



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:21 PM UTC

PDB ID : 7LZ8 / pdb_00007lz8
Title : Tubulin-RB3_SLD-TTL in complex with compound 5t
Authors : White, S.W.; Yun, M.
Deposited on : 2021-03-09
Resolution : 2.92 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

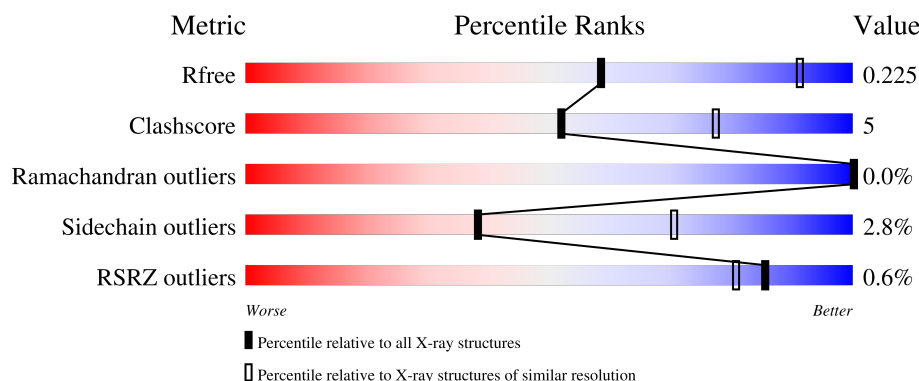
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	83% 14% .
1	C	450	84% 12% ..
2	B	445	86% 9% 5%
2	D	445	75% 18% 6%
3	E	143	67% 17% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	% 58% 8% 33%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 16797 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
			3406	2155	581	649	21			
1	C	438	Total	C	N	O	S	0	0	0
			3428	2170	582	654	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	0	0
			3333	2093	571	643	26			
2	D	417	Total	C	N	O	S	0	0	0
			3278	2061	558	633	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
			993	614	181	193	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	256	Total	C	N	O	S	0	0	0
			2095	1357	357	370	11			

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	B	1	Total	Ca	0	0
			1	1		
6	C	2	Total	Ca	0	0
			2	2		

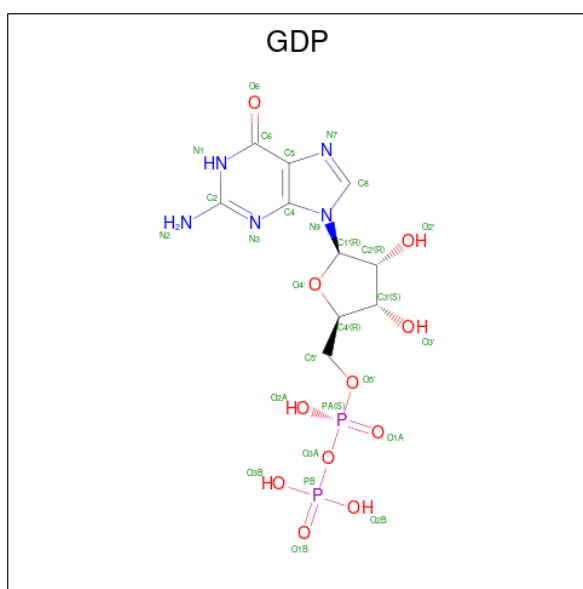
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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		
7	D	1	Total	Mg	0	0
			1	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		
8	D	1	Total	Cl	0	0
			1	1		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



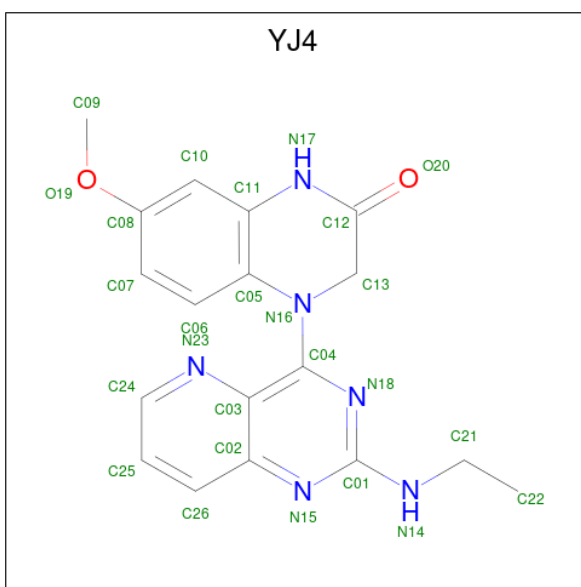
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 11 is 4-[2-(ethylamino)pyrido[3,2-d]pyrimidin-4-yl]-7-methoxy-3,4-dihydroquinoxalin-2(1H)-one (CCD ID: YJ4) (formula: C₁₈H₁₈N₆O₂) (labeled as "Ligand of Interest" by depositor).



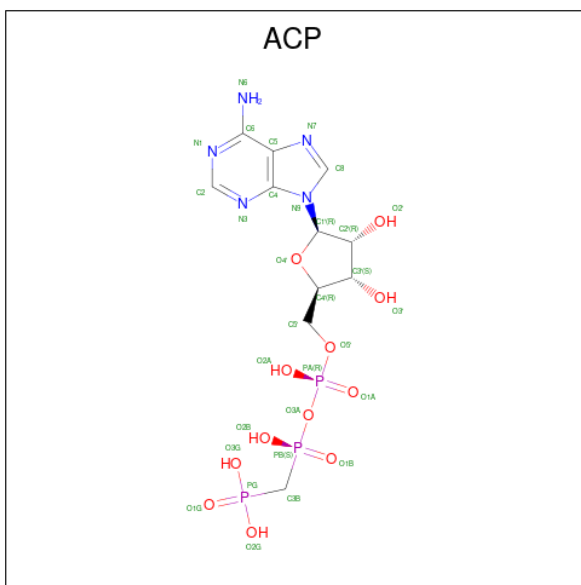
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O		0	0
			26	18	6	2			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	N	O	0	0
			26	18	6	2		

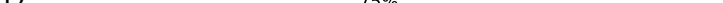
- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

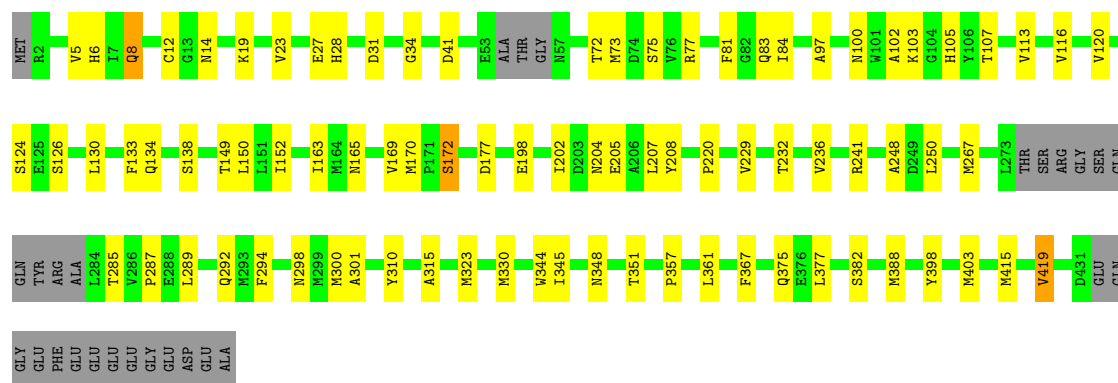


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	F	1	Total	C	N	O	0	0
			17	9	5	3		

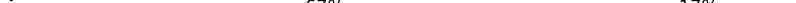
- Molecule 13 is water.

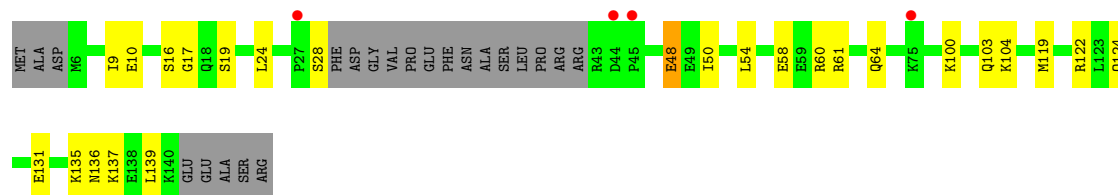
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	7	Total O 7 7	0	0
13	B	10	Total O 10 10	0	0
13	C	17	Total O 17 17	0	0
13	D	3	Total O 3 3	0	0

Chain D:  75% 18% 6%

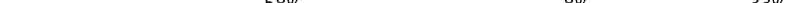


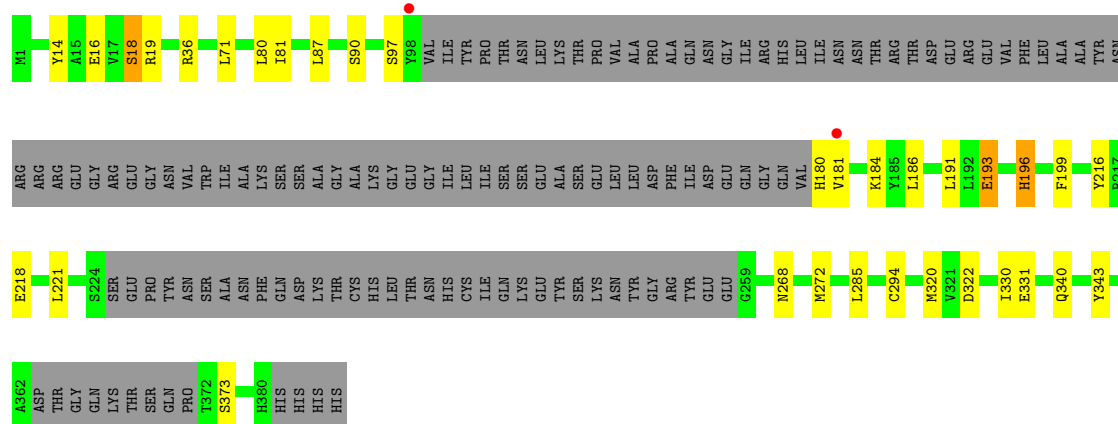
- Molecule 3: Stathmin-4

Chain E:  3% 67% 17% 15%



- Molecule 4: Tubulin Tyrosine Ligase

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.57Å 155.04Å 182.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.36 – 2.92 45.36 – 2.92	Depositor EDS
% Data completeness (in resolution range)	98.1 (45.36-2.92) 92.2 (45.36-2.92)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.184 , 0.228 0.187 , 0.225	Depositor DCC
R_{free} test set	2000 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16797	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: GTP, CL, ACP, MG, YJ4, GDP, CA, 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	0.14	0/3483	0.35	0/4729
1	C	0.15	0/3505	0.40	2/4757 (0.0%)
2	B	0.15	0/3406	0.34	0/4613
2	D	0.14	0/3350	0.35	0/4537
3	E	0.13	0/1001	0.35	0/1328
4	F	0.13	0/2144	0.38	0/2897
All	All	0.14	0/16889	0.36	2/22861 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	ILE	CA-C-N	5.23	127.68	120.67
1	C	171	ILE	C-N-CA	5.23	127.68	120.67

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	3406	0	3316	35	0
1	C	3428	0	3339	33	0
2	B	3333	0	3213	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3278	0	3148	51	0
3	E	993	0	1012	15	0
4	F	2095	0	2097	17	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	2	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
8	A	1	0	0	0	0
8	D	1	0	0	0	0
9	B	28	0	12	0	0
10	B	24	0	24	1	0
11	B	26	0	0	0	0
11	D	26	0	0	1	0
12	F	17	0	8	4	0
13	A	7	0	0	0	0
13	B	10	0	0	0	0
13	C	17	0	0	0	0
13	D	3	0	0	0	0
All	All	16797	0	16205	169	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 5.

All (169) 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:178:THR:HG22	1:C:258:ASN:HD21	1.53	0.74
2:D:170:MET:HE3	2:D:377:LEU:HD11	1.72	0.72
2:D:375:GLN:HB2	2:D:419:VAL:HG23	1.72	0.71
2:D:398:TYR:HB3	2:D:403:MET:HE3	1.75	0.69
1:C:252:LEU:HA	1:C:255:PHE:HD2	1.62	0.65
2:D:330:MET:HG3	2:D:351:THR:HG21	1.78	0.64
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.81	0.63
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.82	0.61
2:B:219:THR:HG21	1:C:326:LYS:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:100:LYS:HA	3:E:103:GLN:HG2	1.83	0.60
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.83	0.60
2:B:202:ILE:HD13	2:B:229:VAL:HG13	1.83	0.59
4:F:81:ILE:HD13	4:F:87:LEU:HD13	1.84	0.59
2:D:31:ASP:OD1	2:D:34:GLY:N	2.34	0.59
1:A:88:HIS:O	1:A:91:GLN:HG2	2.04	0.57
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.86	0.56
2:D:8:GLN:HE21	2:D:14:ASN:HA	1.69	0.56
2:B:293:MET:HG2	2:B:367:PHE:HB2	1.86	0.56
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.87	0.56
3:E:58:GLU:HG3	3:E:61:ARG:HH21	1.71	0.55
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.25	0.54
3:E:60:ARG:O	3:E:64:GLN:HG2	2.07	0.54
4:F:186:LEU:HD11	4:F:322:ASP:HB3	1.90	0.54
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.43	0.54
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.90	0.54
2:D:232:THR:HG21	2:D:300:MET:HG3	1.90	0.54
2:D:12:CYS:SG	2:D:138:SER:HB3	2.49	0.53
2:B:375:GLN:HB2	2:B:419:VAL:HG13	1.90	0.53
2:D:202:ILE:HD13	2:D:229:VAL:HG13	1.91	0.53
1:C:214:ARG:NH1	1:C:220:GLU:O	2.42	0.52
2:D:100:ASN:HD22	2:D:103:LYS:HG3	1.75	0.52
4:F:184:LYS:O	12:F:401:ACP:N6	2.42	0.52
1:A:399:TYR:O	1:A:402:ARG:NH1	2.41	0.51
2:B:2:ARG:HA	2:B:129:CYS:O	2.11	0.51
2:D:172:SER:OG	2:D:205:GLU:N	2.44	0.51
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.46	0.51
2:D:134:GLN:HA	2:D:165:ASN:O	2.11	0.51
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.76	0.50
1:C:320:ARG:HA	1:C:356:ASN:O	2.11	0.50
1:C:211:ASP:OD2	1:C:304:LYS:NZ	2.42	0.50
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.93	0.50
4:F:330:ILE:HD13	12:F:401:ACP:H3'	1.94	0.50
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.94	0.49
2:B:209:ASP:O	2:B:213:ARG:HG2	2.12	0.49
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.95	0.49
1:A:245:ASP:O	3:E:16:SER:OG	2.31	0.49
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.95	0.48
2:B:161:ASP:O	2:B:251:ARG:NH2	2.46	0.48
4:F:320:MET:HB3	4:F:330:ILE:HD11	1.93	0.48
1:C:210:TYR:OH	1:C:221:ARG:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.95	0.48
4:F:199:PHE:CD2	4:F:221:LEU:HD23	2.48	0.48
1:A:325:PRO:O	1:A:328:VAL:HG22	2.14	0.48
2:D:105:HIS:O	2:D:150:LEU:HD22	2.14	0.48
1:C:276:ILE:HG23	1:C:369:ALA:HB3	1.96	0.48
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.49	0.48
2:D:285:THR:HG23	2:D:287:PRO:HD2	1.96	0.48
1:A:209:ILE:HD11	1:A:302:MET:SD	2.54	0.47
1:A:2:ARG:HB3	1:A:133:GLN:HG3	1.95	0.47
1:A:83:TYR:HD2	1:A:86:LEU:HD22	1.80	0.47
2:B:267:MET:HG2	2:B:374:ILE:HD13	1.96	0.47
2:D:107:THR:HG21	3:E:137:LYS:HZ3	1.80	0.47
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.97	0.47
2:B:293:MET:CG	2:B:367:PHE:HB2	2.44	0.47
2:D:294:PHE:HZ	2:D:330:MET:HE1	1.80	0.47
2:D:292:GLN:HG2	2:D:298:ASN:HD21	1.79	0.47
1:A:166:LYS:HE2	1:A:197:HIS:O	2.14	0.47
2:B:335:ASN:OD1	4:F:36:ARG:HD3	2.14	0.47
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.97	0.47
2:D:6:HIS:HE2	2:D:8:GLN:HG2	1.80	0.47
1:C:252:LEU:HA	1:C:255:PHE:CD2	2.46	0.46
2:D:6:HIS:NE2	2:D:8:GLN:HG2	2.31	0.46
2:D:107:THR:HG21	3:E:137:LYS:NZ	2.30	0.46
1:A:296:PHE:CZ	1:A:377:MET:HE1	2.51	0.46
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.30	0.46
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.50	0.46
2:B:134:GLN:HA	2:B:165:ASN:O	2.16	0.46
1:A:241:SER:HB3	1:A:248:LEU:O	2.16	0.46
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.98	0.46
2:D:116:VAL:O	2:D:120:VAL:HG13	2.16	0.46
1:A:406:HIS:HA	1:A:409:VAL:HG22	1.98	0.46
2:B:169:VAL:HA	2:B:202:ILE:O	2.16	0.46
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.97	0.45
1:C:216:ASN:HB3	1:C:275:VAL:O	2.17	0.45
1:A:346:TRP:CD1	1:A:346:TRP:H	2.34	0.45
2:D:310:TYR:CE1	2:D:367:PHE:HZ	2.34	0.45
1:A:274:PRO:HG2	1:A:371:VAL:HG11	1.97	0.45
2:B:324:LYS:NZ	2:B:328:GLU:OE1	2.47	0.45
2:D:102:ALA:HB2	2:D:403:MET:HE2	1.97	0.45
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.51	0.45
3:E:103:GLN:HG3	3:E:104:LYS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.57	0.45
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.00	0.44
1:A:324:VAL:O	1:A:327:ASP:HB2	2.17	0.44
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.99	0.44
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.81	0.44
1:A:141:PHE:O	1:A:147:SER:HB3	2.18	0.44
3:E:135:LYS:HA	3:E:135:LYS:HD3	1.73	0.44
2:B:295:ASP:HA	10:B:503:MES:O3S	2.18	0.44
1:C:255:PHE:CE1	1:C:316:CYS:HB3	2.53	0.44
1:C:250:VAL:HG11	1:C:352:LYS:NZ	2.33	0.44
2:D:170:MET:HE2	2:D:170:MET:HB2	1.85	0.44
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.33	0.44
1:A:39:ASP:OD2	1:A:61:HIS:NE2	2.49	0.43
3:E:48:GLU:H	3:E:48:GLU:HG3	1.47	0.43
2:B:73:MET:HE3	2:B:90:PHE:HD2	1.84	0.43
4:F:320:MET:HE1	12:F:401:ACP:N3	2.33	0.43
2:B:30:ILE:HD11	2:B:47:ILE:HD11	2.00	0.43
3:E:9:ILE:HG22	3:E:10:GLU:HG2	1.99	0.43
1:A:54:SER:O	1:A:61:HIS:HA	2.18	0.43
2:D:315:ALA:HB3	2:D:351:THR:HG22	1.99	0.43
2:D:149:THR:HA	2:D:152:ILE:HG12	2.01	0.43
1:C:271:THR:HG22	1:C:301:GLN:HG2	2.00	0.43
1:A:355:ILE:O	3:E:17:GLY:HA3	2.18	0.43
2:D:165:ASN:HD22	2:D:198:GLU:HB2	1.84	0.43
4:F:16:GLU:HA	4:F:19:ARG:HD2	2.01	0.43
1:C:2:ARG:HB3	1:C:133:GLN:NE2	2.33	0.43
2:D:124:SER:HB2	2:D:130:LEU:HD22	2.01	0.43
2:D:208:TYR:HE1	2:D:220:PRO:HD2	1.82	0.43
1:C:120:ASP:O	1:C:124:LYS:HG2	2.19	0.43
1:A:96:LYS:HG3	1:A:97:GLU:H	1.84	0.43
2:D:382:SER:HB2	2:D:415:MET:HE3	2.01	0.42
2:B:73:MET:HE2	2:B:92:PHE:HB3	2.01	0.42
1:A:134:GLY:HA3	1:A:165:SER:O	2.19	0.42
2:D:415:MET:O	2:D:419:VAL:HG12	2.18	0.42
2:D:81:PHE:O	2:D:84:ILE:HG22	2.20	0.42
2:D:100:ASN:ND2	2:D:103:LYS:HG3	2.34	0.42
1:C:60:LYS:HB3	1:C:60:LYS:HE2	1.74	0.42
2:D:28:HIS:NE2	2:D:241:ARG:HB3	2.35	0.42
1:A:63:PRO:HG2	1:A:87:PHE:CE2	2.55	0.42
2:B:68:LEU:HD12	2:B:97:ALA:HB2	2.01	0.42
4:F:186:LEU:HB3	12:F:401:ACP:H2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.84	0.42
4:F:14:TYR:O	4:F:18:SER:OG	2.36	0.42
4:F:193:GLU:HG3	4:F:196:HIS:H	1.85	0.42
2:B:40:SER:OG	2:B:42:LEU:HB2	2.19	0.41
2:D:19:LYS:O	2:D:23:VAL:HG12	2.19	0.41
2:D:204:ASN:HA	2:D:207:LEU:HD12	2.02	0.41
1:A:90:GLU:O	1:A:121:ARG:HD3	2.20	0.41
2:B:23:VAL:HG21	2:B:230:SER:HB2	2.02	0.41
1:C:241:SER:HB3	1:C:250:VAL:O	2.21	0.41
1:C:320:ARG:HD3	1:C:360:PRO:HB3	2.03	0.41
4:F:180:HIS:HB3	4:F:181:VAL:H	1.74	0.41
1:A:210:TYR:OH	1:A:221:ARG:NH1	2.51	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.55	0.41
2:D:169:VAL:HA	2:D:202:ILE:O	2.20	0.41
2:B:267:MET:HE3	2:B:267:MET:HB3	1.85	0.41
1:C:85:GLN:H	1:C:85:GLN:HG2	1.49	0.41
2:D:344:TRP:CE3	2:D:345:ILE:HG13	2.55	0.41
1:C:276:ILE:HG12	1:C:281:ALA:HB2	2.02	0.41
1:A:234:ILE:O	1:A:238:ILE:HG13	2.20	0.41
1:C:157:LEU:HD23	1:C:157:LEU:HA	1.89	0.41
2:D:73:MET:O	2:D:77:ARG:HG3	2.20	0.41
2:D:357:PRO:HB2	2:D:361:LEU:O	2.20	0.41
2:D:5:VAL:HB	2:D:133:PHE:CD2	2.57	0.41
2:D:23:VAL:O	2:D:27:GLU:HG3	2.21	0.41
2:B:178:THR:HG22	1:C:258:ASN:ND2	2.28	0.40
1:A:296:PHE:CE2	1:A:377:MET:HE1	2.56	0.40
2:D:97:ALA:HB3	5:D:501:GTP:O3G	2.20	0.40
2:D:289:LEU:HD12	2:D:289:LEU:HA	1.92	0.40
2:D:292:GLN:HG2	2:D:298:ASN:ND2	2.36	0.40
1:C:278:ALA:HA	1:C:369:ALA:HB2	2.03	0.40
2:D:170:MET:HE1	2:D:202:ILE:N	2.36	0.40
4:F:268:ASN:O	4:F:272:MET:HG3	2.21	0.40
2:D:248:ALA:HB1	11:D:504:YJ4:N14	2.37	0.40
3:E:54:LEU:HD23	3:E:54:LEU:HA	1.95	0.40
1:A:86:LEU:HD12	1:A:86:LEU:HA	1.95	0.40
2:B:403:MET:HE2	2:B:403:MET:HB3	1.98	0.40
3:E:119:MET:O	3:E:122:ARG:HG2	2.21	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%)	422 (97%)	13 (3%)	0	100	100
1	C	434/450 (96%)	423 (98%)	11 (2%)	0	100	100
2	B	420/445 (94%)	413 (98%)	7 (2%)	0	100	100
2	D	411/445 (92%)	401 (98%)	10 (2%)	0	100	100
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	248/384 (65%)	236 (95%)	11 (4%)	1 (0%)	30	58
All	All	2065/2317 (89%)	2011 (97%)	53 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	373	SER

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	366/378 (97%)	358 (98%)	8 (2%)	45	75
1	C	371/378 (98%)	361 (97%)	10 (3%)	39	71
2	B	366/383 (96%)	363 (99%)	3 (1%)	73	89
2	D	360/383 (94%)	347 (96%)	13 (4%)	31	63
3	E	107/127 (84%)	99 (92%)	8 (8%)	12	35
4	F	230/342 (67%)	221 (96%)	9 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1800/1991 (90%)	1749 (97%)	51 (3%)	38 70

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	48	SER
1	A	85	GLN
1	A	168	GLU
1	A	176	GLN
1	A	241	SER
1	A	324	VAL
1	A	419	SER
2	B	8	GLN
2	B	77	ARG
2	B	375	GLN
1	C	38	SER
1	C	71	GLU
1	C	85	GLN
1	C	128	GLN
1	C	196	GLU
1	C	241	SER
1	C	253	THR
1	C	335	ILE
1	C	381	THR
1	C	384	ILE
2	D	8	GLN
2	D	41	ASP
2	D	72	THR
2	D	75	SER
2	D	83	GLN
2	D	113	VAL
2	D	126	SER
2	D	172	SER
2	D	177	ASP
2	D	236	VAL
2	D	323	MET
2	D	388	MET
2	D	419	VAL
3	E	19	SER
3	E	24	LEU
3	E	48	GLU

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Mol	Chain	Res	Type
3	E	50	ILE
3	E	124	GLN
3	E	131	GLU
3	E	136	ASN
3	E	139	LEU
4	F	18	SER
4	F	80	LEU
4	F	90	SER
4	F	97	SER
4	F	191	LEU
4	F	193	GLU
4	F	196	HIS
4	F	285	LEU
4	F	331	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
1	A	309	HIS
1	A	356	ASN
1	A	393	HIS
2	B	99	ASN
2	B	165	ASN
2	B	337	ASN
1	C	15	GLN
1	C	61	HIS
1	C	133	GLN
1	C	293	ASN
1	C	356	ASN
1	C	393	HIS
2	D	8	GLN
2	D	100	ASN
2	D	332	ASN
4	F	333	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 10 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$
12	ACP	F	401	-	19,19,33	1.86	5 (26%)	27,28,52	2.19	10 (37%)
11	YJ4	D	504	-	29,29,29	0.94	1 (3%)	35,41,41	1.75	9 (25%)
9	GDP	B	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.74	6 (13%)
5	GTP	C	501	7	33,34,34	0.99	2 (6%)	50,54,54	1.62	9 (18%)
5	GTP	A	501	7	33,34,34	0.94	1 (3%)	50,54,54	1.64	9 (18%)
11	YJ4	B	506	-	29,29,29	0.95	1 (3%)	35,41,41	1.82	8 (22%)
5	GTP	D	501	7	33,34,34	0.97	2 (6%)	50,54,54	1.60	8 (16%)
10	MES	B	502	-	12,12,12	2.33	1 (8%)	15,16,16	1.90	3 (20%)
10	MES	B	503	-	12,12,12	2.30	1 (8%)	15,16,16	1.80	3 (20%)

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
12	ACP	F	401	-	-	0/4/17/38	0/3/3/3
11	YJ4	D	504	-	-	3/9/21/21	0/4/4/4
9	GDP	B	501	-	-	5/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	501	7	-	5/22/38/38	0/3/3/3
5	GTP	A	501	7	-	6/22/38/38	0/3/3/3
11	YJ4	B	506	-	-	3/9/21/21	0/4/4/4
5	GTP	D	501	7	-	3/22/38/38	0/3/3/3
10	MES	B	502	-	-	4/6/14/14	0/1/1/1
10	MES	B	503	-	-	0/6/14/14	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	502	MES	C8-S	-7.82	1.66	1.77
10	B	503	MES	C8-S	-7.72	1.66	1.77
12	F	401	ACP	C6-N6	4.43	1.45	1.34
12	F	401	ACP	O3'-C3'	-3.40	1.36	1.43
9	B	501	GDP	C5-C4	3.02	1.47	1.38
12	F	401	ACP	C5-C4	-2.76	1.34	1.39
12	F	401	ACP	C5-N7	-2.46	1.34	1.39
5	C	501	GTP	PA-O3A	2.36	1.62	1.59
11	B	506	YJ4	C05-N16	2.34	1.44	1.40
9	B	501	GDP	C6-N1	-2.28	1.34	1.38
9	B	501	GDP	C5-N7	-2.21	1.34	1.39
5	A	501	GTP	C2-N3	2.20	1.38	1.33
11	D	504	YJ4	C05-N16	2.19	1.44	1.40
12	F	401	ACP	C8-N9	-2.17	1.33	1.37
5	D	501	GTP	C2-N3	2.16	1.38	1.33
5	C	501	GTP	C2-N3	2.14	1.38	1.33
5	D	501	GTP	PB-O3A	2.06	1.61	1.59

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	C5-C4-N3	-6.06	118.74	128.39
12	F	401	ACP	N3-C2-N1	-5.27	120.61	128.58
9	B	501	GDP	C2-N3-C4	5.08	121.05	112.30
5	A	501	GTP	C5-C4-N3	-5.07	120.32	128.39
5	A	501	GTP	C2-N3-C4	4.96	120.85	112.30
5	D	501	GTP	C5-C4-N3	-4.88	120.62	128.39
11	B	506	YJ4	O20-C12-N17	-4.86	116.24	121.39
5	C	501	GTP	C5-C4-N3	-4.83	120.70	128.39
5	C	501	GTP	C2-N3-C4	4.80	120.56	112.30
5	D	501	GTP	C2-N3-C4	4.64	120.30	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	C5-N4-C3	4.64	118.83	108.84
11	D	504	YJ4	O20-C12-N17	-4.64	116.47	121.39
10	B	502	MES	C5-N4-C3	4.51	118.56	108.84
9	B	501	GDP	N9-C4-N3	4.34	134.63	125.95
12	F	401	ACP	C5-C4-N3	-4.22	120.90	126.72
12	F	401	ACP	N9-C8-N7	-4.14	108.07	113.94
11	B	506	YJ4	C09-O19-C08	3.83	125.71	117.50
11	B	506	YJ4	C21-N14-C01	-3.78	118.78	124.35
11	D	504	YJ4	C05-N16-C04	3.65	125.95	119.21
11	D	504	YJ4	C09-O19-C08	3.60	125.23	117.50
11	B	506	YJ4	C05-N16-C04	3.42	125.52	119.21
9	B	501	GDP	C6-C5-N7	3.41	136.50	130.29
5	D	501	GTP	N9-C4-N3	3.38	132.71	125.95
5	A	501	GTP	N9-C4-N3	3.24	132.43	125.95
5	A	501	GTP	C2-N1-C6	-3.19	119.33	125.11
5	C	501	GTP	N9-C4-N3	3.11	132.18	125.95
5	D	501	GTP	C2-N1-C6	-3.07	119.54	125.11
11	B	506	YJ4	C13-C12-N17	3.03	119.90	116.13
12	F	401	ACP	C2-N3-C4	2.95	119.04	111.83
5	C	501	GTP	C2-N1-C6	-2.94	119.79	125.11
11	D	504	YJ4	C13-C12-N17	2.89	119.73	116.13
12	F	401	ACP	C3'-C2'-C1'	2.85	104.69	101.76
5	A	501	GTP	C5-C6-N1	2.82	120.44	113.25
5	D	501	GTP	O6-C6-C5	-2.82	119.08	126.53
5	C	501	GTP	N9-C8-N7	-2.82	108.17	113.40
5	D	501	GTP	N9-C8-N7	-2.78	108.25	113.40
9	B	501	GDP	C4-C5-N7	-2.74	106.32	110.67
5	A	501	GTP	O6-C6-C5	-2.73	119.33	126.53
12	F	401	ACP	C5-N7-C8	2.70	107.69	103.45
10	B	502	MES	O1S-S-C8	2.69	110.80	106.73
5	C	501	GTP	C5-C6-N1	2.65	120.00	113.25
5	A	501	GTP	N9-C8-N7	-2.63	108.52	113.40
5	C	501	GTP	C8-N7-C5	2.62	108.92	104.26
5	C	501	GTP	O6-C6-C5	-2.61	119.64	126.53
11	B	506	YJ4	C24-N23-C03	2.59	120.36	117.31
5	D	501	GTP	C5-C6-N1	2.58	119.83	113.25
5	A	501	GTP	C8-N7-C5	2.54	108.79	104.26
10	B	502	MES	C6-C5-N4	-2.50	106.33	110.12
11	D	504	YJ4	C24-N23-C03	2.49	120.24	117.31
12	F	401	ACP	C4-N9-C8	2.46	108.32	105.74
11	D	504	YJ4	C21-N14-C01	-2.43	120.77	124.35
5	D	501	GTP	C8-N7-C5	2.41	108.55	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	504	YJ4	C11-N17-C12	-2.38	121.60	124.45
12	F	401	ACP	C2'-C1'-N9	-2.38	107.40	113.30
12	F	401	ACP	N3-C4-N9	2.36	131.17	127.17
11	B	506	YJ4	C11-N17-C12	-2.35	121.64	124.45
11	D	504	YJ4	N14-C01-N18	-2.33	113.13	117.16
11	D	504	YJ4	C22-C21-N14	-2.28	104.22	111.45
12	F	401	ACP	C4-C5-N7	-2.26	108.00	110.58
10	B	503	MES	O1S-S-C8	2.24	110.11	106.73
5	C	501	GTP	O3G-PG-O3B	2.19	111.98	104.64
10	B	503	MES	C7-N4-C5	2.13	116.92	111.24
5	A	501	GTP	O2G-PG-O3B	2.07	111.59	104.64
9	B	501	GDP	O6-C6-C5	-2.02	121.21	126.53
11	B	506	YJ4	C22-C21-N14	-2.01	105.09	111.45

There are no chirality outliers.

All (29) 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	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
5	D	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
10	B	502	MES	C7-C8-S-O2S
10	B	502	MES	C7-C8-S-O3S
11	B	506	YJ4	C03-C04-N16-C05
11	D	504	YJ4	N18-C04-N16-C13
11	B	506	YJ4	N18-C04-N16-C13
10	B	502	MES	C7-C8-S-O1S
9	B	501	GDP	PB-O3A-PA-O1A
11	B	506	YJ4	C03-C04-N16-C13
5	A	501	GTP	PB-O3B-PG-O1G
10	B	502	MES	C8-C7-N4-C3

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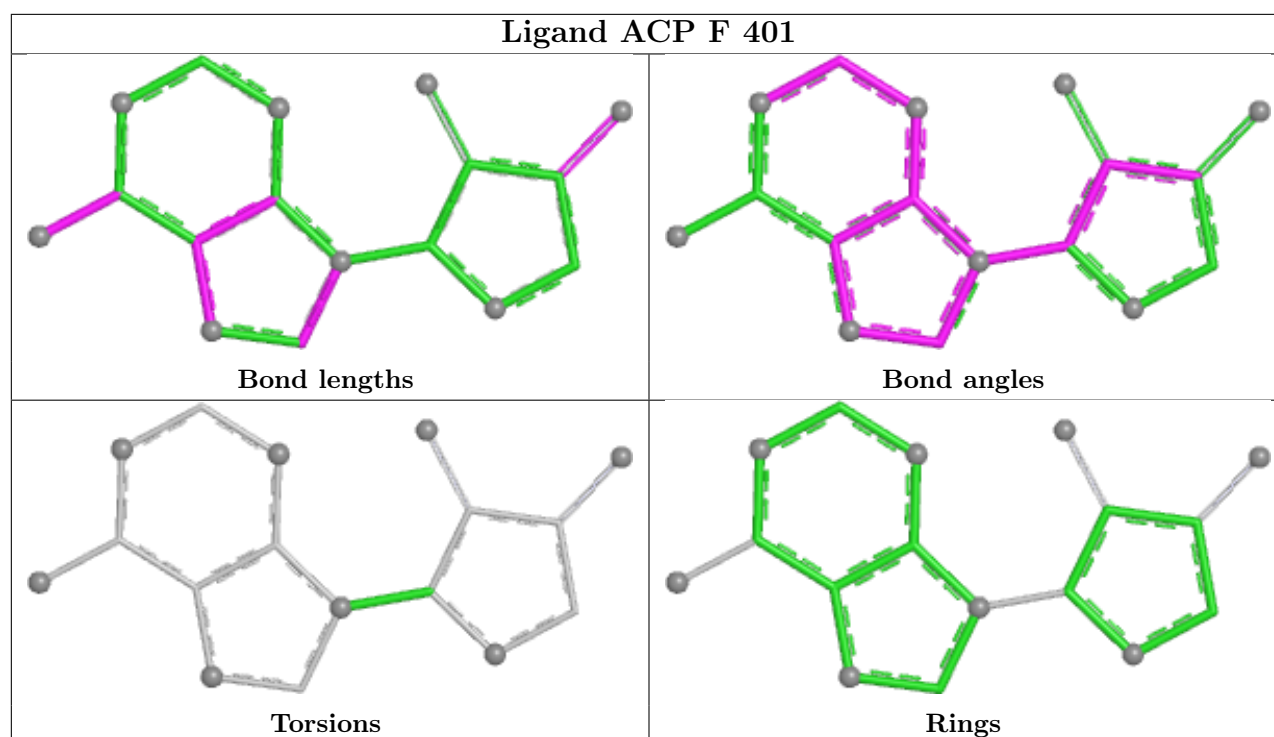
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
11	D	504	YJ4	C03-C04-N16-C05
11	D	504	YJ4	C03-C04-N16-C13
9	B	501	GDP	PB-O3A-PA-O2A

There are no ring outliers.

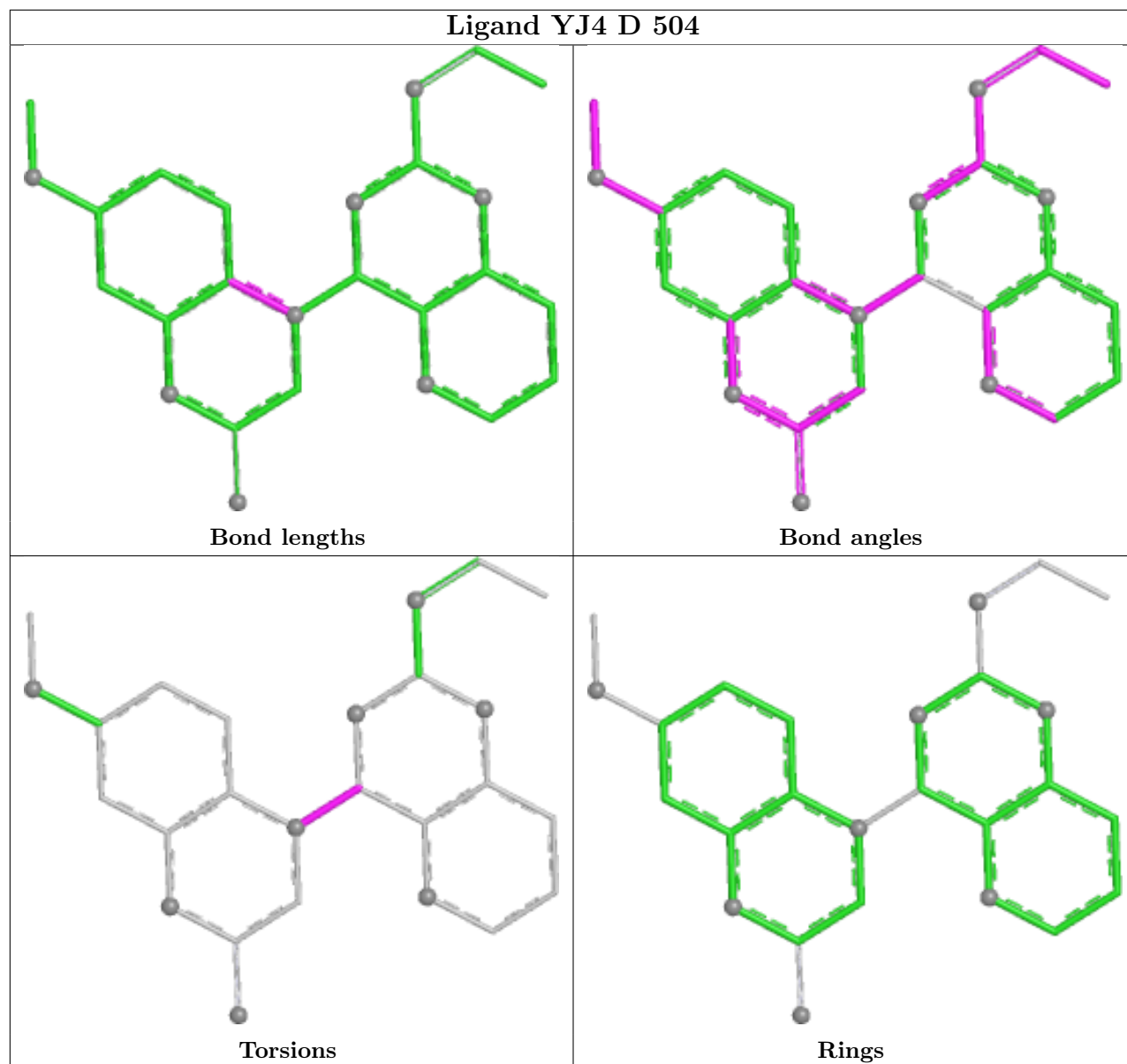
4 monomers are involved in 7 short contacts:

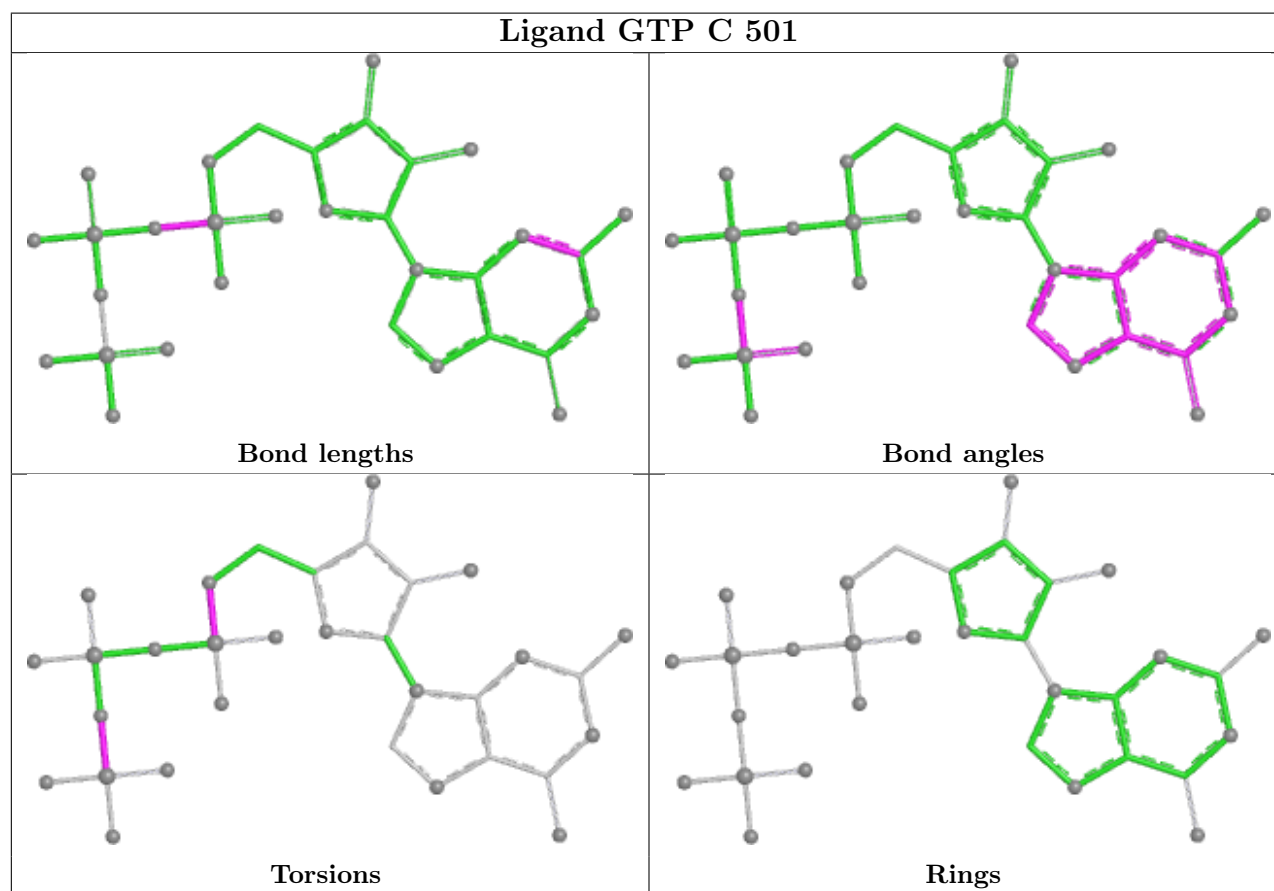
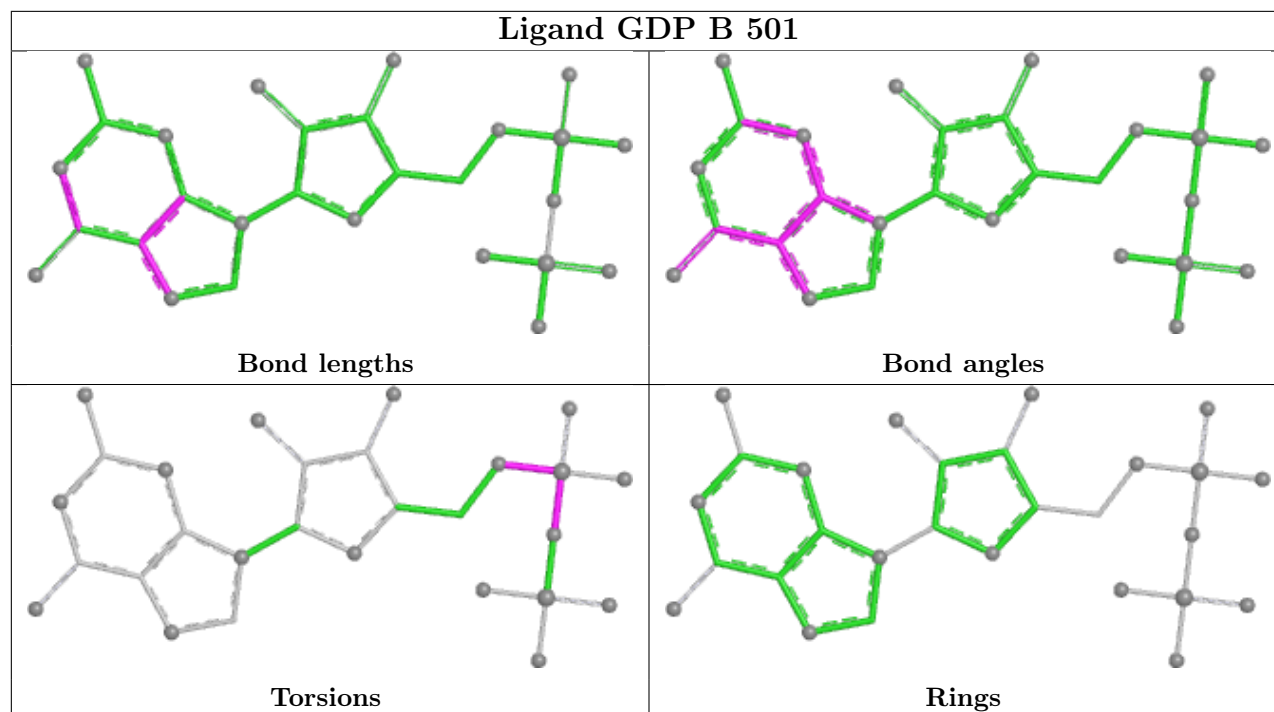
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	401	ACP	4	0
11	D	504	YJ4	1	0
5	D	501	GTP	1	0
10	B	503	MES	1	0

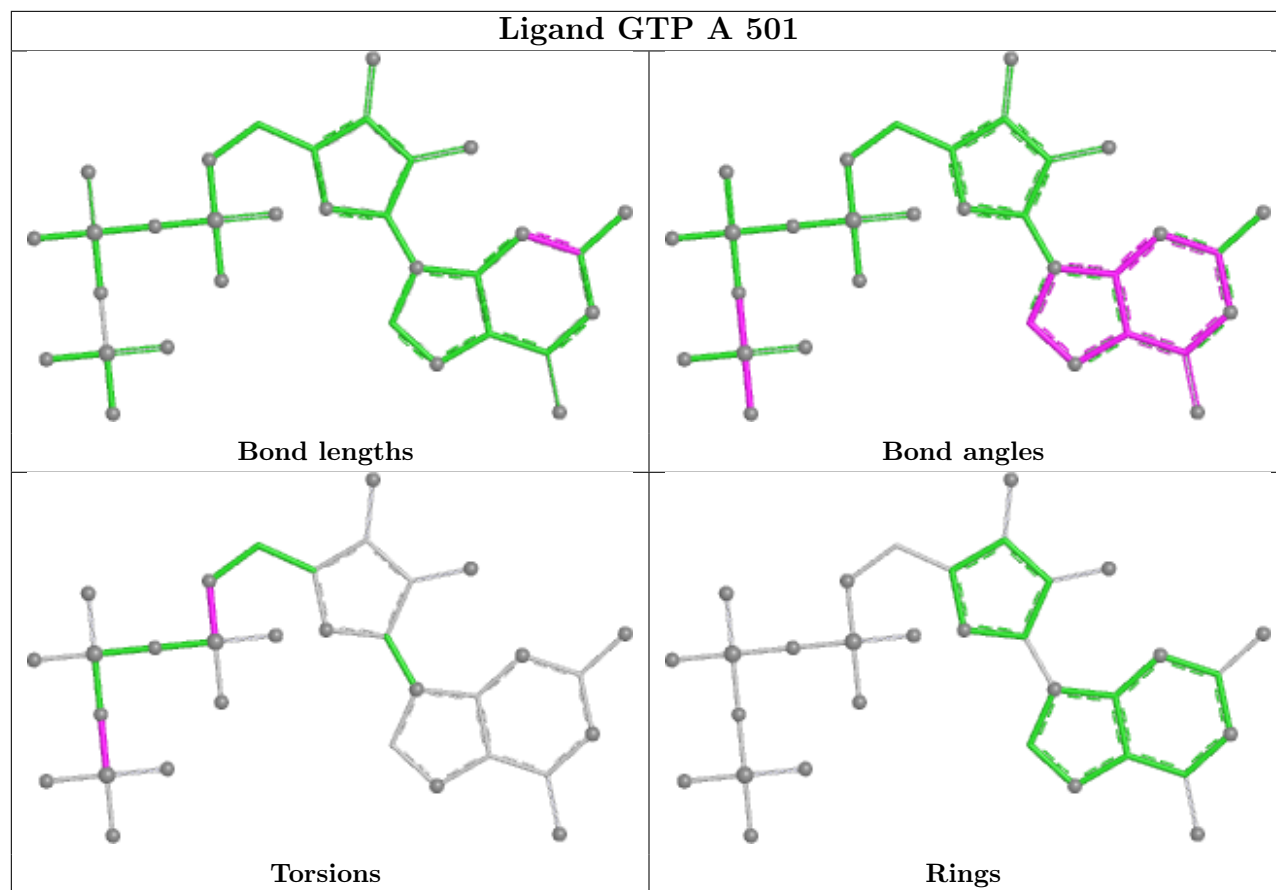
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



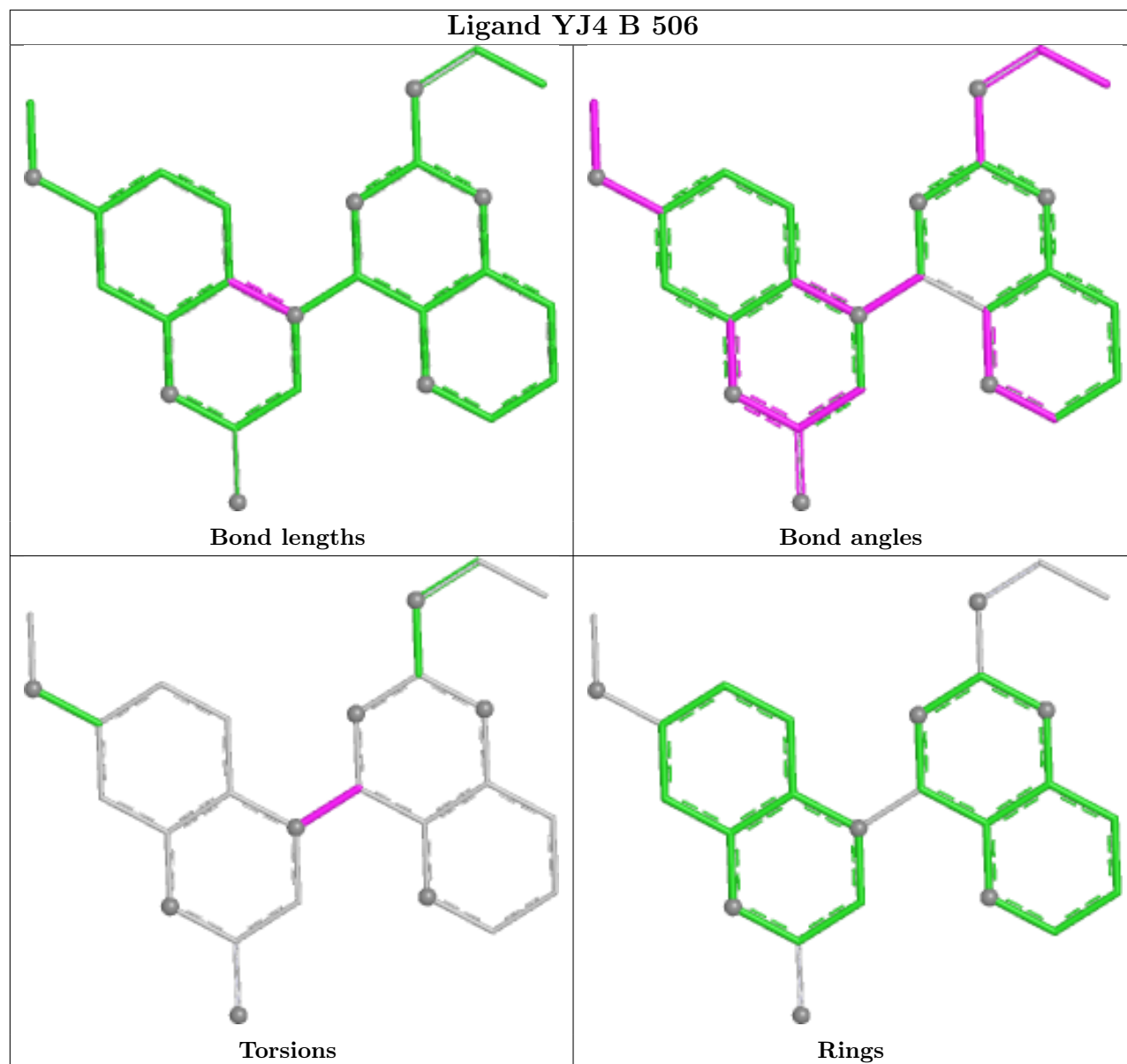
Ligand YJ4 D 504

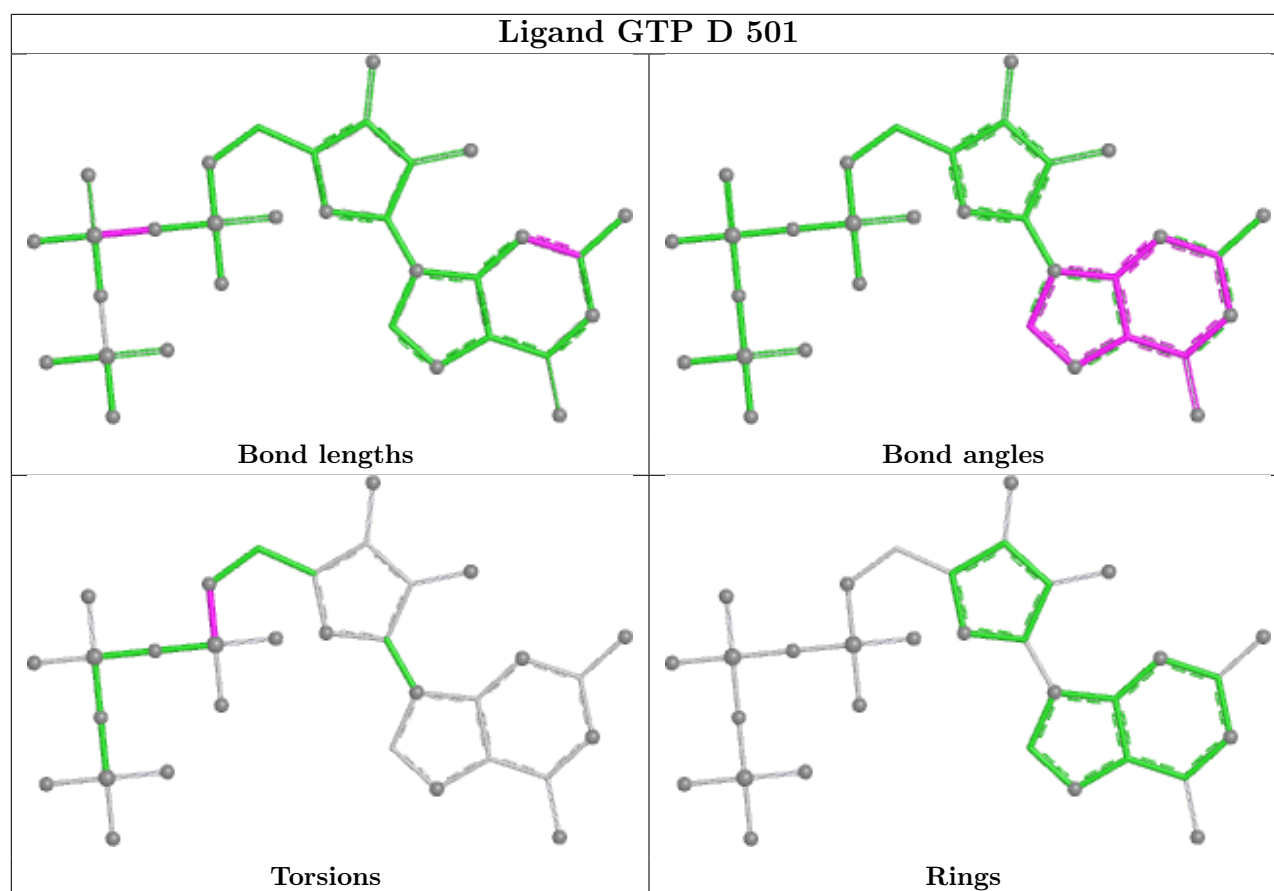






Ligand YJ4 B 506





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.17	4 (0%) 81 74	57, 81, 121, 164	0
1	C	438/450 (97%)	-0.25	0 100 100	50, 66, 99, 147	0
2	B	424/445 (95%)	-0.22	3 (0%) 84 79	48, 68, 111, 153	0
2	D	417/445 (93%)	-0.03	0 100 100	61, 95, 131, 156	0
3	E	121/143 (84%)	0.07	4 (3%) 49 39	57, 94, 136, 167	0
4	F	256/384 (66%)	0.05	2 (0%) 82 76	65, 103, 146, 177	0
All	All	2093/2317 (90%)	-0.13	13 (0%) 85 81	48, 82, 128, 177	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	281	TYR	3.5
4	F	181	VAL	2.8
1	A	1	MET	2.7
3	E	44	ASP	2.6
4	F	98	TYR	2.5
3	E	45	PRO	2.5
1	A	437	VAL	2.4
2	B	360	GLY	2.4
3	E	75	LYS	2.2
3	E	27	PRO	2.2
2	B	428	ALA	2.1
1	A	282	TYR	2.1
1	A	247	ALA	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](#)

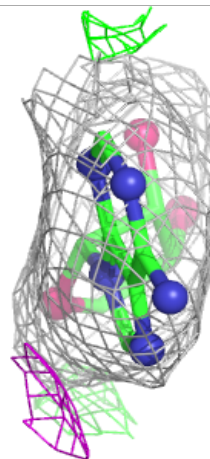
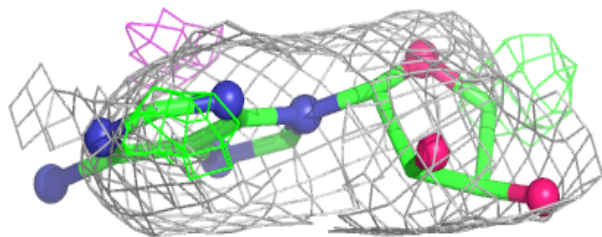
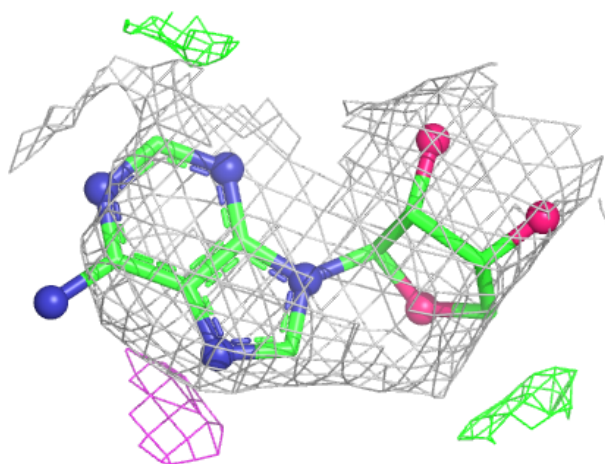
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	ACP	F	401	17/31	0.71	0.14	119,132,155,166	0
6	CA	C	504	1/1	0.76	0.23	124,124,124,124	0
6	CA	B	505	1/1	0.86	0.22	120,120,120,120	0
8	CL	A	504	1/1	0.88	0.15	102,102,102,102	0
7	MG	D	502	1/1	0.92	0.10	104,104,104,104	0
10	MES	B	503	12/12	0.94	0.11	89,103,134,147	0
8	CL	D	503	1/1	0.94	0.21	86,86,86,86	0
10	MES	B	502	12/12	0.95	0.09	61,73,90,103	0
7	MG	B	504	1/1	0.95	0.07	109,109,109,109	0
5	GTP	D	501	32/32	0.95	0.07	80,99,115,120	0
6	CA	A	502	1/1	0.96	0.06	133,133,133,133	0
7	MG	A	503	1/1	0.96	0.04	58,58,58,58	0
11	YJ4	D	504	26/26	0.96	0.08	58,69,89,93	0
9	GDP	B	501	28/28	0.96	0.06	47,56,64,81	0
11	YJ4	B	506	26/26	0.97	0.08	50,63,78,81	0
6	CA	C	502	1/1	0.97	0.05	97,97,97,97	0
5	GTP	C	501	32/32	0.97	0.06	54,58,77,82	0
5	GTP	A	501	32/32	0.98	0.05	56,60,75,83	0
7	MG	C	503	1/1	1.00	0.02	62,62,62,62	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.

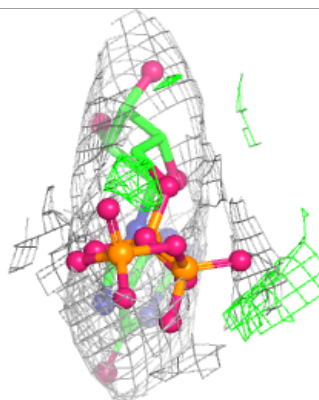
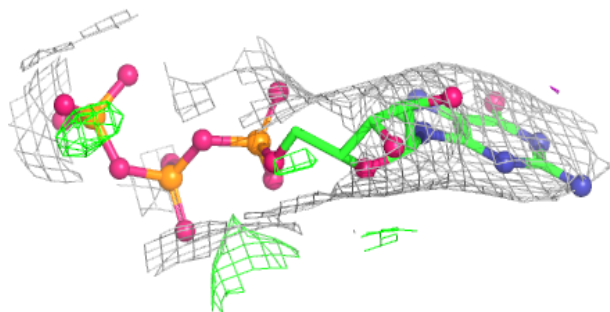
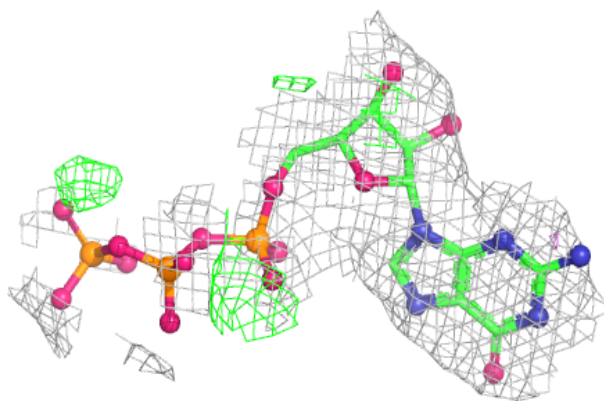
Electron density around ACP F 401:

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

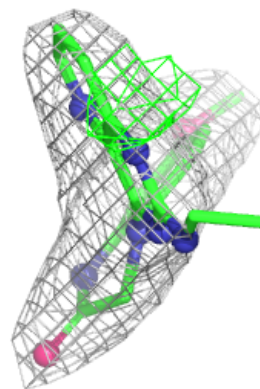
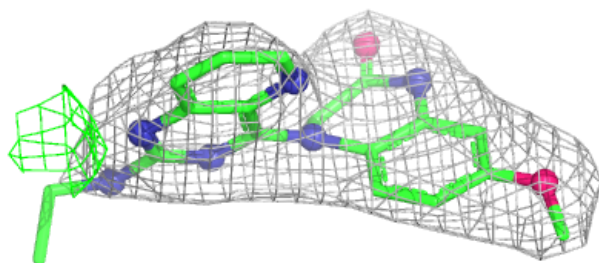
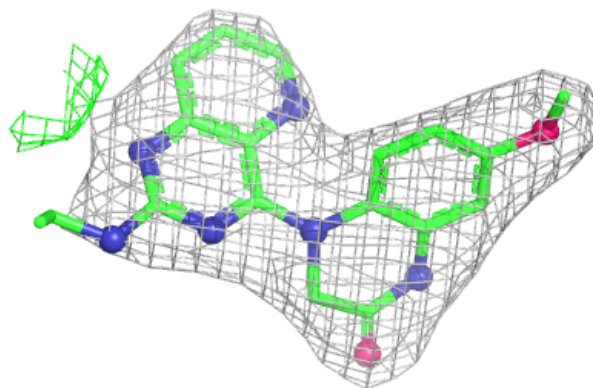


Electron density around GTP D 501:

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

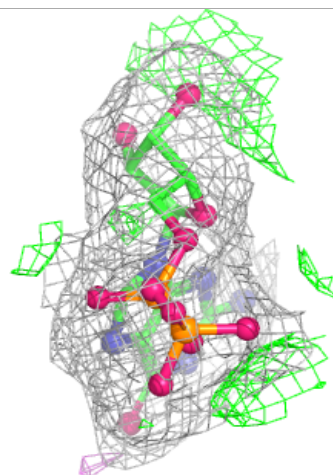
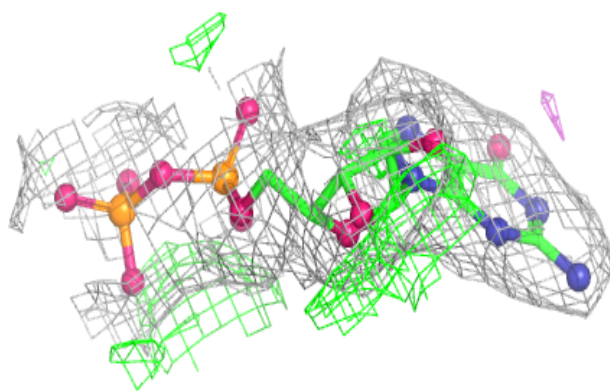
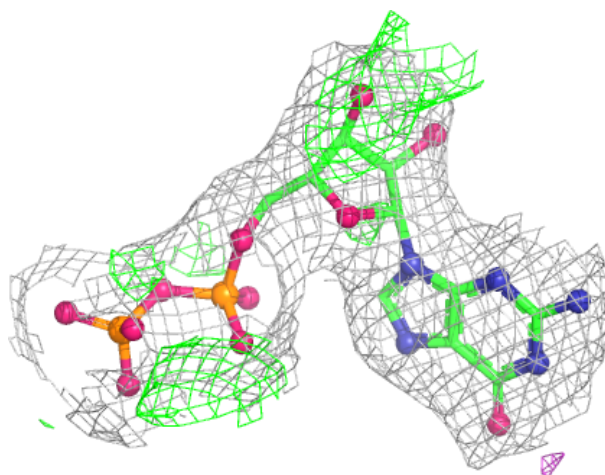
**Electron density around YJ4 D 504:**

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



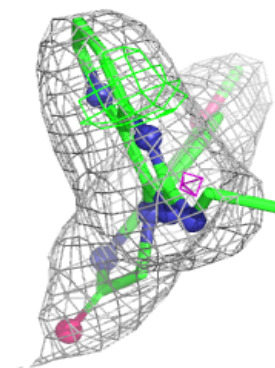
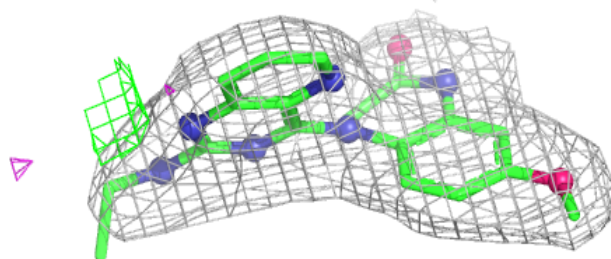
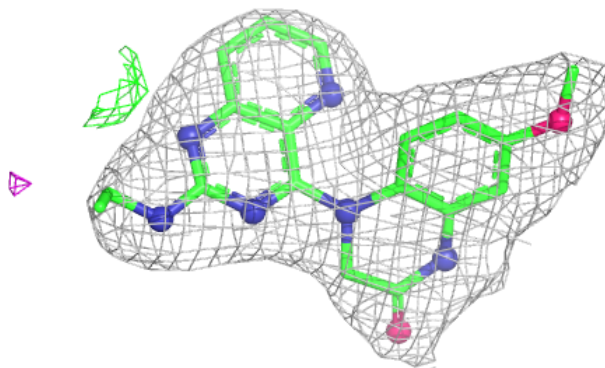
Electron density around GDP B 501:

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

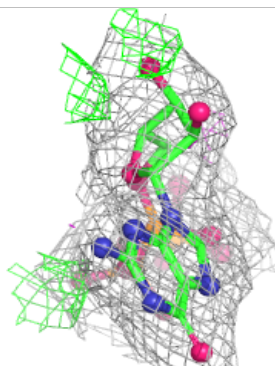
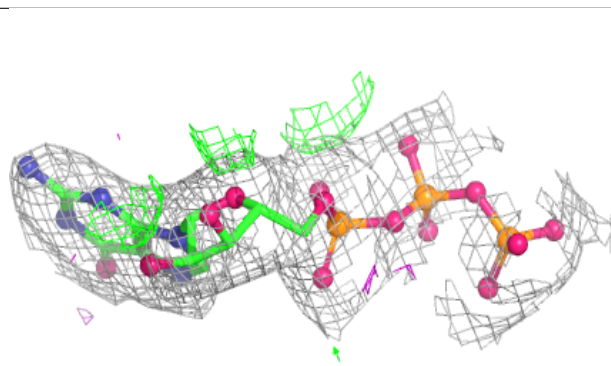
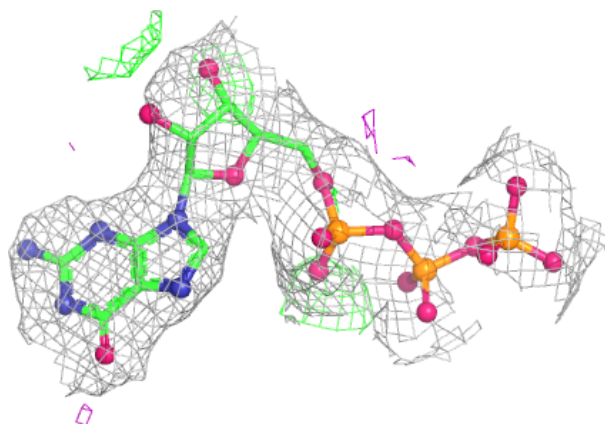


Electron density around YJ4 B 506:

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

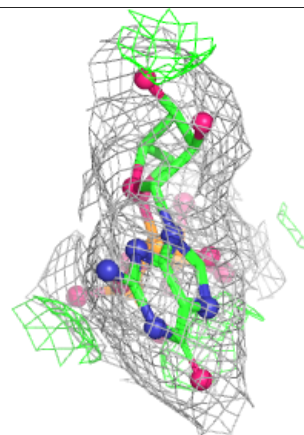
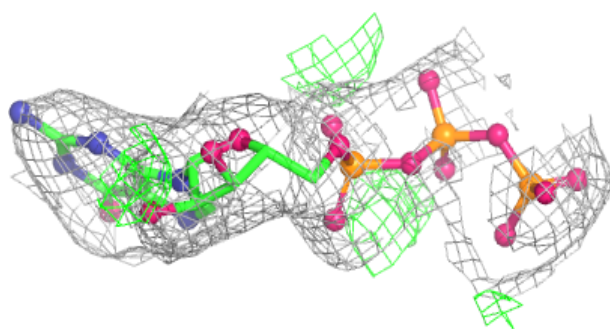
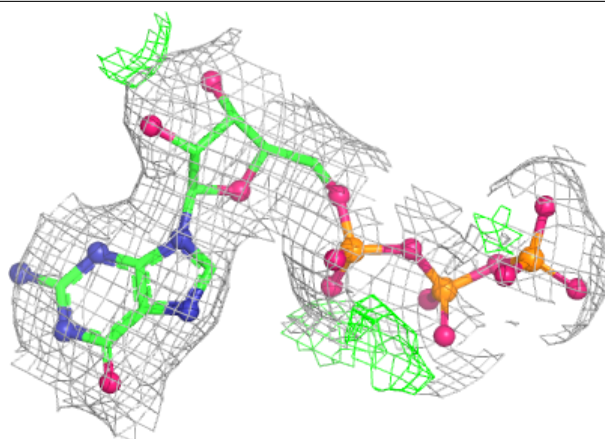
**Electron density around GTP C 501:**

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



Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.