



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2021 – 03:09 PM EDT

PDB ID : 7LZ7
Title : Tubulin-RB3_SLD-TTL in complex with compound 5k
Authors : White, S.W.; Yun, M.
Deposited on : 2021-03-09
Resolution : 2.80 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

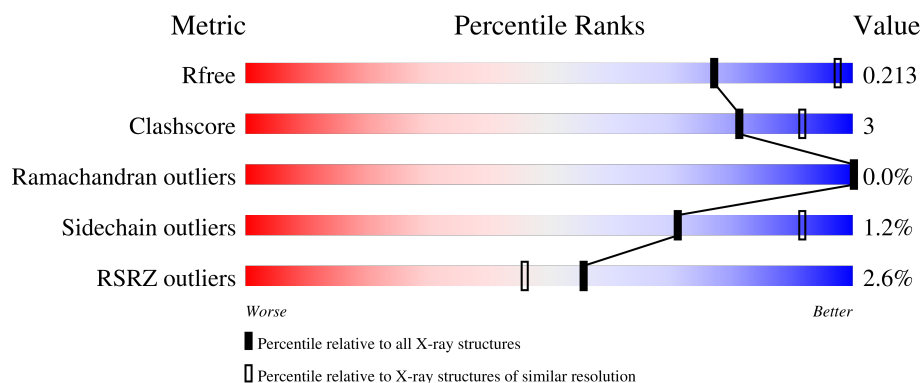
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	 90% 8% .
1	C	450	 91% 7% .
2	B	445	 87% 9% .
2	D	445	 87% 7% 5%
3	E	143	 79% 6% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div>11%</div><div>78%</div><div>7%</div><div>15%</div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17560 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

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

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

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

- Molecule 3 is a protein called Stathmin-4.

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

There are 2 discrepancies between the modelled and reference sequences:

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

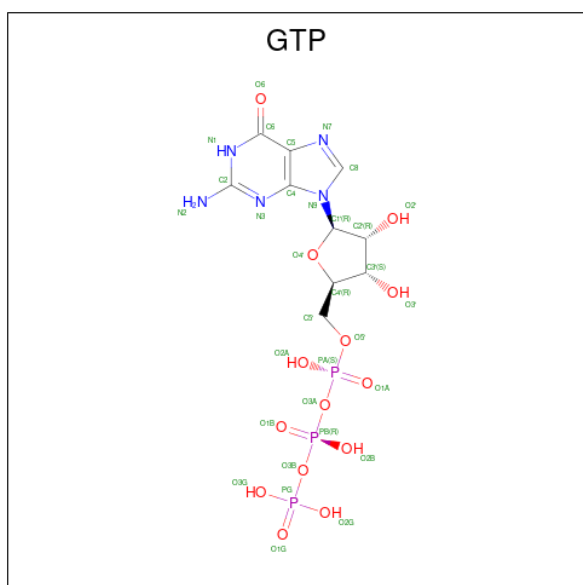
- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	328	Total	C	N	O	S	0	0	0
			2672	1718	459	481	14			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (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		

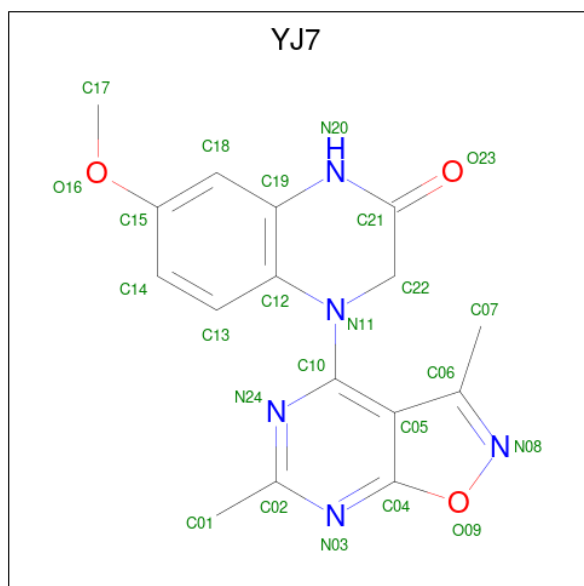
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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).

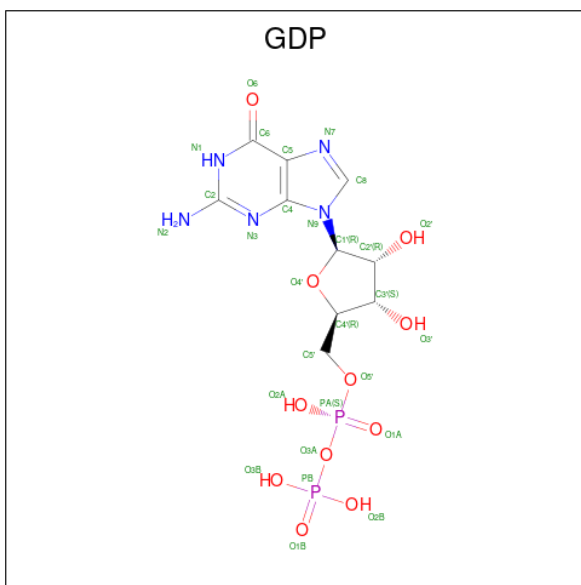
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		
7	F	1	Total	Mg	0	0
			1	1		

- Molecule 8 is 4-(3,6-dimethyl[1,2]oxazolo[5,4-d]pyrimidin-4-yl)-7-methoxy-3,4-dihydroquinoxalin-2(1H)-one (three-letter code: YJ7) (formula: C₁₆H₁₅N₅O₃) (labeled as "Ligand of Interest" by depositor).



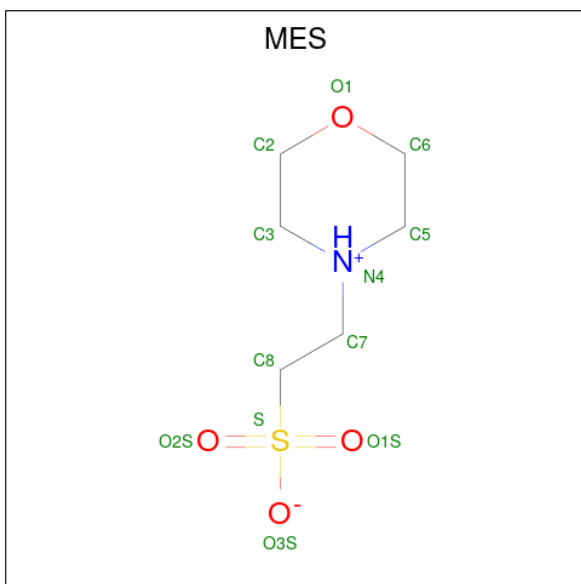
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			24	16	5	3		
8	D	1	Total	C	N	O	0	0
			24	16	5	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



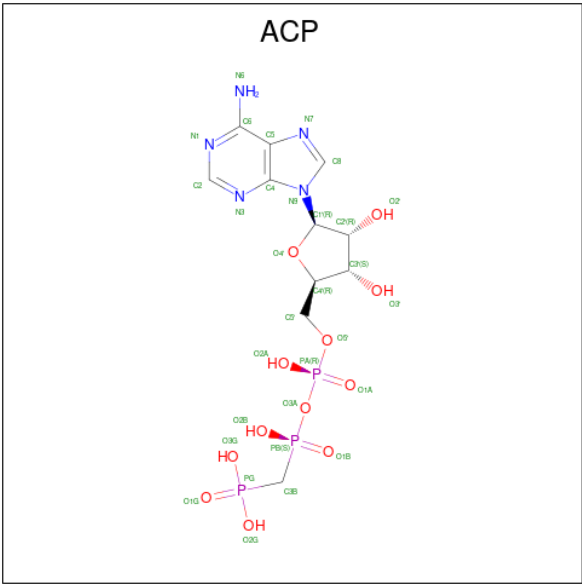
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



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

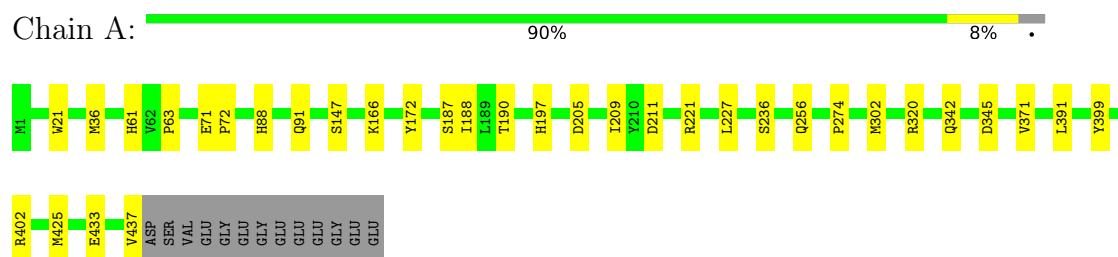
- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



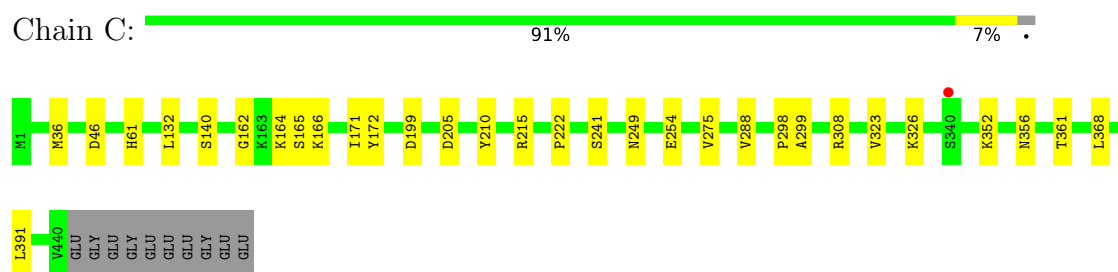
3 Residue-property plots

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.

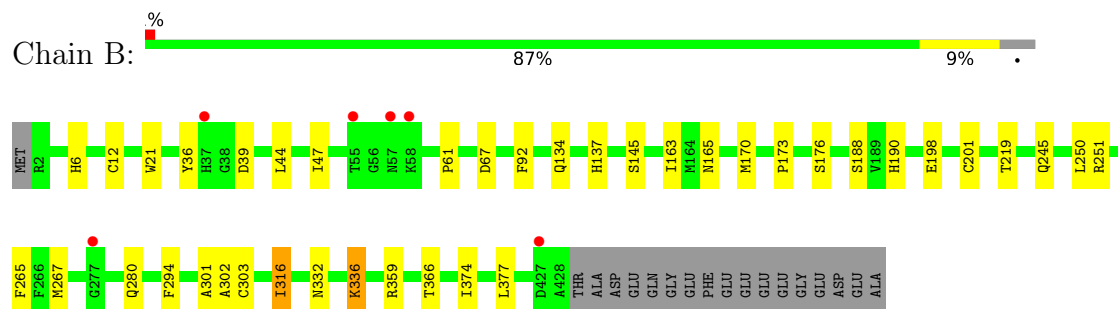
• Molecule 1: Tubulin alpha-1B chain



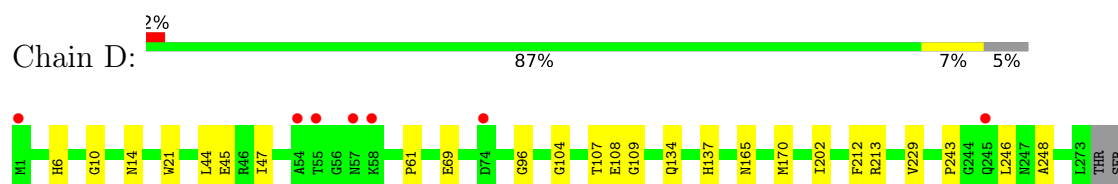
• Molecule 1: Tubulin alpha-1B chain

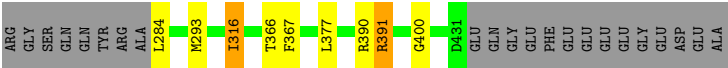


• Molecule 2: Tubulin beta-2B chain

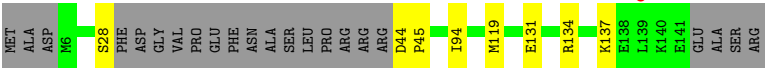
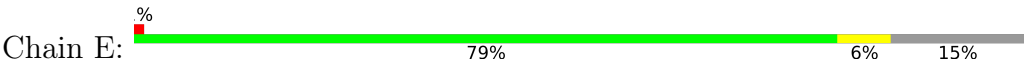


• Molecule 2: Tubulin beta-2B chain

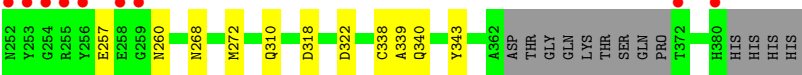
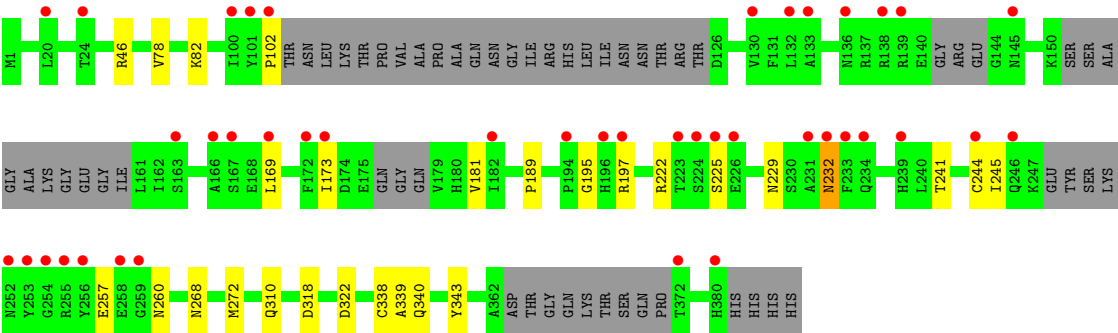
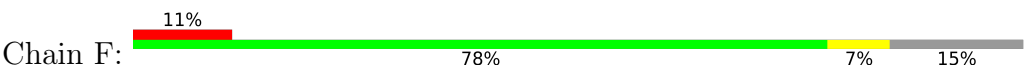




● Molecule 3: Stathmin-4



● 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	105.21Å 158.00Å 182.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 2.80 49.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.88-2.80) 94.3 (49.88-2.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.171 , 0.211 0.172 , 0.213	Depositor DCC
R_{free} test set	2000 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17560	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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, MES, CA, YJ7, ACP, GTP, GDP

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	0.25	0/3494	0.42	0/4743
1	C	0.26	0/3515	0.43	0/4772
2	B	0.25	0/3436	0.43	0/4654
2	D	0.25	0/3378	0.42	0/4577
3	E	0.24	0/1008	0.37	0/1337
4	F	0.24	0/2731	0.41	0/3689
All	All	0.25	0/17562	0.42	0/23772

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	15	0
1	C	3437	0	3348	18	0
2	B	3361	0	3238	21	0
2	D	3305	0	3179	17	0
3	E	1000	0	1018	5	0
4	F	2672	0	2626	16	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	B	24	0	0	0	0
8	D	24	0	0	0	0
9	B	28	0	12	1	0
10	B	24	0	24	3	0
11	F	31	0	13	1	0
12	A	31	0	0	0	0
12	B	30	0	0	0	0
12	C	54	0	0	1	0
12	D	10	0	0	0	0
12	E	2	0	0	0	0
12	F	8	0	0	0	0
All	All	17560	0	16824	89	0

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

All (89) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:SER:HA	1:C:249:ASN:HD21	1.53	0.73
4:F:229:ASN:OD1	4:F:232:ASN:ND2	2.28	0.66
4:F:102:PRO:HB3	4:F:173:ILE:HG22	1.80	0.64
4:F:222:ARG:NH1	4:F:318:ASP:OD2	2.31	0.63
2:B:170:MET:HG3	2:B:377:LEU:HD21	1.81	0.63
2:B:165:ASN:HD22	2:B:198:GLU:HB2	1.64	0.62
1:A:345:ASP:HB3	3:E:28:SER:HB3	1.82	0.61
2:B:251:ARG:NH2	10:B:503:MES:O3S	2.32	0.60
2:D:246:LEU:HD13	2:D:248:ALA:HB2	1.84	0.60
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.85	0.58
2:D:316:ILE:HG23	2:D:366:THR:HB	1.85	0.58
3:E:44:ASP:HB3	3:E:45:PRO:HD3	1.86	0.57
2:B:36:TYR:CZ	2:B:44:LEU:HD11	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:LEU:HA	2:B:47:ILE:HB	1.86	0.56
2:B:173:PRO:HA	2:B:176:SER:HB2	1.87	0.56
2:B:145:SER:HG	2:B:188:SER:HG	1.52	0.56
2:B:134:GLN:HA	2:B:165:ASN:O	2.05	0.56
2:B:316:ILE:HG23	2:B:366:THR:HB	1.87	0.56
1:A:88:HIS:O	1:A:91:GLN:HG2	2.06	0.56
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.41	0.55
2:D:69:GLU:HG2	2:D:96:GLY:HA2	1.89	0.55
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.89	0.54
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.91	0.53
2:D:10:GLY:O	2:D:14:ASN:ND2	2.36	0.53
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.90	0.53
2:D:134:GLN:HA	2:D:165:ASN:O	2.09	0.52
4:F:241:THR:OG1	11:F:402:ACP:O3'	2.28	0.52
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.50	0.51
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.91	0.51
2:B:219:THR:HG21	1:C:326:LYS:HA	1.92	0.51
2:B:301:ALA:O	2:B:303:CYS:N	2.43	0.51
1:A:399:TYR:O	1:A:402:ARG:NH1	2.39	0.50
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.94	0.49
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.31	0.49
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.47	0.49
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.94	0.49
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.94	0.49
1:C:215:ARG:NH2	1:C:299:ALA:O	2.46	0.49
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.48	0.48
1:C:140:SER:HA	1:C:171:ILE:HB	1.95	0.48
2:B:332:ASN:O	2:B:336:LYS:HB3	2.15	0.47
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.97	0.47
1:C:46:ASP:OD1	1:C:46:ASP:N	2.46	0.47
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.50	0.47
4:F:78:VAL:HG21	4:F:181:VAL:HG11	1.95	0.47
1:A:147:SER:HB2	1:A:190:THR:HB	1.95	0.47
1:A:166:LYS:HE2	1:A:197:HIS:O	2.14	0.47
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.33	0.46
2:B:12:CYS:HB2	9:B:502:GDP:C8	2.51	0.46
3:E:131:GLU:OE1	3:E:134:ARG:NH1	2.48	0.46
4:F:195:GLY:HA3	4:F:197:ARG:HD2	1.98	0.46
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.49	0.46
1:A:236:SER:OG	1:A:320:ARG:NH2	2.49	0.45
1:C:249:ASN:ND2	1:C:356:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:LEU:HG	1:C:164:LYS:HD3	1.98	0.45
2:B:267:MET:HG2	2:B:374:ILE:HD12	1.98	0.45
1:C:166:LYS:NZ	12:C:602:HOH:O	2.39	0.45
1:A:209:ILE:HD11	1:A:302:MET:SD	2.57	0.45
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.52	0.45
2:B:67:ASP:O	2:B:92:PHE:HA	2.17	0.44
2:D:107:THR:OG1	2:D:108:GLU:N	2.49	0.44
2:D:390:ARG:HG3	2:D:391:ARG:HG3	1.98	0.44
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.33	0.44
4:F:225:SER:HB3	4:F:260:ASN:HD21	1.82	0.44
1:C:165:SER:HA	1:C:199:ASP:OD2	2.17	0.44
2:D:202:ILE:HD13	2:D:229:VAL:HG13	2.00	0.43
2:B:294:PHE:O	10:B:504:MES:H82	2.18	0.43
1:C:162:GLY:HA2	3:E:94:ILE:HD11	2.00	0.43
1:A:209:ILE:HG22	1:A:227:LEU:HD22	2.00	0.43
4:F:78:VAL:O	4:F:82:LYS:HG3	2.19	0.43
4:F:189:PRO:HA	4:F:322:ASP:HA	2.01	0.42
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.55	0.42
2:D:44:LEU:HA	2:D:47:ILE:HB	2.02	0.42
4:F:268:ASN:O	4:F:272:MET:HG3	2.20	0.42
1:C:288:VAL:HG22	1:C:323:VAL:HG22	2.02	0.41
2:D:400:GLY:O	3:E:137:LYS:HG3	2.20	0.41
4:F:338:CYS:SG	4:F:339:ALA:N	2.93	0.41
4:F:169:LEU:O	4:F:173:ILE:HG13	2.20	0.41
2:D:104:GLY:O	2:D:109:GLY:HA3	2.20	0.41
10:B:504:MES:H51	10:B:504:MES:H81	1.81	0.41
1:C:391:LEU:HD23	1:C:391:LEU:HA	1.91	0.41
1:A:274:PRO:HG2	1:A:371:VAL:HG11	2.01	0.41
4:F:244:CYS:SG	4:F:245:ILE:HD12	2.61	0.41
2:B:39:ASP:OD1	2:B:39:ASP:N	2.55	0.40
2:D:45:GLU:OE1	2:D:243:PRO:HG3	2.21	0.40
2:D:293:MET:CG	2:D:367:PHE:HB2	2.52	0.40
4:F:197:ARG:HH12	4:F:257:GLU:CD	2.25	0.40
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.86	0.40
2:D:212:PHE:HD1	2:D:213:ARG:HG2	1.86	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%)	433 (99%)	5 (1%)	0	100	100
2	B	425/445 (96%)	418 (98%)	6 (1%)	1 (0%)	47	78
2	D	417/445 (94%)	407 (98%)	10 (2%)	0	100	100
3	E	117/143 (82%)	117 (100%)	0	0	100	100
4	F	314/384 (82%)	305 (97%)	9 (3%)	0	100	100
All	All	2146/2317 (93%)	2106 (98%)	39 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	302	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%)	362 (98%)	6 (2%)	62	88
1	C	371/378 (98%)	370 (100%)	1 (0%)	92	98
2	B	369/383 (96%)	362 (98%)	7 (2%)	57	85
2	D	362/383 (94%)	358 (99%)	4 (1%)	73	92
3	E	109/127 (86%)	108 (99%)	1 (1%)	78	94
4	F	290/342 (85%)	287 (99%)	3 (1%)	76	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1869/1991 (94%)	1847 (99%)	22 (1%)	71 92

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	ASP
1	A	221	ARG
1	A	256	GLN
1	A	342	GLN
1	A	433	GLU
1	A	437	VAL
2	B	137	HIS
2	B	190	HIS
2	B	245	GLN
2	B	280	GLN
2	B	316	ILE
2	B	336	LYS
2	B	359	ARG
1	C	361	THR
2	D	137	HIS
2	D	284	LEU
2	D	316	ILE
2	D	391	ARG
3	E	119	MET
4	F	46	ARG
4	F	232	ASN
4	F	310	GLN

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

Mol	Chain	Res	Type
1	A	301	GLN
2	B	15	GLN
2	B	165	ASN
2	B	245	GLN
2	B	337	ASN
1	C	31	GLN
1	C	128	GLN
1	C	249	ASN
1	C	356	ASN
1	C	372	GLN

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Mol	Chain	Res	Type
2	D	292	GLN
2	D	396	HIS
4	F	229	ASN
4	F	232	ASN
4	F	246	GLN
4	F	260	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 7 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
10	MES	B	504	-	12,12,12	2.29	1 (8%)	14,16,16	1.88	4 (28%)
5	GTP	C	501	7	26,34,34	0.98	1 (3%)	33,54,54	1.77	6 (18%)
8	YJ7	D	502	-	23,27,27	2.96	9 (39%)	26,40,40	2.05	3 (11%)
11	ACP	F	402	7	27,33,33	2.01	6 (22%)	32,52,52	1.32	2 (6%)
5	GTP	D	501	7	26,34,34	1.02	2 (7%)	33,54,54	1.82	7 (21%)
9	GDP	B	502	7	24,30,30	1.21	2 (8%)	31,47,47	1.96	7 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	A	501	7	26,34,34	1.00	1 (3%)	33,54,54	1.75	8 (24%)
8	YJ7	B	501	-	23,27,27	3.00	9 (39%)	26,40,40	2.03	4 (15%)
10	MES	B	503	-	12,12,12	2.22	1 (8%)	14,16,16	1.84	3 (21%)

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
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
5	GTP	C	501	7	-	7/18/38/38	0/3/3/3
8	YJ7	D	502	-	-	4/6/18/18	0/4/4/4
11	ACP	F	402	7	-	7/15/38/38	0/3/3/3
5	GTP	D	501	7	-	9/18/38/38	0/3/3/3
9	GDP	B	502	7	-	3/12/32/32	0/3/3/3
5	GTP	A	501	7	-	6/18/38/38	0/3/3/3
8	YJ7	B	501	-	-	4/6/18/18	0/4/4/4
10	MES	B	503	-	-	4/6/14/14	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	502	YJ7	C21-N20	9.46	1.45	1.35
8	B	501	YJ7	C21-N20	9.46	1.45	1.35
10	B	504	MES	C8-S	-7.65	1.66	1.77
10	B	503	MES	C8-S	-7.39	1.67	1.77
11	F	402	ACP	PB-O3A	7.27	1.66	1.58
8	B	501	YJ7	C19-N20	5.38	1.49	1.39
8	D	502	YJ7	C19-N20	5.34	1.49	1.39
9	B	502	GDP	C6-C5	4.23	1.48	1.41
8	B	501	YJ7	C22-C21	3.93	1.56	1.51
8	D	502	YJ7	C22-C21	3.83	1.56	1.51
8	B	501	YJ7	C07-C06	3.61	1.53	1.50
8	D	502	YJ7	C22-N11	-3.55	1.42	1.46
8	B	501	YJ7	C12-N11	3.53	1.46	1.40
8	D	502	YJ7	C07-C06	3.44	1.53	1.50
8	B	501	YJ7	C22-N11	-3.44	1.42	1.46
5	D	501	GTP	C6-N1	3.36	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	502	YJ7	C12-N11	3.27	1.45	1.40
5	A	501	GTP	C6-N1	3.13	1.38	1.33
5	C	501	GTP	C6-N1	3.13	1.38	1.33
8	B	501	YJ7	C10-N11	3.12	1.46	1.39
8	D	502	YJ7	C10-N11	3.07	1.46	1.39
11	F	402	ACP	C6-N6	3.04	1.45	1.34
11	F	402	ACP	O3'-C3'	-2.92	1.36	1.43
11	F	402	ACP	C5-C4	-2.70	1.33	1.40
9	B	502	GDP	C5-C4	2.37	1.47	1.40
8	D	502	YJ7	C19-C12	-2.28	1.38	1.40
8	B	501	YJ7	C19-C12	-2.24	1.38	1.40
11	F	402	ACP	C2-N3	2.16	1.35	1.32
11	F	402	ACP	PB-O2B	-2.14	1.51	1.56
8	B	501	YJ7	O23-C21	-2.10	1.19	1.23
8	D	502	YJ7	O23-C21	-2.09	1.19	1.23
5	D	501	GTP	C2-N1	2.04	1.39	1.35

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	502	YJ7	C05-C10-N24	-6.16	117.64	124.05
8	B	501	YJ7	C05-C10-N24	-6.10	117.70	124.05
8	B	501	YJ7	C02-N03-C04	5.69	120.15	115.52
8	D	502	YJ7	C02-N03-C04	5.55	120.03	115.52
5	A	501	GTP	N3-C2-N1	-5.35	120.09	127.22
5	D	501	GTP	N3-C2-N1	-5.23	120.24	127.22
11	F	402	ACP	N3-C2-N1	-5.22	120.52	128.68
5	C	501	GTP	N3-C2-N1	-5.22	120.26	127.22
9	B	502	GDP	C2-N3-C4	4.86	120.91	115.36
10	B	503	MES	C5-N4-C3	4.76	119.55	108.83
10	B	504	MES	C5-N4-C3	4.63	119.25	108.83
5	D	501	GTP	C2-N3-C4	4.33	120.30	115.36
9	B	502	GDP	C6-N1-C2	4.27	122.71	115.93
9	B	502	GDP	C6-C5-C4	-4.22	116.77	120.80
5	A	501	GTP	C2-N3-C4	4.15	120.10	115.36
5	C	501	GTP	C2-N3-C4	4.11	120.05	115.36
9	B	502	GDP	C5-C6-N1	-4.04	117.91	123.43
8	D	502	YJ7	C19-N20-C21	-3.69	119.93	124.49
5	D	501	GTP	PB-O3B-PG	-3.64	120.32	132.83
9	B	502	GDP	N3-C2-N1	-3.53	122.51	127.22
5	C	501	GTP	PA-O3A-PB	-3.45	120.97	132.83
8	B	501	YJ7	C19-N20-C21	-3.35	120.34	124.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	GTP	C5-C6-N1	-3.34	118.86	123.43
9	B	502	GDP	PA-O3A-PB	-3.09	122.22	132.83
5	A	501	GTP	C5-C6-N1	-3.05	119.26	123.43
5	C	501	GTP	C5-C6-N1	-3.02	119.30	123.43
9	B	502	GDP	C4-C5-N7	-2.94	106.34	109.40
5	C	501	GTP	PB-O3B-PG	-2.91	122.84	132.83
5	A	501	GTP	PA-O3A-PB	-2.89	122.89	132.83
11	F	402	ACP	C5-C6-N6	2.73	124.50	120.35
5	D	501	GTP	PA-O3A-PB	-2.72	123.49	132.83
5	A	501	GTP	C6-N1-C2	2.65	120.14	115.93
10	B	503	MES	O2S-S-C8	2.60	110.05	106.92
5	D	501	GTP	C6-N1-C2	2.59	120.04	115.93
5	C	501	GTP	C6-N1-C2	2.56	120.00	115.93
5	A	501	GTP	PB-O3B-PG	-2.46	124.39	132.83
10	B	504	MES	O2S-S-C8	2.29	109.67	106.92
10	B	504	MES	O3S-S-C8	2.22	109.36	105.77
10	B	503	MES	O3S-S-C8	2.17	109.28	105.77
10	B	504	MES	C6-C5-N4	-2.16	106.83	110.10
5	A	501	GTP	O2G-PG-O3B	2.14	111.82	104.64
8	B	501	YJ7	N24-C10-N11	2.14	118.52	116.26
5	D	501	GTP	C4-C5-N7	-2.12	107.19	109.40
5	A	501	GTP	N2-C2-N1	2.03	120.41	117.25

There are no chirality outliers.

All (48) 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	YJ7	C05-C10-N11-C12
8	B	501	YJ7	C05-C10-N11-C22
8	B	501	YJ7	N24-C10-N11-C12
8	D	502	YJ7	C05-C10-N11-C12
8	D	502	YJ7	C05-C10-N11-C22

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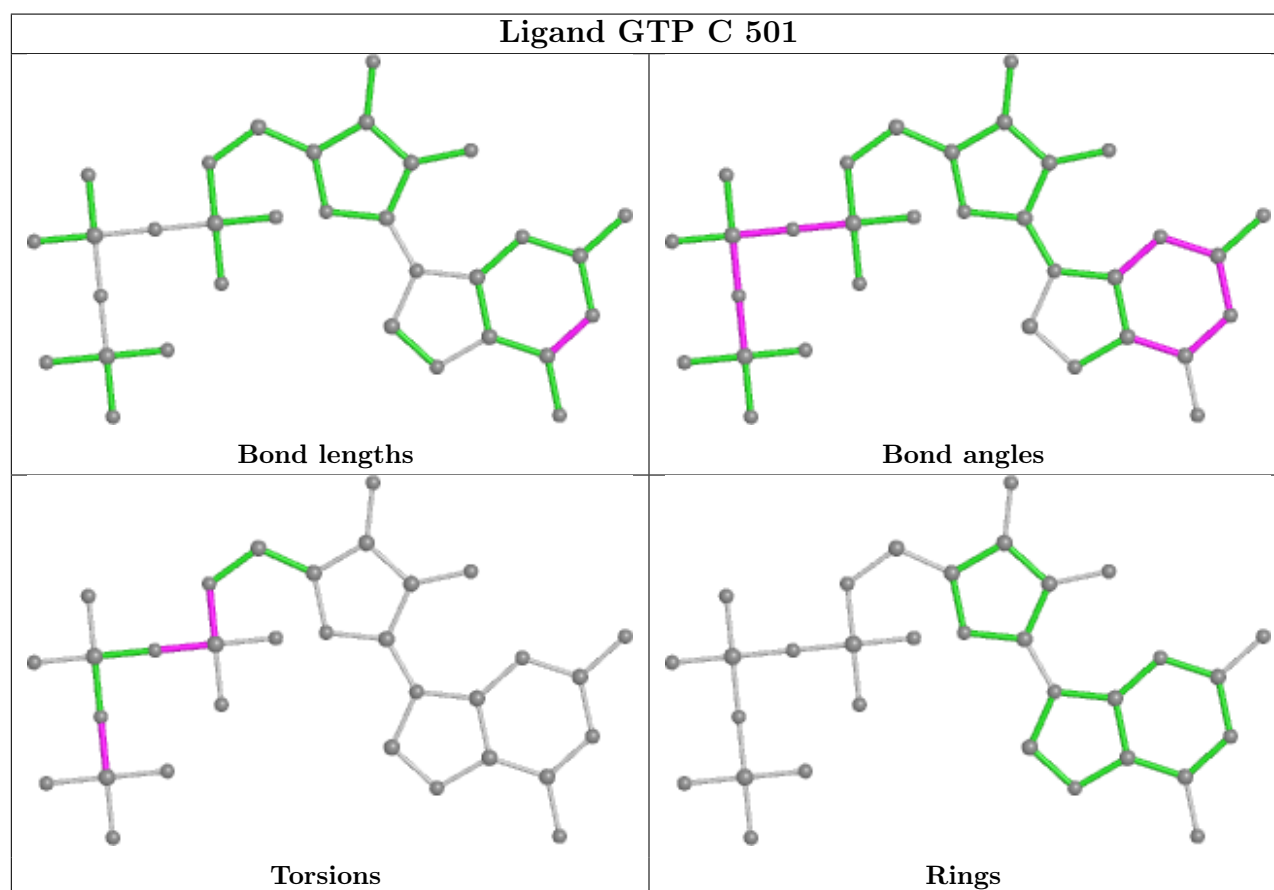
Mol	Chain	Res	Type	Atoms
8	D	502	YJ7	N24-C10-N11-C12
9	B	502	GDP	C5'-O5'-PA-O1A
9	B	502	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C7-C8-S-O1S
11	F	402	ACP	PG-C3B-PB-O1B
11	F	402	ACP	PG-C3B-PB-O2B
11	F	402	ACP	PG-C3B-PB-O3A
8	B	501	YJ7	N24-C10-N11-C22
11	F	402	ACP	O4'-C4'-C5'-O5'
10	B	504	MES	C7-C8-S-O3S
8	D	502	YJ7	N24-C10-N11-C22
10	B	503	MES	C7-C8-S-O3S
10	B	503	MES	C8-C7-N4-C3
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
10	B	503	MES	C7-C8-S-O2S
10	B	504	MES	C7-C8-S-O1S
10	B	504	MES	C7-C8-S-O2S
11	F	402	ACP	PB-C3B-PG-O2G
11	F	402	ACP	C3'-C4'-C5'-O5'
5	D	501	GTP	O4'-C4'-C5'-O5'
5	D	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3B-PG-O1G
11	F	402	ACP	PB-C3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
9	B	502	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	PB-O3A-PA-O2A
10	B	504	MES	C8-C7-N4-C3

There are no ring outliers.

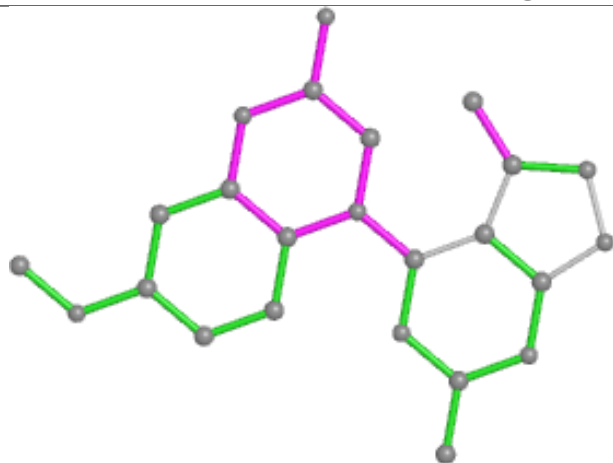
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	504	MES	2	0
11	F	402	ACP	1	0
9	B	502	GDP	1	0
10	B	503	MES	1	0

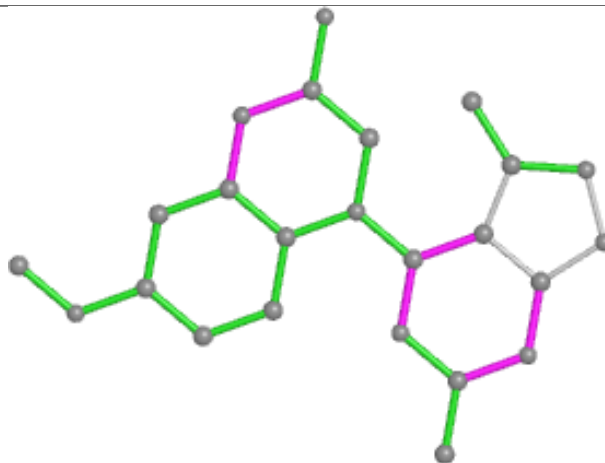
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



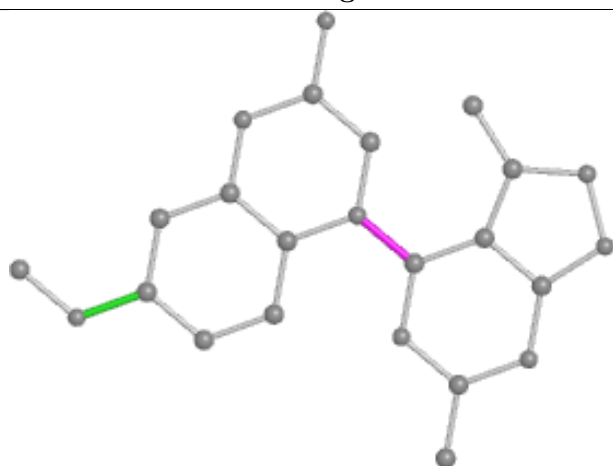
Ligand YJ7 D 502



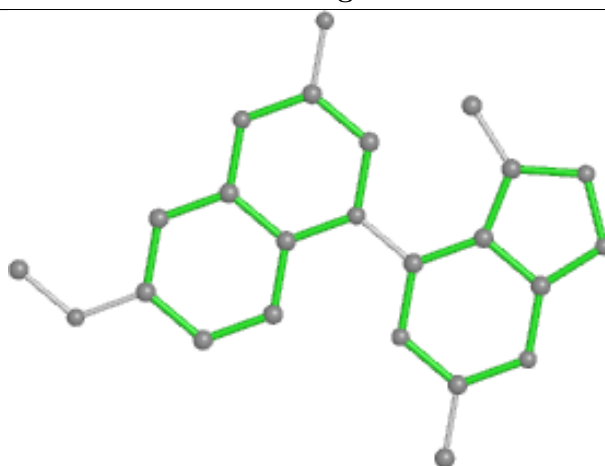
Bond lengths



Bond angles

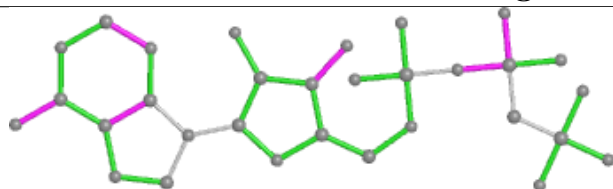


Torsions

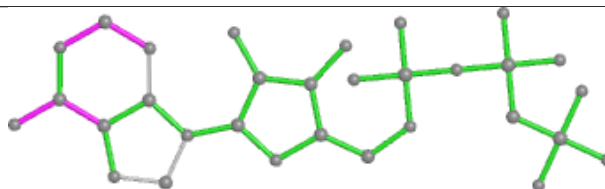


Rings

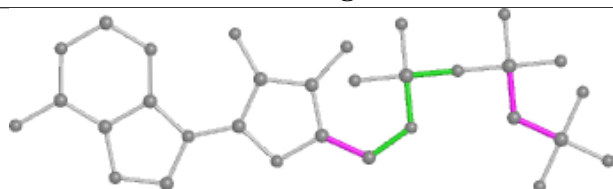
Ligand ACP F 402



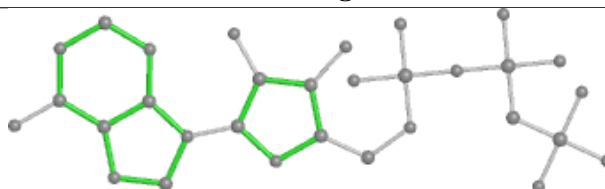
Bond lengths



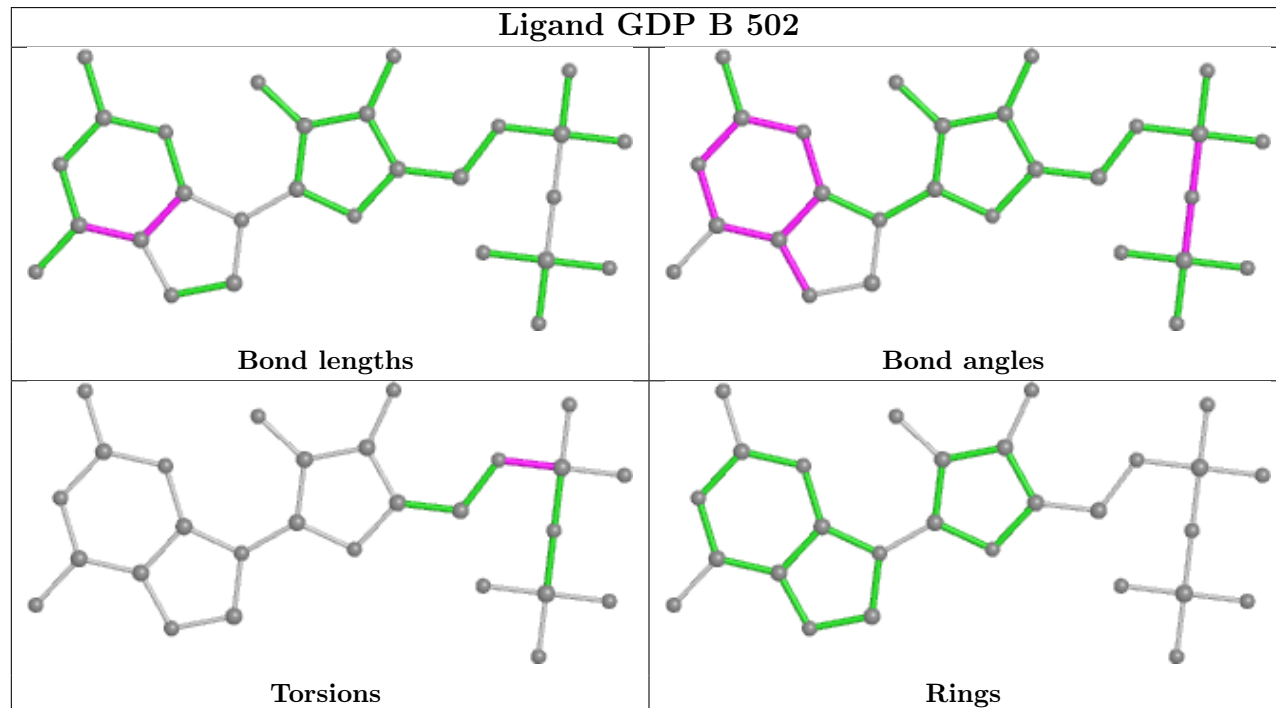
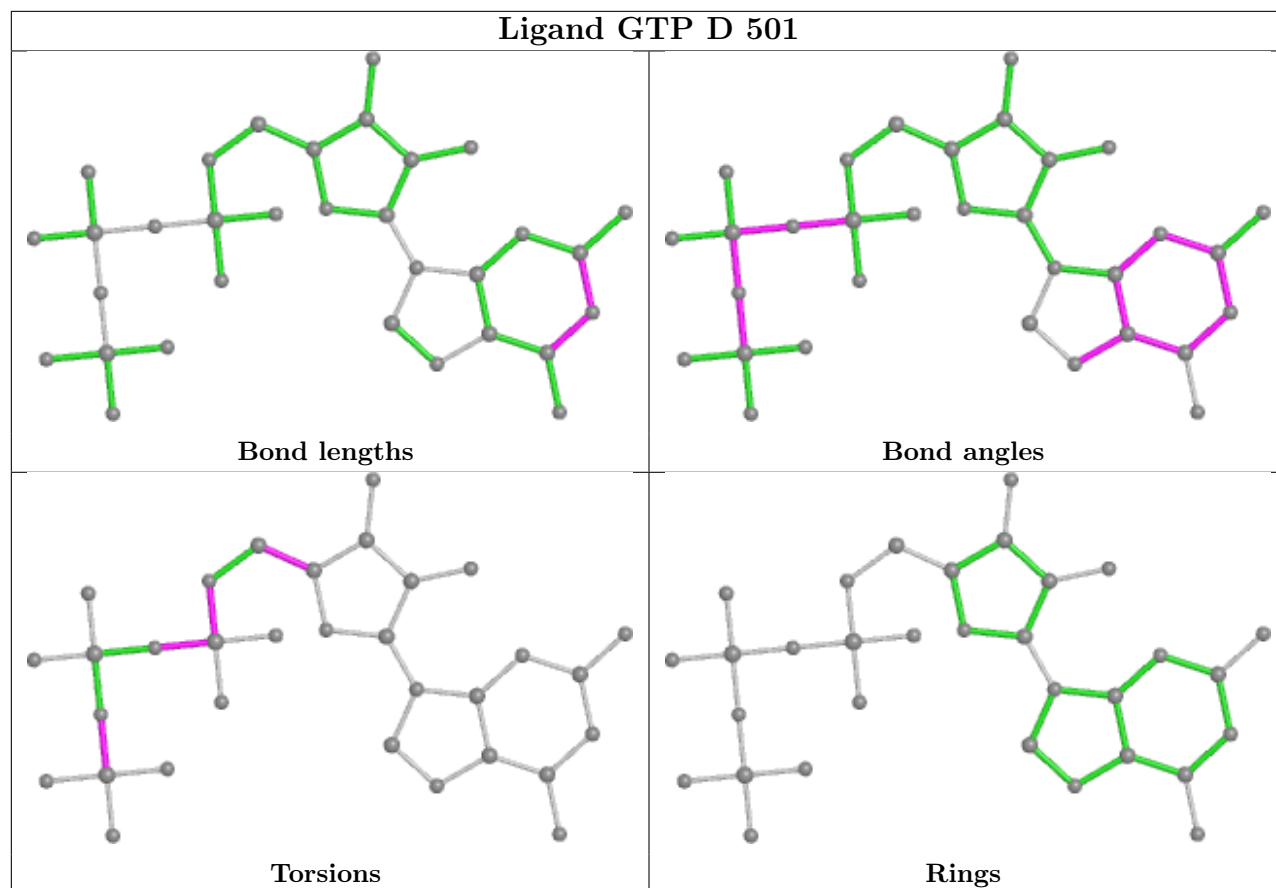
Bond angles

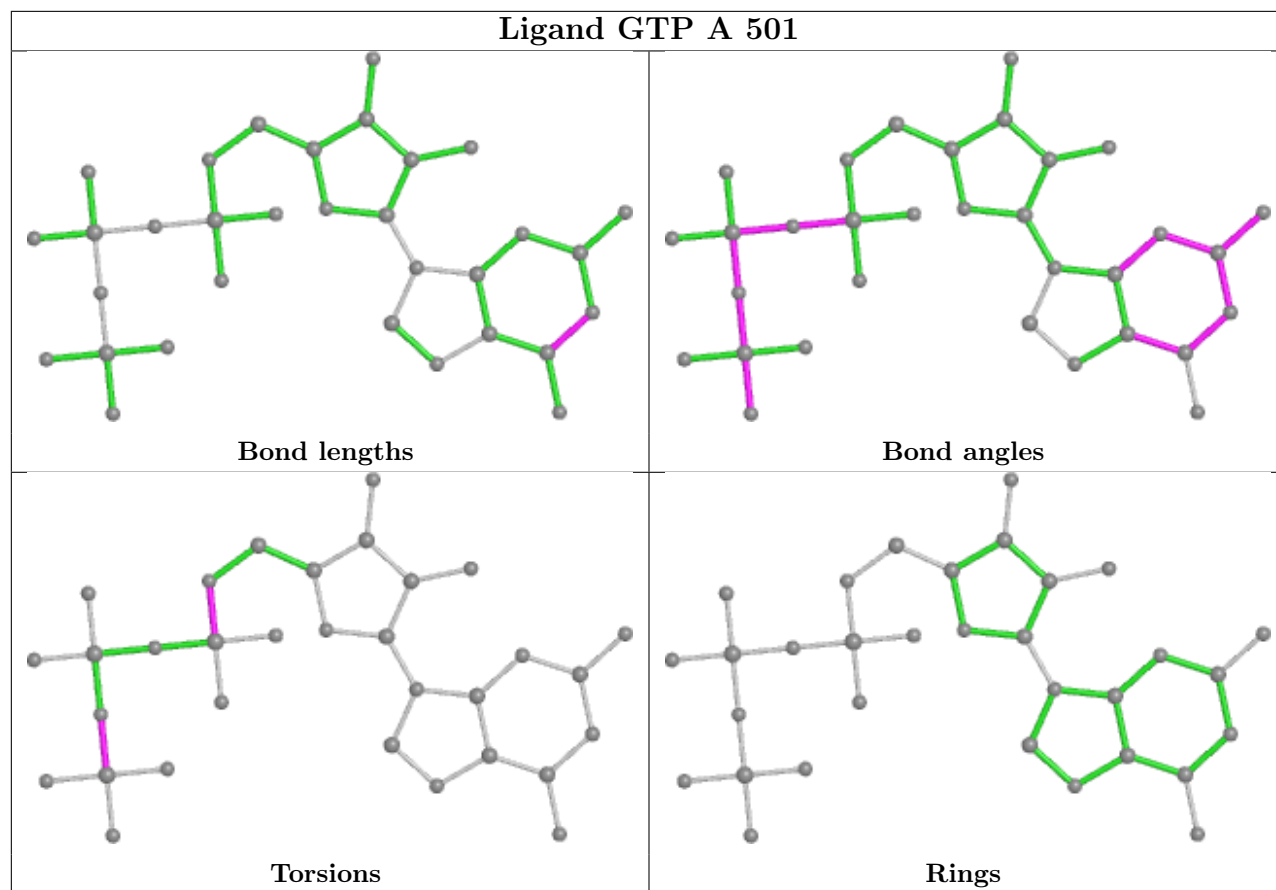


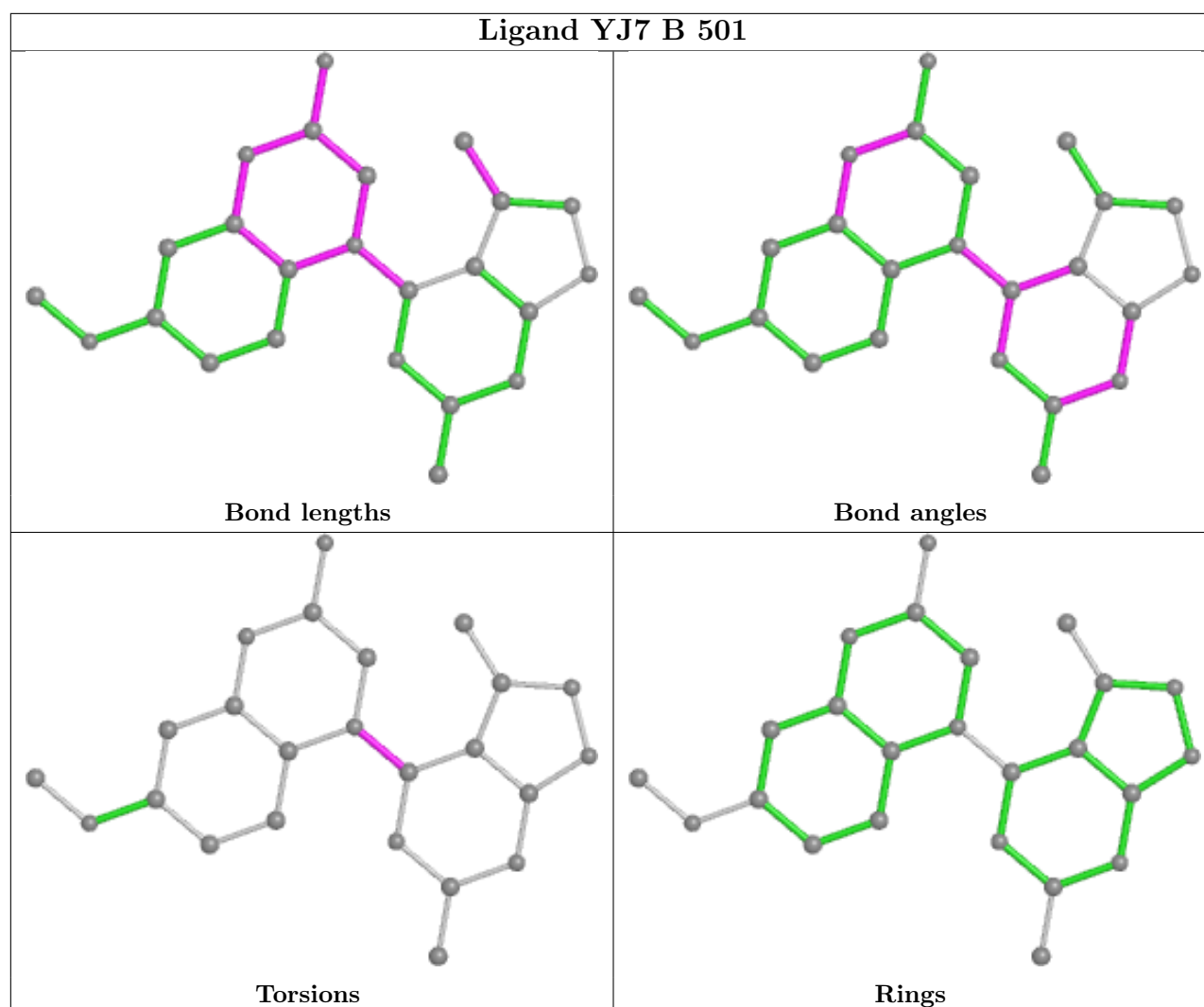
Torsions



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%)	-0.50	0 100 100	25, 42, 73, 93	0
1	C	440/450 (97%)	-0.62	1 (0%) 95 94	19, 33, 62, 92	0
2	B	427/445 (95%)	-0.39	6 (1%) 75 70	21, 40, 81, 138	0
2	D	421/445 (94%)	-0.25	7 (1%) 70 63	28, 60, 99, 124	0
3	E	121/143 (84%)	-0.16	1 (0%) 86 81	32, 57, 99, 118	0
4	F	328/384 (85%)	0.35	42 (12%) 3 2	35, 68, 130, 148	0
All	All	2174/2317 (93%)	-0.31	57 (2%) 56 46	19, 48, 98, 148	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	57	ASN	4.4
2	B	55	THR	4.4
4	F	233	PHE	4.2
4	F	256	TYR	4.0
4	F	225	SER	3.7
4	F	380	HIS	3.7
2	B	277	GLY	3.7
2	D	1	MET	3.7
4	F	253	TYR	3.6
2	B	427	ASP	3.6
4	F	194	PRO	3.5
4	F	132	LEU	3.4
4	F	234	GLN	3.3
4	F	223	THR	3.3
4	F	133	ALA	3.3
4	F	244	CYS	3.3
4	F	226	GLU	3.3
4	F	224	SER	3.2
2	D	55	THR	3.0

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Mol	Chain	Res	Type	RSRZ
4	F	136	ASN	3.0
4	F	169	LEU	2.8
4	F	100	ILE	2.8
4	F	138	ARG	2.8
4	F	145	ASN	2.8
4	F	173	ILE	2.8
4	F	139	ARG	2.8
4	F	259	GLY	2.7
4	F	232	ASN	2.7
4	F	130	VAL	2.7
4	F	101	TYR	2.7
4	F	163	SER	2.6
4	F	166	ALA	2.6
4	F	167	SER	2.5
4	F	102	PRO	2.5
2	D	57	ASN	2.5
4	F	255	ARG	2.5
4	F	182	ILE	2.5
4	F	372	THR	2.4
4	F	24	THR	2.3
2	D	54	ALA	2.3
4	F	254	GLY	2.3
2	D	245	GLN	2.3
4	F	239	HIS	2.3
2	B	37	HIS	2.3
4	F	258	GLU	2.2
4	F	172	PHE	2.2
4	F	20	LEU	2.2
2	B	58	LYS	2.2
4	F	197	ARG	2.2
4	F	231	ALA	2.2
2	D	58	LYS	2.1
4	F	246	GLN	2.1
4	F	252	ASN	2.1
4	F	196	HIS	2.0
2	D	74	ASP	2.0
3	E	139	LEU	2.0
1	C	340	SER	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 ⓘ

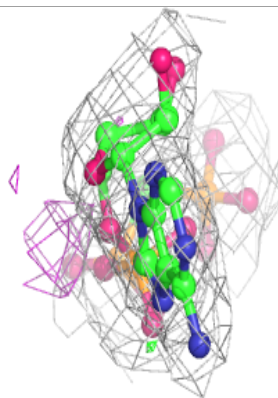
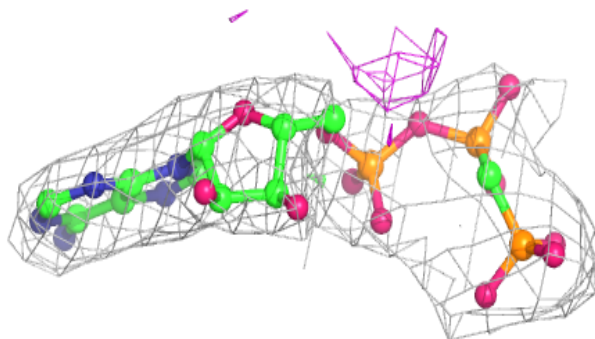
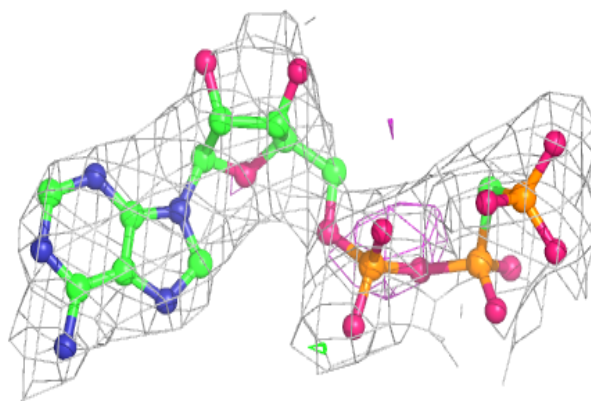
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MG	D	503	1/1	0.81	0.15	62,62,62,62	0
7	MG	F	401	1/1	0.84	0.13	95,95,95,95	0
11	ACP	F	402	31/31	0.92	0.18	66,89,131,138	0
6	CA	A	502	1/1	0.95	0.05	62,62,62,62	0
10	MES	B	504	12/12	0.95	0.14	61,65,72,82	0
5	GTP	D	501	32/32	0.95	0.16	42,51,106,109	0
8	YJ7	B	501	24/24	0.96	0.20	31,44,91,111	0
8	YJ7	D	502	24/24	0.96	0.21	42,61,96,106	0
10	MES	B	503	12/12	0.97	0.14	33,47,67,69	0
6	CA	C	502	1/1	0.97	0.07	47,47,47,47	0
7	MG	B	505	1/1	0.97	0.13	22,22,22,22	0
7	MG	C	503	1/1	0.98	0.10	28,28,28,28	0
7	MG	A	503	1/1	0.98	0.13	32,32,32,32	0
5	GTP	A	501	32/32	0.99	0.17	15,29,37,40	0
5	GTP	C	501	32/32	0.99	0.13	18,25,34,38	0
9	GDP	B	502	28/28	0.99	0.16	8,27,36,40	0

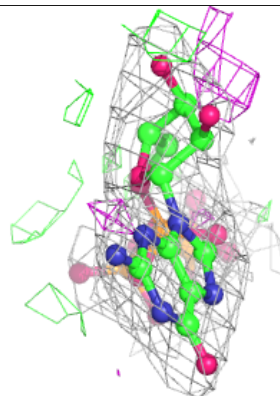
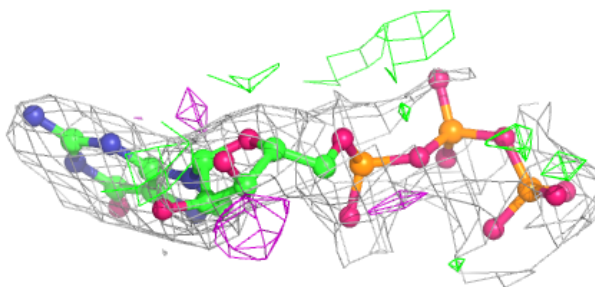
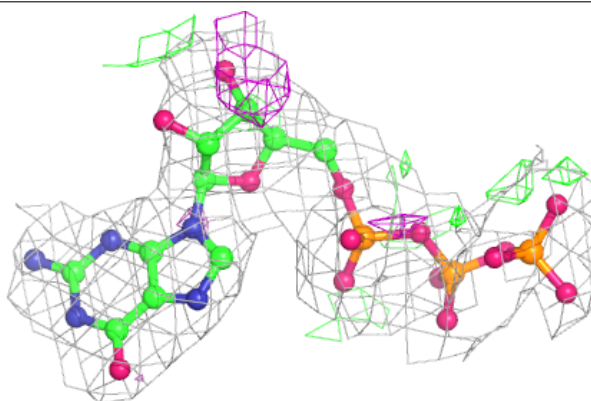
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 402:

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

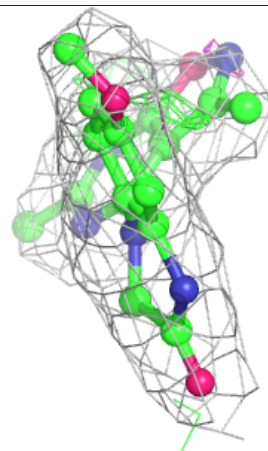
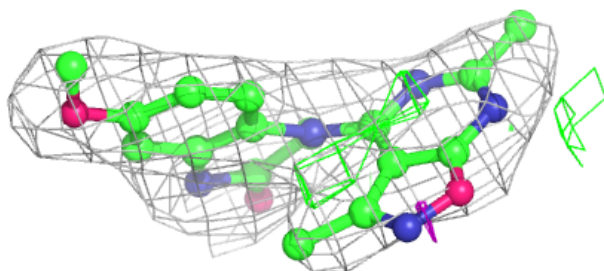
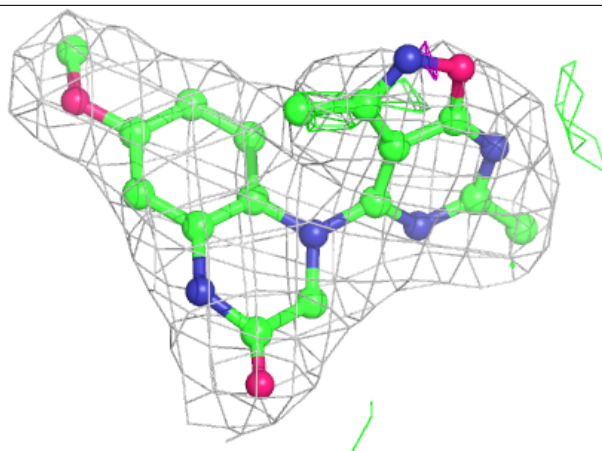
**Electron density around GTP D 501:**

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

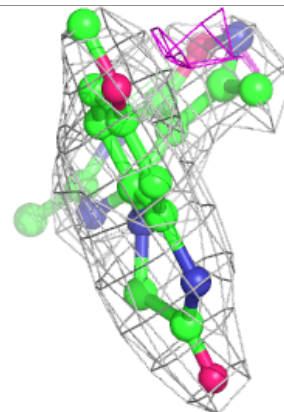
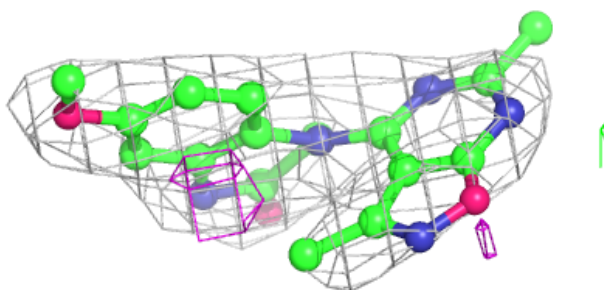
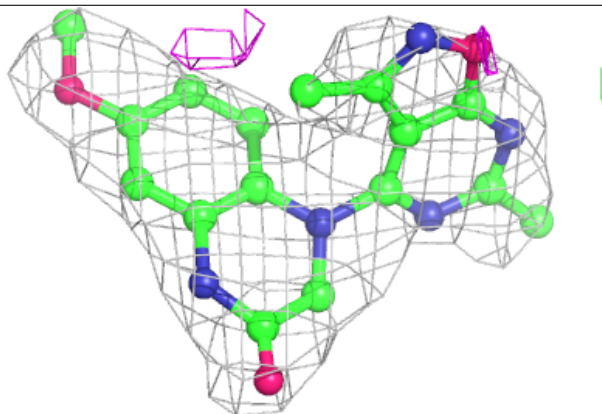


Electron density around YJ7 B 501:

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

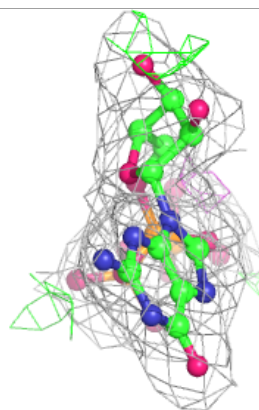
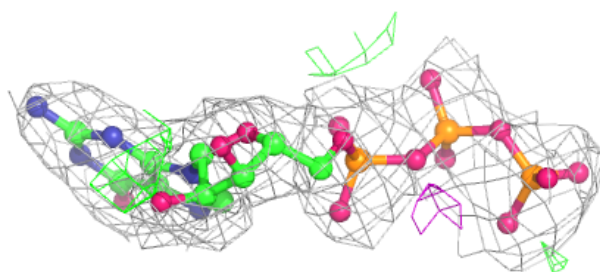
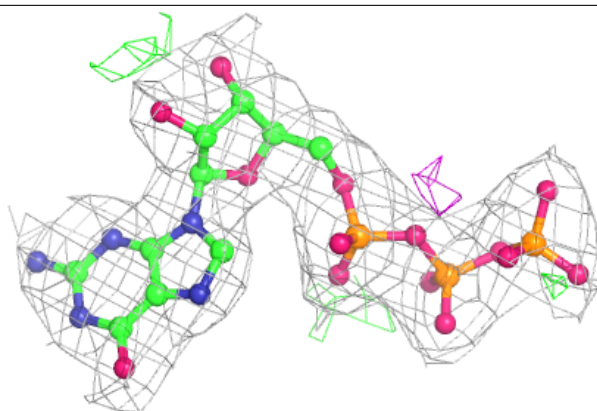
**Electron density around YJ7 D 502:**

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

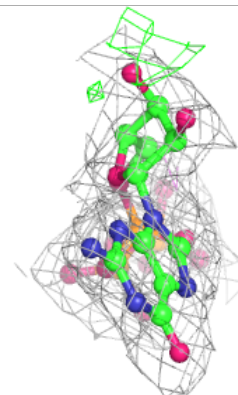
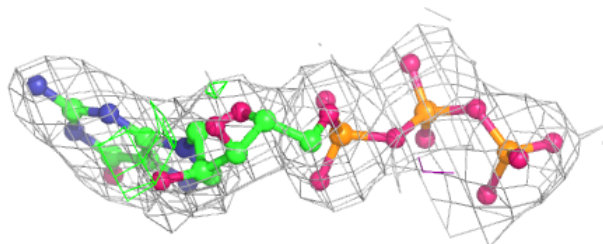
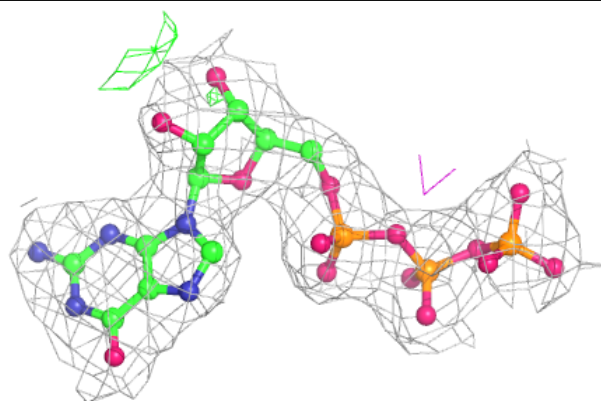


Electron density around GTP A 501:

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

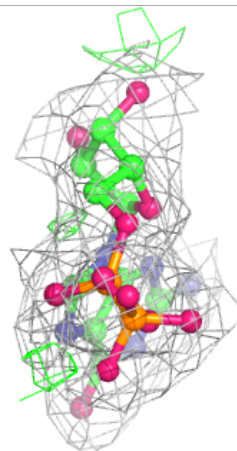
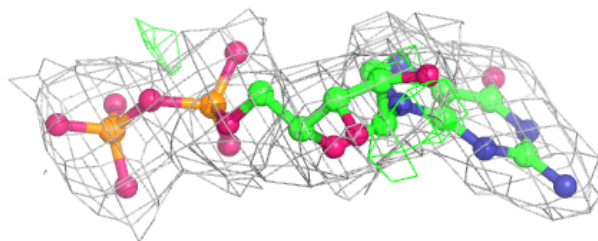
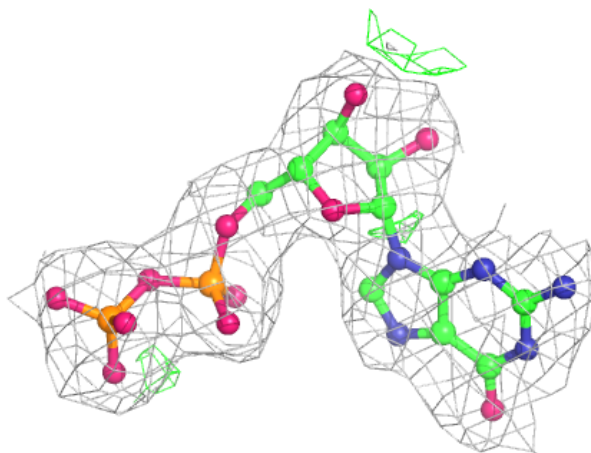
**Electron density around GTP C 501:**

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



Electron density around GDP B 502:

$2mF_o-DF_c$ (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.