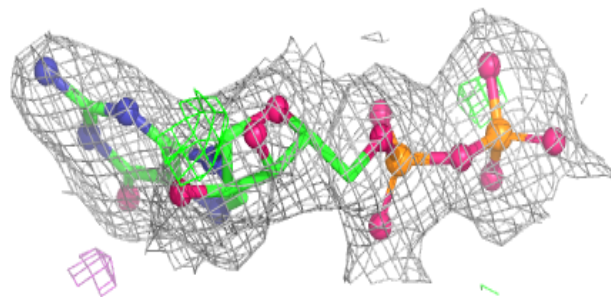
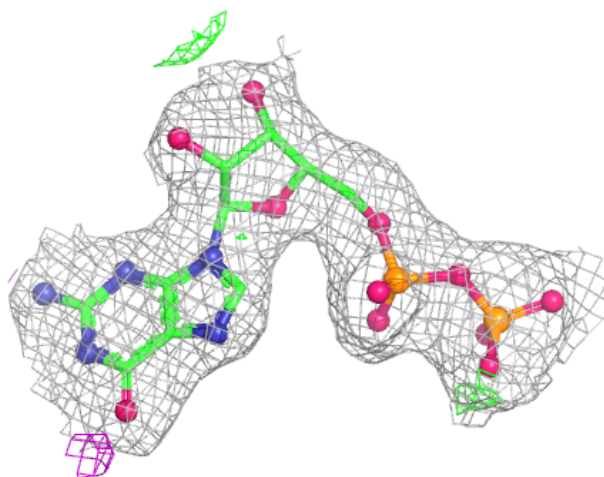
Electron density around GTP A 501:

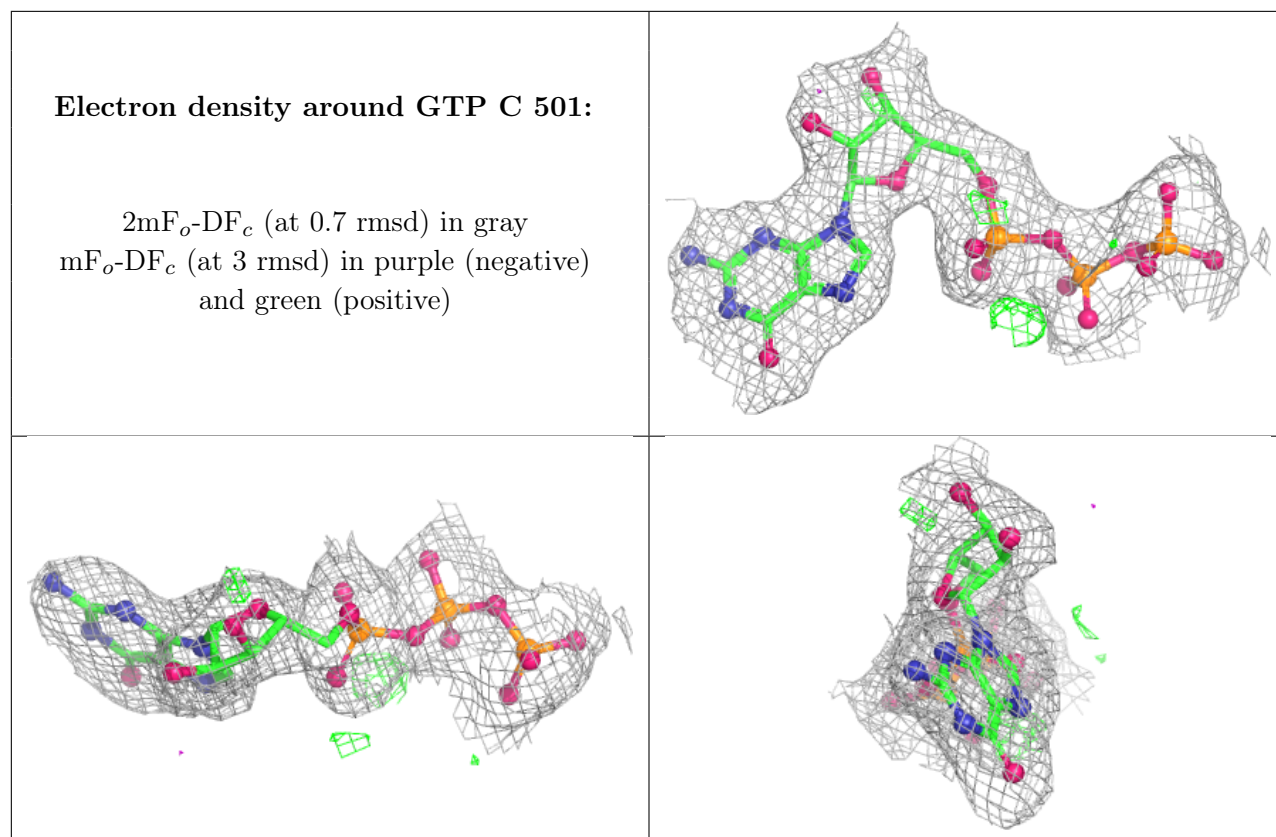
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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 [i](#)

There are no such residues in this entry.