



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2021 – 03:12 PM EDT

PDB ID : 6X1C  
Title : Tubulin-RB3\_SLD-TTL in complex with compound 5j  
Authors : White, S.W.; Yun, M.  
Deposited on : 2020-05-18  
Resolution : 2.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

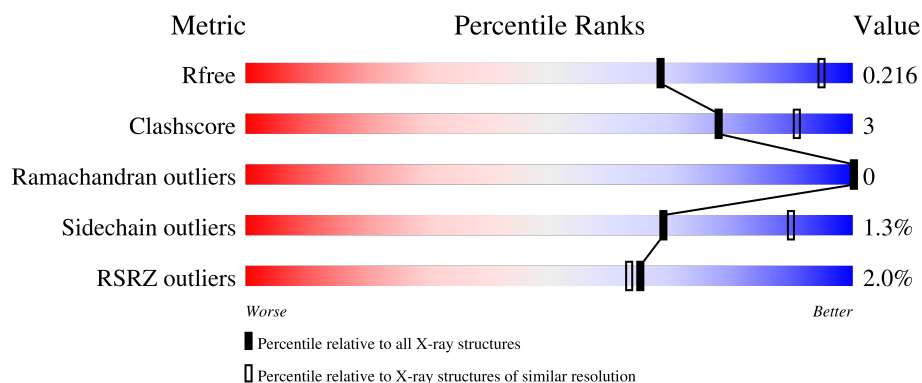
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


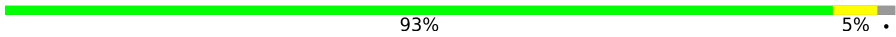



The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	 88% 9% .
1	C	450	 93% 5% .
2	B	445	 2% 85% 11% .
2	D	445	 2% 86% 9% 5%
3	E	143	 81% . 15%

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Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div>7%</div><div>76%</div><div>9%</div><div>15%</div></div>

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17509 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

- Molecule 3 is a protein called Stathmin-4.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

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

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

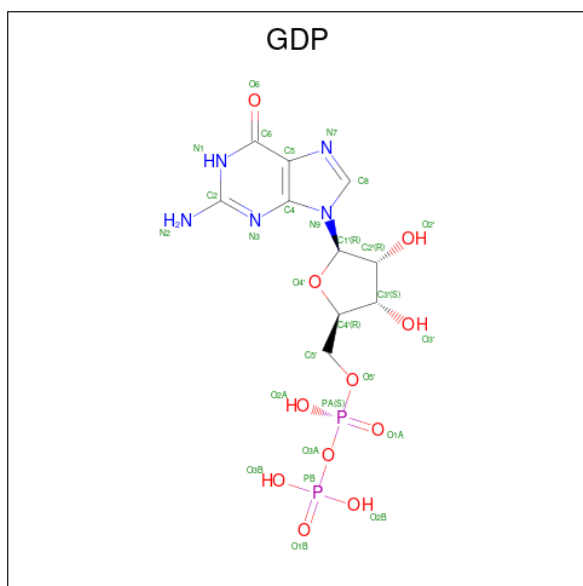
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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



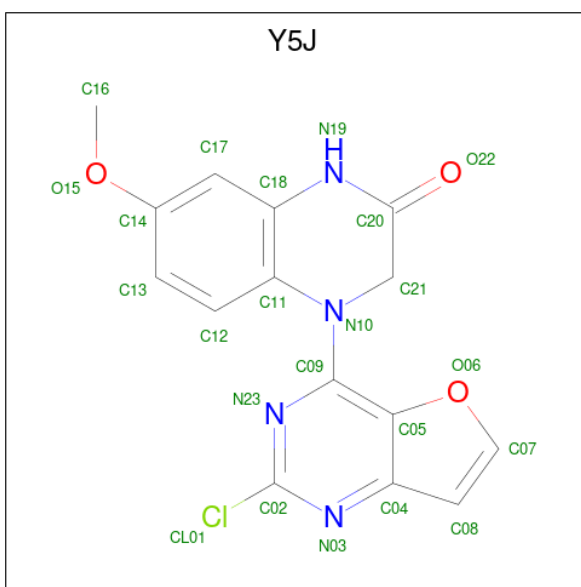
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: 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 4-(2-chlorofuro[3,2-d]pyrimidin-4-yl)-7-methoxy-3,4-dihydroquinoxalin-2(1H)-one (three-letter code: Y5J) (formula: C<sub>15</sub>H<sub>11</sub>ClN<sub>4</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



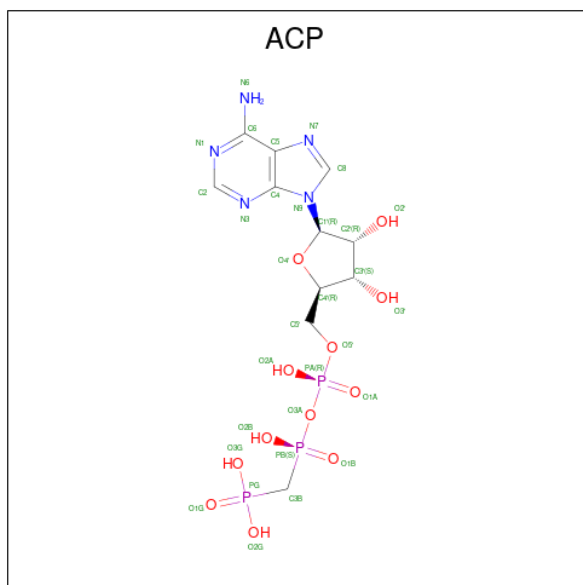
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	Cl	N	O	0	0
			23	15	1	4	3		

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

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



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

- Molecule 12 is water.

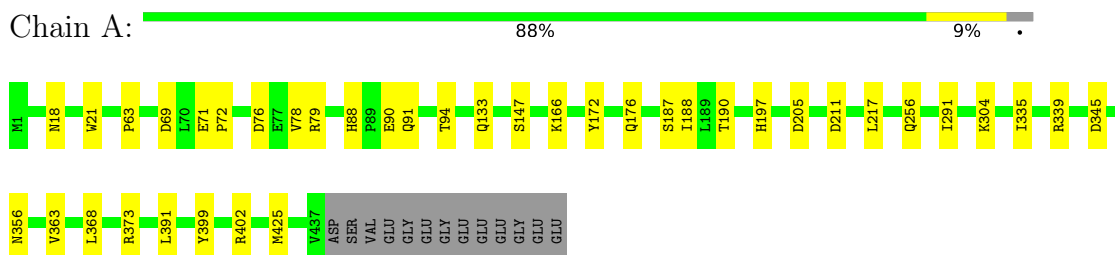
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	25	Total	O		
			25	25	0	0
12	B	23	Total	O		
			23	23	0	0
12	C	41	Total	O		
			41	41	0	0
12	D	5	Total	O		
			5	5	0	0
12	E	4	Total	O		
			4	4	0	0
12	F	6	Total	O		
			6	6	0	0



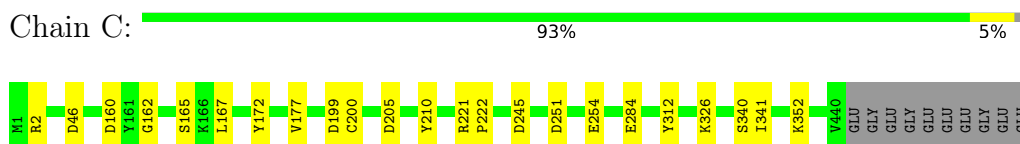
### 3 Residue-property plots

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.

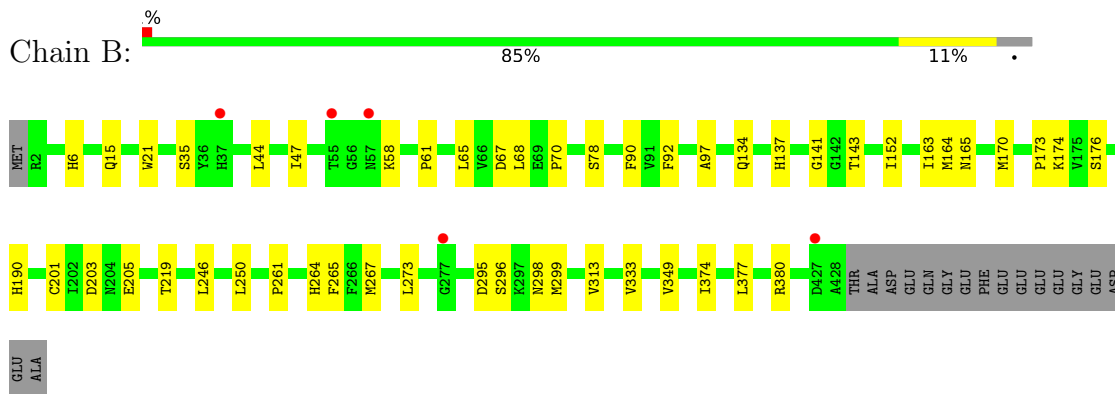
#### • Molecule 1: Tubulin alpha-1B chain



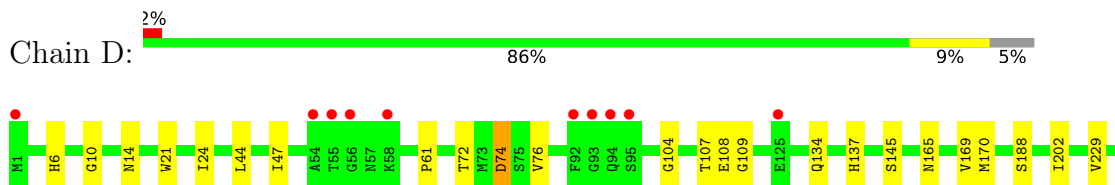
#### • Molecule 1: Tubulin alpha-1B chain



#### • Molecule 2: Tubulin beta-2B chain

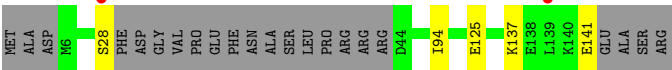
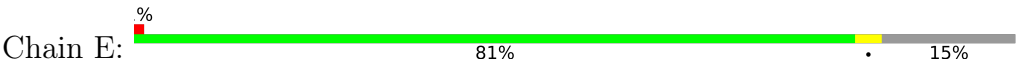


#### • Molecule 2: Tubulin beta-2B chain

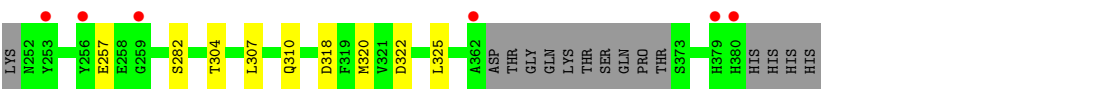
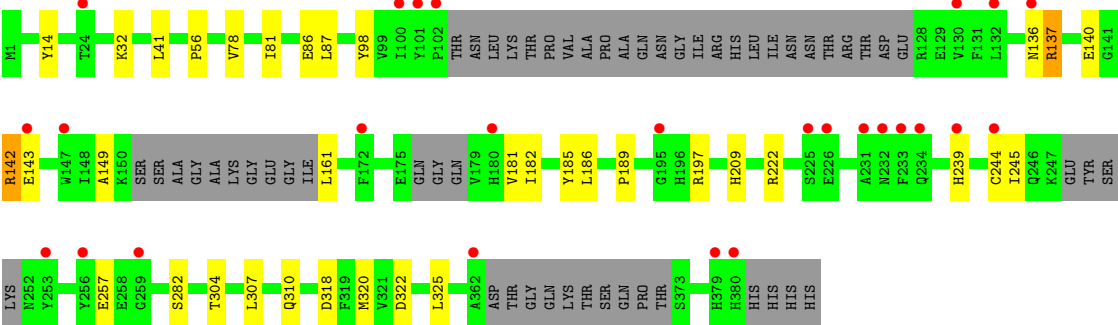
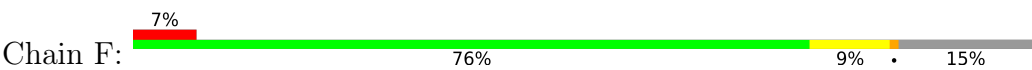




● Molecule 3: Stathmin-4



● 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, $\alpha$ , $\beta$ , $\gamma$	105.34Å 158.32Å 181.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 2.90 48.19 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.14-2.90) 93.9 (48.19-2.87)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.174 , 0.216 0.174 , 0.216	Depositor DCC
$R_{free}$ test set	2000 reflections (2.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17509	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, MG, CA, Y5J, GDP, ACP, 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	0.25	0/3494	0.41	0/4743
1	C	0.25	0/3515	0.42	0/4772
2	B	0.25	0/3436	0.42	0/4654
2	D	0.24	0/3378	0.41	0/4577
3	E	0.23	0/1008	0.35	0/1337
4	F	0.24	0/2714	0.41	0/3669
All	All	0.24	0/17545	0.41	0/23752

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3330	20	0
1	C	3437	0	3348	10	0
2	B	3361	0	3238	27	0
2	D	3305	0	3179	21	0
3	E	1000	0	1018	3	0
4	F	2654	0	2592	21	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	B	28	0	12	2	0
9	B	24	0	24	3	0
10	B	23	0	0	0	0
10	D	23	0	0	0	0
11	F	31	0	13	0	0
12	A	25	0	0	0	0
12	B	23	0	0	0	0
12	C	41	0	0	0	0
12	D	5	0	0	0	0
12	E	4	0	0	0	0
12	F	6	0	0	0	0
All	All	17509	0	16790	99	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 (99) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:MET:HG3	2:B:377:LEU:HD21	1.77	0.67
2:D:375:GLN:HB2	2:D:419:VAL:HG13	1.77	0.65
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.77	0.64
4:F:209:HIS:HB2	4:F:310:GLN:HG3	1.82	0.61
2:D:10:GLY:O	2:D:14:ASN:ND2	2.27	0.58
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.85	0.58
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.87	0.57
4:F:197:ARG:NH1	4:F:257:GLU:OE1	2.37	0.56
4:F:222:ARG:NH1	4:F:318:ASP:OD2	2.38	0.56
1:A:345:ASP:HB3	3:E:28:SER:HB3	1.87	0.56
1:A:335:ILE:HG23	1:A:339:ARG:HD2	1.88	0.55
4:F:86:GLU:OE1	4:F:86:GLU:N	2.28	0.55
3:E:137:LYS:O	3:E:141:GLU:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:O	1:A:91:GLN:HG2	2.07	0.54
2:D:134:GLN:HA	2:D:165:ASN:O	2.07	0.54
2:B:174:LYS:HD2	2:B:205:GLU:HG3	1.90	0.54
2:B:219:THR:HG21	1:C:326:LYS:HA	1.89	0.53
4:F:137:ARG:HD2	4:F:140:GLU:HB3	1.92	0.52
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.91	0.51
4:F:185:TYR:OH	4:F:239:HIS:ND1	2.32	0.51
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.29	0.50
2:B:134:GLN:HA	2:B:165:ASN:O	2.10	0.50
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.93	0.50
2:B:15:GLN:NE2	8:B:501:GDP:O6	2.45	0.50
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.38	0.50
1:C:46:ASP:OD1	1:C:46:ASP:N	2.44	0.49
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.94	0.49
2:B:313:VAL:HB	2:B:349:VAL:HG22	1.92	0.49
1:A:166:LYS:HE2	1:A:197:HIS:O	2.13	0.48
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.53	0.48
4:F:98:TYR:HD2	4:F:182:ILE:HD11	1.78	0.48
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.94	0.48
1:A:399:TYR:O	1:A:402:ARG:NH1	2.46	0.48
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.95	0.48
2:B:67:ASP:HA	2:B:143:THR:HG21	1.95	0.47
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.32	0.47
2:B:35:SER:HG	2:B:58:LYS:HZ3	1.60	0.47
1:A:188:ILE:HG13	1:A:425:MET:HG3	1.97	0.47
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.46	0.47
2:D:74:ASP:OD1	2:D:74:ASP:N	2.47	0.47
4:F:142:ARG:HB2	4:F:142:ARG:HH11	1.79	0.47
4:F:78:VAL:HG21	4:F:181:VAL:HG11	1.96	0.47
9:B:503:MES:H51	9:B:503:MES:H81	1.71	0.46
2:D:72:THR:O	2:D:76:VAL:HG23	2.15	0.46
4:F:304:THR:HG22	4:F:307:LEU:HD12	1.97	0.46
2:B:67:ASP:O	2:B:92:PHE:HA	2.15	0.46
1:A:88:HIS:CE1	1:A:90:GLU:HB2	2.52	0.45
2:B:173:PRO:HA	2:B:176:SER:HB2	1.97	0.45
1:A:176:GLN:NE2	4:F:56:PRO:HB3	2.32	0.45
2:B:333:VAL:HG13	9:B:503:MES:H22	1.97	0.45
2:D:202:ILE:HD13	2:D:229:VAL:HG13	1.98	0.45
2:B:295:ASP:HA	9:B:503:MES:O3S	2.17	0.45
2:D:145:SER:HG	2:D:188:SER:HG	1.65	0.45
2:B:44:LEU:HA	2:B:47:ILE:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.52	0.44
1:C:165:SER:HA	1:C:199:ASP:OD2	2.17	0.44
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.99	0.44
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.53	0.44
2:D:247:ASN:O	2:D:252:LYS:HD2	2.17	0.44
4:F:149:ALA:HB2	4:F:182:ILE:HG22	1.99	0.44
2:B:65:LEU:HD22	2:B:90:PHE:CE2	2.53	0.44
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.00	0.44
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.53	0.44
1:A:147:SER:HB2	1:A:190:THR:HB	2.00	0.43
4:F:149:ALA:O	4:F:161:LEU:HB3	2.18	0.43
2:B:152:ILE:HG23	2:B:164:MET:HG2	2.00	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.53	0.43
2:D:44:LEU:HA	2:D:47:ILE:HB	1.99	0.43
2:B:141:GLY:HA3	8:B:501:GDP:O3A	2.19	0.43
2:B:203:ASP:OD2	2:B:380:ARG:NH1	2.47	0.43
2:B:267:MET:HG2	2:B:374:ILE:HD13	2.01	0.43
4:F:137:ARG:HD2	4:F:137:ARG:HA	1.76	0.43
2:B:261:PRO:O	2:B:264:HIS:ND1	2.49	0.43
4:F:81:ILE:HA	4:F:87:LEU:HD12	2.00	0.43
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.54	0.43
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.01	0.43
2:D:267:MET:HG2	2:D:301:ALA:HB3	1.99	0.43
1:A:69:ASP:O	1:A:94:THR:HA	2.19	0.42
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.53	0.42
2:D:104:GLY:O	2:D:109:GLY:HA3	2.19	0.42
2:B:246:LEU:HD12	2:B:246:LEU:HA	1.75	0.42
1:A:88:HIS:ND1	1:A:90:GLU:HB2	2.35	0.42
1:A:291:ILE:HD13	1:A:373:ARG:HG3	2.02	0.42
2:B:296:SER:HA	2:B:299:MET:HG2	2.02	0.42
2:B:273:LEU:HD11	2:B:298:ASN:HA	2.01	0.42
4:F:189:PRO:HA	4:F:322:ASP:HA	2.01	0.42
2:B:68:LEU:HD12	2:B:97:ALA:HB2	2.02	0.42
2:D:396:HIS:CD2	2:D:397:TRP:HD1	2.37	0.41
2:D:301:ALA:O	2:D:303:CYS:N	2.53	0.41
4:F:32:LYS:HB3	4:F:32:LYS:HE2	1.86	0.41
4:F:186:LEU:HD12	4:F:320:MET:HG2	2.02	0.41
2:D:404:ASP:OD1	2:D:405:GLU:N	2.53	0.41
1:C:245:ASP:OD1	1:C:245:ASP:N	2.54	0.41
2:D:239:CYS:O	2:D:248:ALA:HB3	2.20	0.41
2:D:107:THR:OG1	2:D:108:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.86	0.41
4:F:244:CYS:SG	4:F:245:ILE:HD12	2.61	0.41
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.04	0.40
2:D:169:VAL:HA	2:D:202:ILE:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

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

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/378 (97%)	364 (99%)	4 (1%)	73	92
1	C	371/378 (98%)	364 (98%)	7 (2%)	57	84
2	B	369/383 (96%)	365 (99%)	4 (1%)	73	92
2	D	362/383 (94%)	358 (99%)	4 (1%)	73	92
3	E	109/127 (86%)	108 (99%)	1 (1%)	78	93
4	F	284/342 (83%)	280 (99%)	4 (1%)	67	89
All	All	1863/1991 (94%)	1839 (99%)	24 (1%)	69	90

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	256	GLN
1	A	356	ASN
1	A	363	VAL
2	B	70	PRO
2	B	78	SER
2	B	137	HIS
2	B	190	HIS
1	C	2	ARG
1	C	160	ASP
1	C	177	VAL
1	C	221	ARG
1	C	251	ASP
1	C	284	GLU
1	C	340	SER
2	D	74	ASP
2	D	137	HIS
2	D	343	GLU
2	D	350	LYS
3	E	125	GLU
4	F	136	ASN
4	F	137	ARG
4	F	142	ARG
4	F	143	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN

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Mol	Chain	Res	Type
2	B	15	GLN
2	D	247	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
5	GTP	D	501	7	26,34,34	0.95	1 (3%)	33,54,54	1.69	6 (18%)
5	GTP	C	501	7	26,34,34	0.93	1 (3%)	33,54,54	1.74	6 (18%)
5	GTP	A	501	7	26,34,34	0.95	1 (3%)	33,54,54	1.69	6 (18%)
10	Y5J	B	505	-	22,26,26	3.09	9 (40%)	24,38,38	2.30	7 (29%)
9	MES	B	502	-	12,12,12	2.12	1 (8%)	14,16,16	1.68	3 (21%)
9	MES	B	503	-	12,12,12	2.11	1 (8%)	14,16,16	1.78	3 (21%)
11	ACP	F	401	7	27,33,33	1.89	5 (18%)	32,52,52	1.45	3 (9%)
10	Y5J	D	502	-	22,26,26	3.04	9 (40%)	24,38,38	2.31	6 (25%)
8	GDP	B	501	7	24,30,30	1.19	2 (8%)	31,47,47	1.94	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	D	501	7	-	2/18/38/38	0/3/3/3
5	GTP	C	501	7	-	8/18/38/38	0/3/3/3
5	GTP	A	501	7	-	6/18/38/38	0/3/3/3
10	Y5J	B	505	-	-	5/6/18/18	0/4/4/4
9	MES	B	502	-	-	0/6/14/14	0/1/1/1
9	MES	B	503	-	-	0/6/14/14	0/1/1/1
11	ACP	F	401	7	-	5/15/38/38	0/3/3/3
10	Y5J	D	502	-	-	5/6/18/18	0/4/4/4
8	GDP	B	501	7	-	3/12/32/32	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	Y5J	C20-N19	9.56	1.45	1.35
10	D	502	Y5J	C20-N19	9.36	1.45	1.35
9	B	502	MES	C8-S	-7.13	1.67	1.77
9	B	503	MES	C8-S	-7.08	1.67	1.77
11	F	401	ACP	PB-O3A	6.52	1.65	1.58
10	B	505	Y5J	C18-N19	5.56	1.49	1.39
10	D	502	Y5J	C18-N19	5.41	1.49	1.39
8	B	501	GDP	C6-C5	4.21	1.48	1.41
10	B	505	Y5J	C02-N03	3.78	1.33	1.30
10	D	502	Y5J	C21-C20	3.68	1.55	1.51
10	B	505	Y5J	C21-C20	3.67	1.55	1.51
10	D	502	Y5J	C02-N03	3.51	1.33	1.30
10	D	502	Y5J	C11-N10	3.50	1.46	1.40
10	B	505	Y5J	C21-N10	-3.48	1.42	1.46
10	D	502	Y5J	C21-N10	-3.39	1.42	1.46
10	B	505	Y5J	C11-N10	3.38	1.45	1.40
11	F	401	ACP	C6-N6	3.09	1.45	1.34
5	D	501	GTP	C6-N1	2.98	1.38	1.33
11	F	401	ACP	O3'-C3'	-2.98	1.36	1.43
10	D	502	Y5J	C09-N10	2.93	1.45	1.39
5	A	501	GTP	C6-N1	2.92	1.38	1.33
5	C	501	GTP	C6-N1	2.88	1.38	1.33
10	B	505	Y5J	C09-N10	2.83	1.45	1.39
11	F	401	ACP	C5-C4	-2.63	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	GDP	C5-C4	2.46	1.47	1.40
10	D	502	Y5J	O22-C20	-2.22	1.18	1.23
10	B	505	Y5J	O22-C20	-2.19	1.18	1.23
11	F	401	ACP	C2-N3	2.11	1.35	1.32
10	D	502	Y5J	C18-C11	-2.11	1.38	1.40
10	B	505	Y5J	C18-C11	-2.08	1.38	1.40

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	502	Y5J	N03-C02-N23	-7.92	122.64	130.62
10	B	505	Y5J	N03-C02-N23	-7.73	122.83	130.62
11	F	401	ACP	N3-C2-N1	-5.33	120.35	128.68
5	A	501	GTP	N3-C2-N1	-5.15	120.35	127.22
5	C	501	GTP	N3-C2-N1	-5.09	120.43	127.22
5	D	501	GTP	N3-C2-N1	-5.01	120.53	127.22
8	B	501	GDP	C2-N3-C4	4.75	120.78	115.36
9	B	502	MES	C5-N4-C3	4.29	118.47	108.83
8	B	501	GDP	C6-N1-C2	4.19	122.58	115.93
8	B	501	GDP	C6-C5-C4	-4.13	116.86	120.80
5	D	501	GTP	C2-N3-C4	4.05	119.98	115.36
8	B	501	GDP	C5-C6-N1	-4.02	117.93	123.43
5	A	501	GTP	C2-N3-C4	3.99	119.91	115.36
9	B	503	MES	C5-N4-C3	3.98	117.79	108.83
10	B	505	Y5J	CL01-C02-N03	3.90	119.03	115.70
5	C	501	GTP	C2-N3-C4	3.88	119.78	115.36
10	D	502	Y5J	CL01-C02-N03	3.71	118.87	115.70
11	F	401	ACP	C5-C6-N6	3.45	125.60	120.35
5	D	501	GTP	PB-O3B-PG	-3.39	121.19	132.83
10	D	502	Y5J	C02-N23-C09	3.37	121.03	111.04
8	B	501	GDP	N3-C2-N1	-3.34	122.77	127.22
10	B	505	Y5J	C02-N23-C09	3.32	120.88	111.04
10	B	505	Y5J	C18-N19-C20	-3.27	120.44	124.49
5	C	501	GTP	PA-O3A-PB	-3.26	121.62	132.83
5	C	501	GTP	PB-O3B-PG	-3.24	121.72	132.83
5	A	501	GTP	PB-O3B-PG	-3.19	121.87	132.83
10	D	502	Y5J	C18-N19-C20	-3.13	120.62	124.49
5	D	501	GTP	C5-C6-N1	-3.00	119.33	123.43
5	C	501	GTP	C5-C6-N1	-2.93	119.43	123.43
10	D	502	Y5J	N23-C09-N10	2.93	119.35	116.26
9	B	503	MES	O1S-S-C8	2.91	110.42	106.92
8	B	501	GDP	C4-C5-N7	-2.91	106.37	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	501	GTP	PA-O3A-PB	-2.84	123.08	132.83
10	B	505	Y5J	N23-C09-N10	2.83	119.25	116.26
5	A	501	GTP	C5-C6-N1	-2.72	119.70	123.43
8	B	501	GDP	PA-O3A-PB	-2.59	123.94	132.83
5	A	501	GTP	PA-O3A-PB	-2.58	123.97	132.83
5	C	501	GTP	C6-N1-C2	2.55	119.98	115.93
5	D	501	GTP	C6-N1-C2	2.47	119.86	115.93
5	A	501	GTP	C6-N1-C2	2.46	119.84	115.93
9	B	502	MES	O2S-S-C8	2.44	109.85	106.92
10	D	502	Y5J	CL01-C02-N23	2.34	118.49	115.15
9	B	503	MES	O2S-S-C8	2.14	109.49	106.92
11	F	401	ACP	N6-C6-N1	-2.13	114.15	118.57
8	B	501	GDP	C3'-C2'-C1'	2.13	104.19	100.98
10	B	505	Y5J	CL01-C02-N23	2.09	118.14	115.15
9	B	502	MES	O1S-S-C8	2.07	109.41	106.92
10	B	505	Y5J	O22-C20-N19	2.02	123.22	121.43

There are no chirality outliers.

All (34) torsion outliers are listed below:

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

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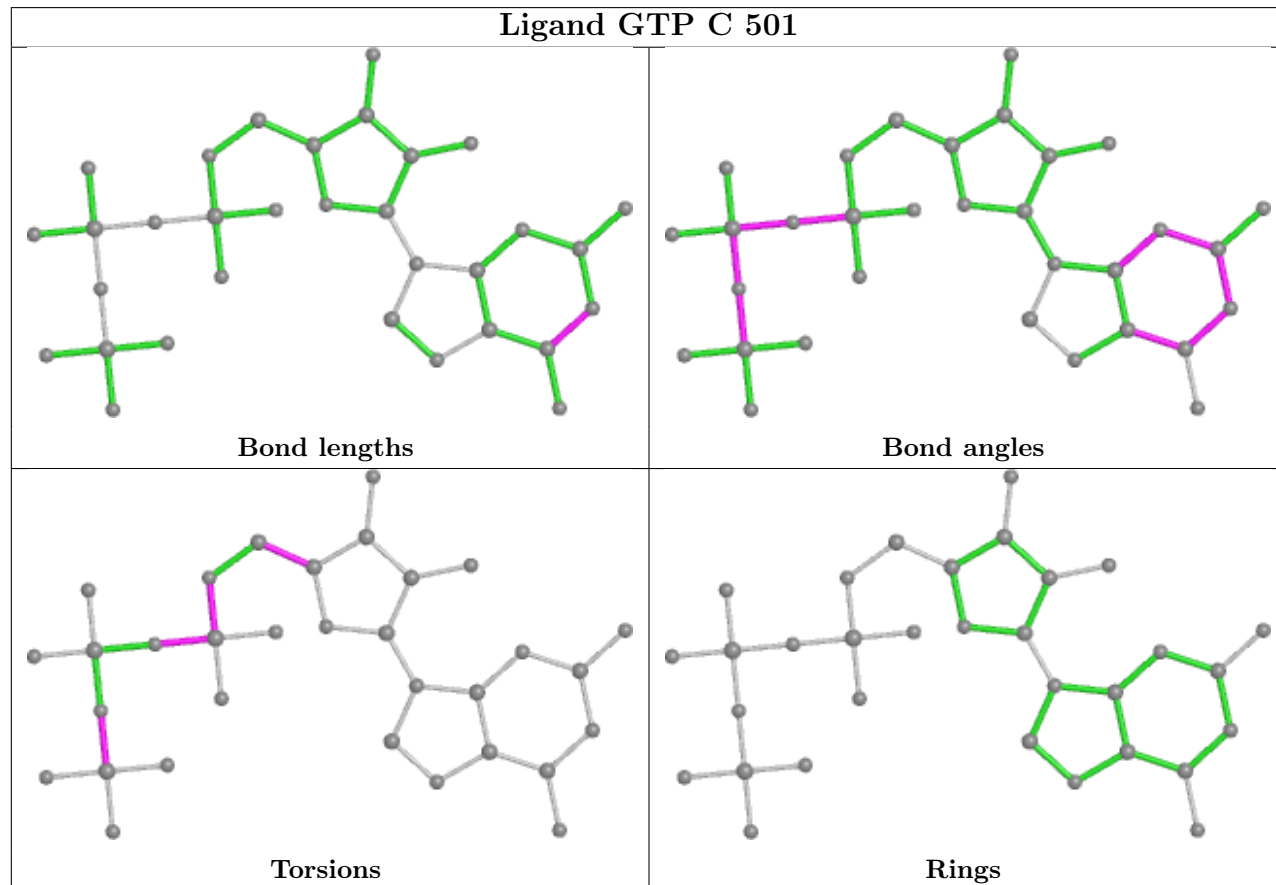
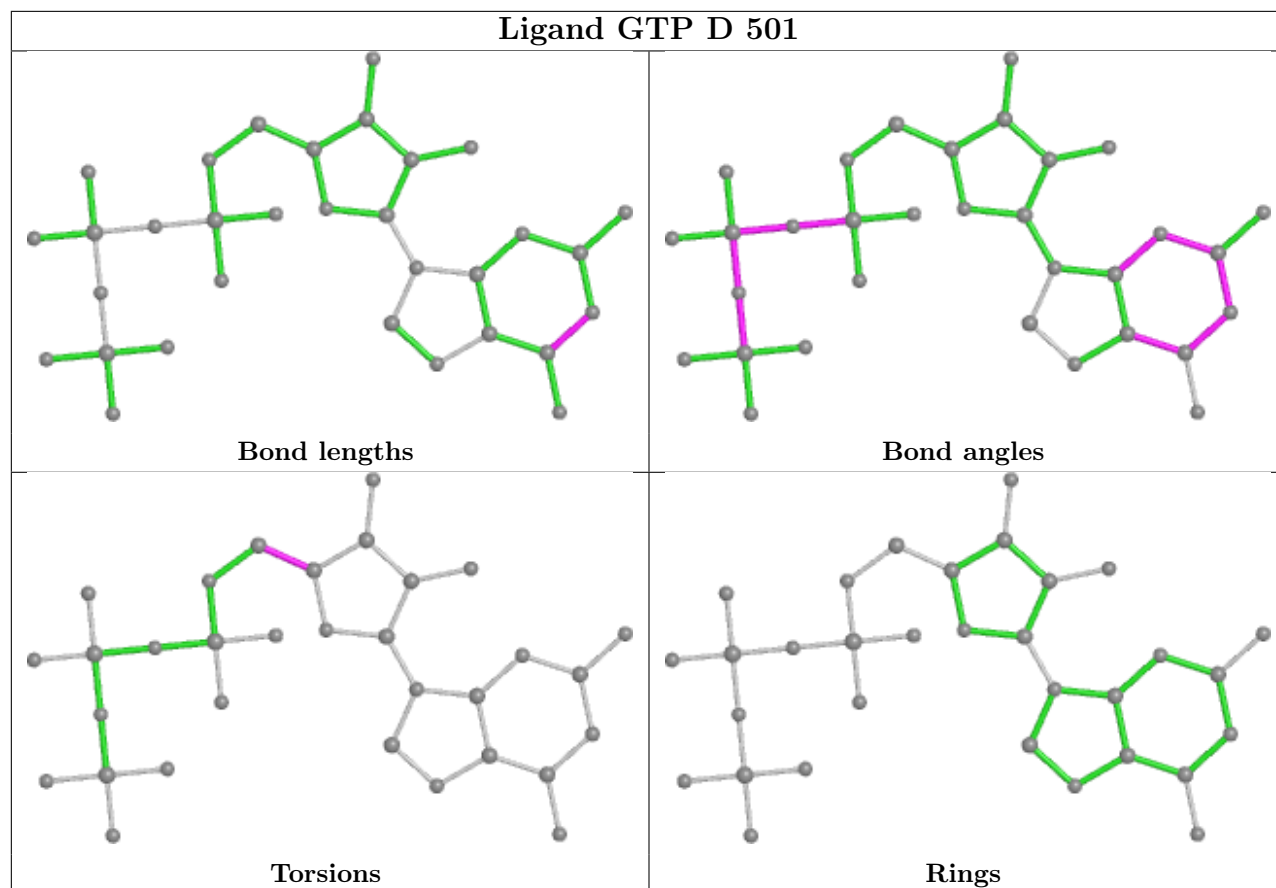
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
10	B	505	Y5J	N23-C09-N10-C21
10	B	505	Y5J	C17-C14-O15-C16
5	C	501	GTP	C3'-C4'-C5'-O5'
10	B	505	Y5J	C13-C14-O15-C16
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O2B
5	C	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3A-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C3'-C4'-C5'-O5'

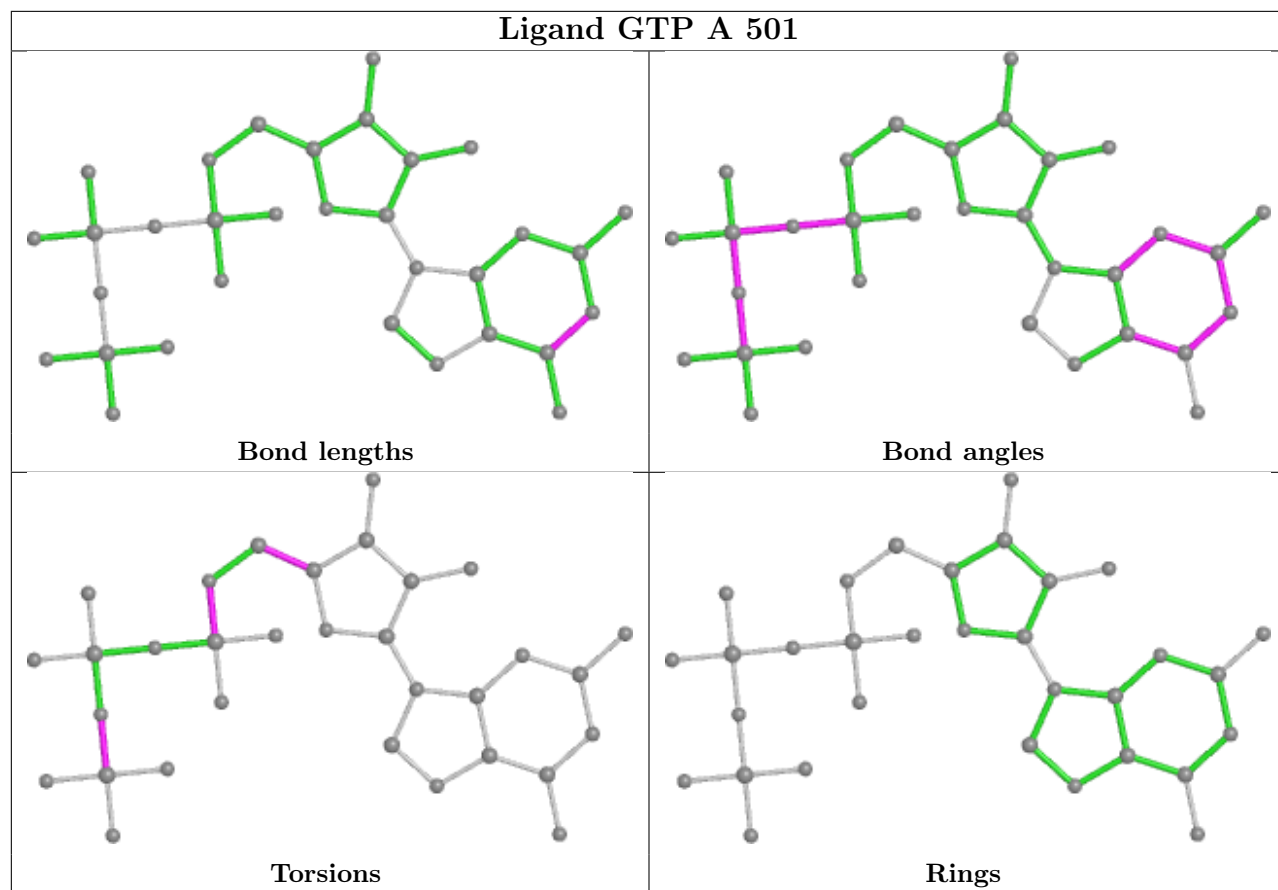
There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

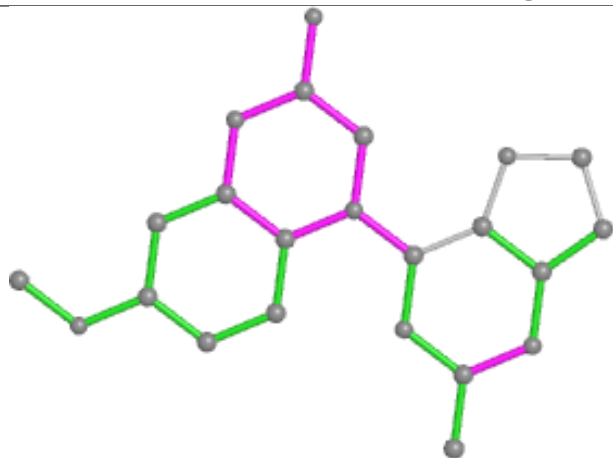
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



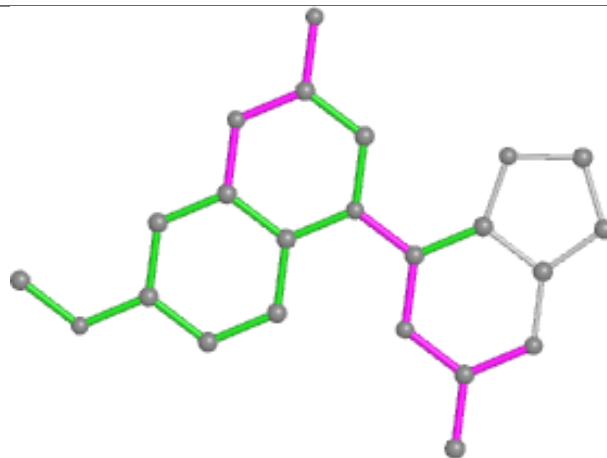




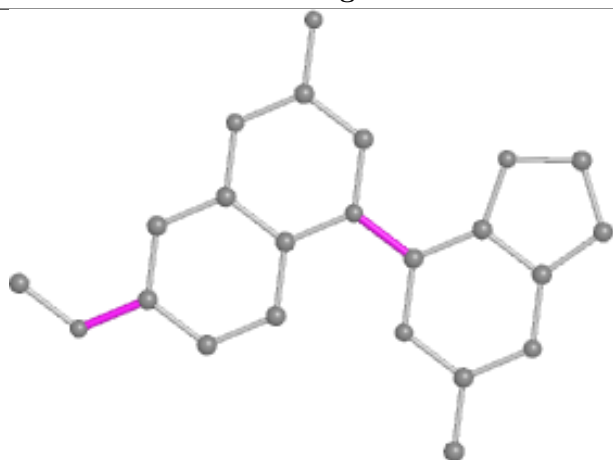
## Ligand Y5J B 505



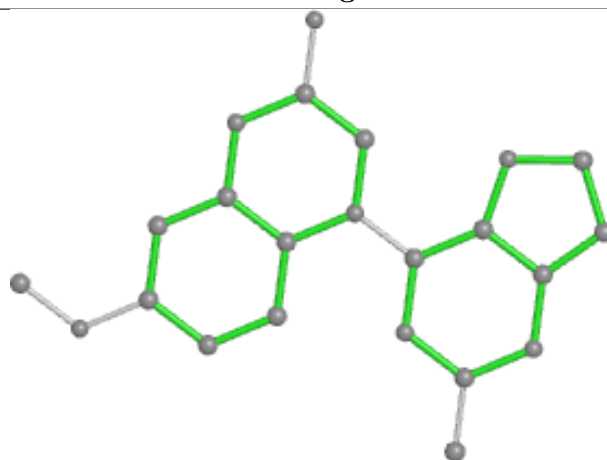
Bond lengths



Bond angles

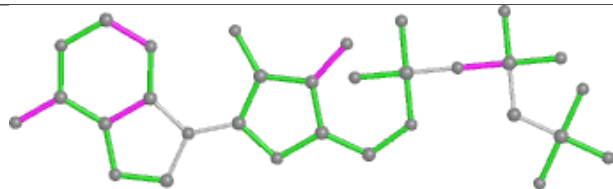


Torsions

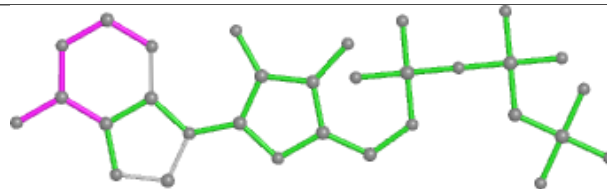


Rings

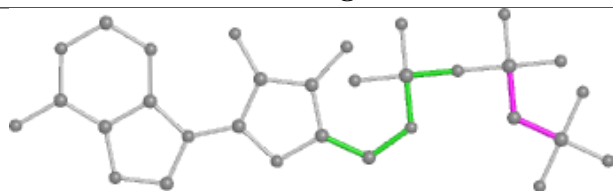
## Ligand ACP F 401



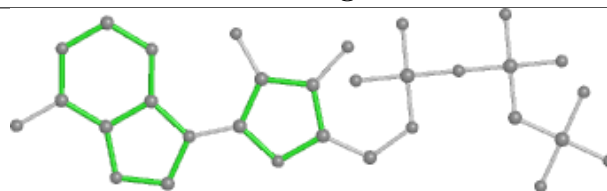
Bond lengths



Bond angles

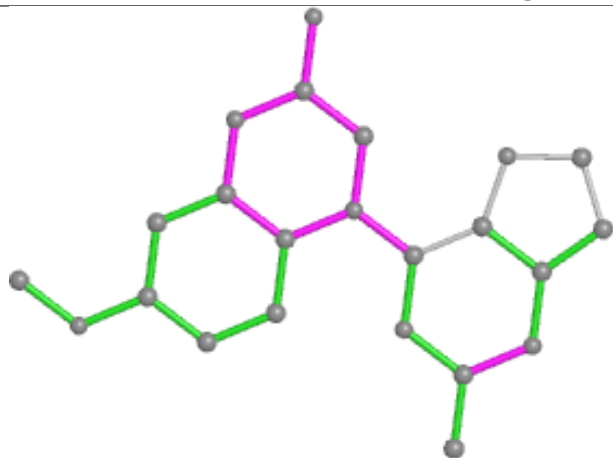


Torsions

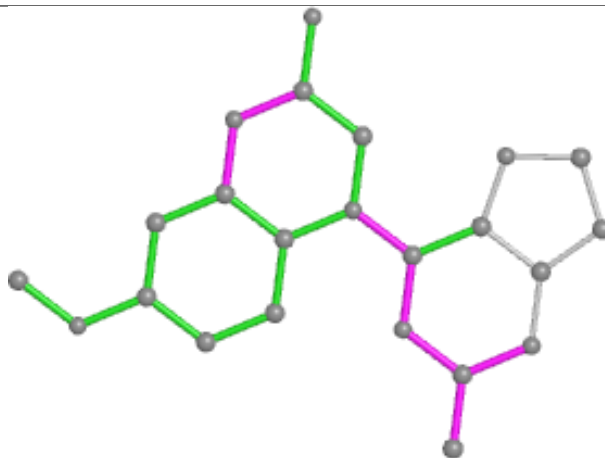


Rings

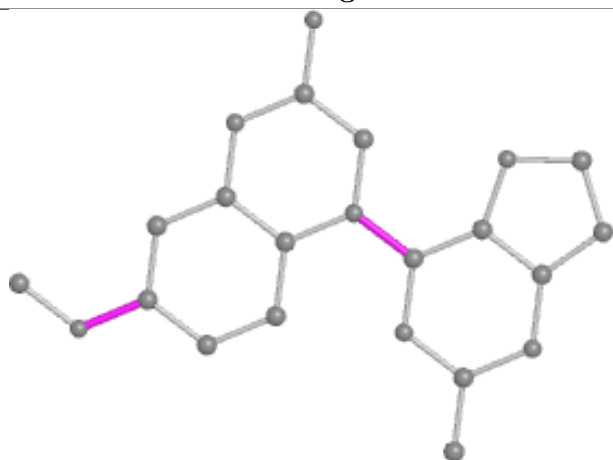
## Ligand Y5J D 502



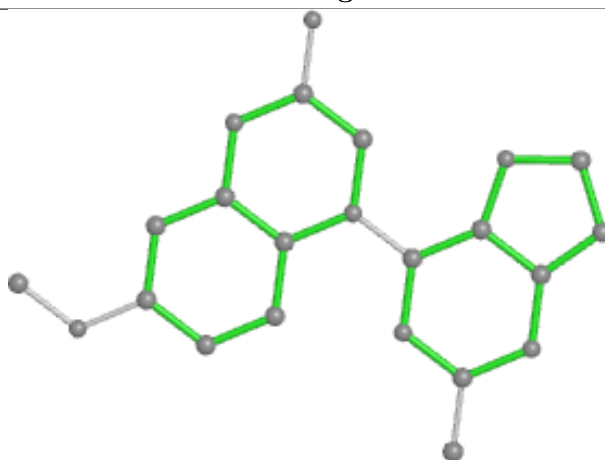
Bond lengths



Bond angles

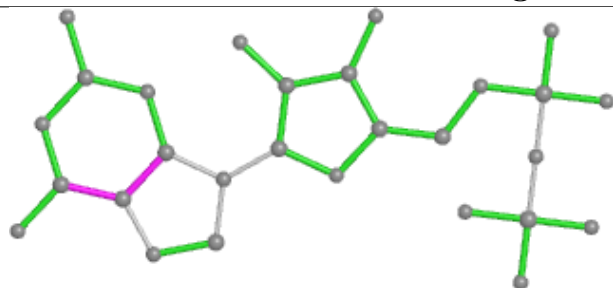


Torsions

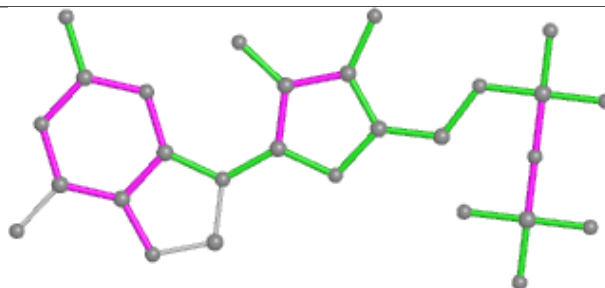


Rings

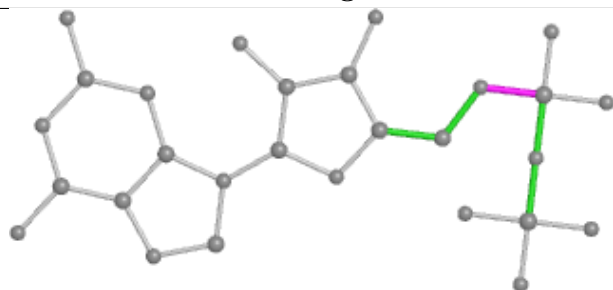
## Ligand GDP B 501



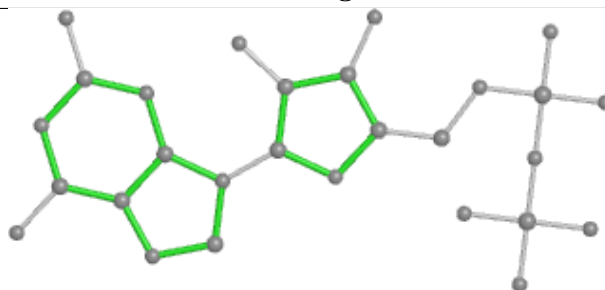
Bond lengths



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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	437/450 (97%)	-0.50	0 100 100	24, 41, 74, 90	0
1	C	440/450 (97%)	-0.59	0 100 100	18, 32, 62, 89	0
2	B	427/445 (95%)	-0.42	5 (1%) 79 79	19, 40, 84, 152	0
2	D	421/445 (94%)	-0.18	10 (2%) 59 56	29, 61, 104, 133	0
3	E	121/143 (84%)	-0.21	2 (1%) 70 69	33, 59, 102, 116	0
4	F	328/384 (85%)	0.33	26 (7%) 12 10	34, 69, 134, 146	0
All	All	2174/2317 (93%)	-0.30	43 (1%) 65 63	18, 47, 102, 152	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	57	ASN	4.6
4	F	234	GLN	4.0
2	B	427	ASP	3.8
4	F	130	VAL	3.7
4	F	136	ASN	3.6
2	D	1	MET	3.5
4	F	232	ASN	3.5
4	F	233	PHE	3.5
2	D	55	THR	3.2
2	D	54	ALA	3.1
4	F	231	ALA	3.1
4	F	172	PHE	3.0
4	F	225	SER	3.0
2	B	55	THR	3.0
4	F	253	TYR	2.9
4	F	143	GLU	2.8
2	D	92	PHE	2.7
4	F	256	TYR	2.7
4	F	244	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	56	GLY	2.7
2	B	37	HIS	2.6
2	D	93	GLY	2.6
4	F	102	PRO	2.6
4	F	380	HIS	2.5
2	B	277	GLY	2.4
4	F	239	HIS	2.4
4	F	195	GLY	2.4
3	E	28	SER	2.4
4	F	100	ILE	2.3
2	D	125	GLU	2.2
2	D	58	LYS	2.2
4	F	379	HIS	2.2
4	F	362	ALA	2.2
2	D	95	SER	2.2
4	F	101	TYR	2.2
4	F	259	GLY	2.1
4	F	132	LEU	2.1
2	D	94	GLN	2.1
4	F	180	HIS	2.0
4	F	226	GLU	2.0
4	F	24	THR	2.0
4	F	147	TRP	2.0
3	E	139	LEU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

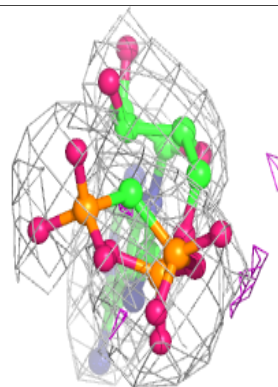
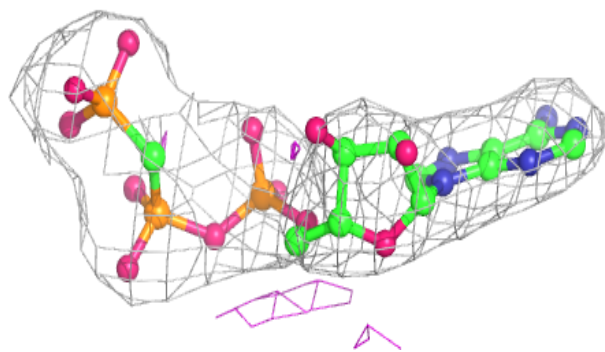
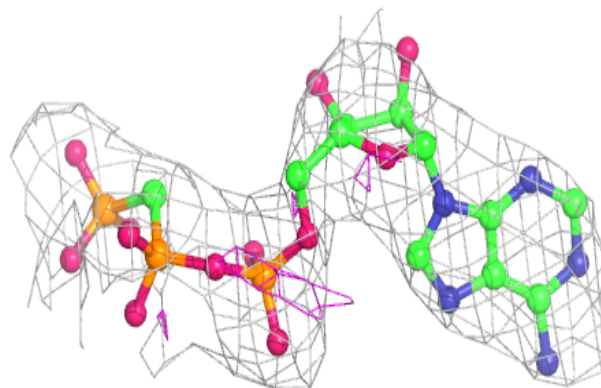
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	MG	F	402	1/1	0.78	0.14	101,101,101,101	0
6	CA	A	502	1/1	0.86	0.08	65,65,65,65	0
7	MG	D	503	1/1	0.87	0.15	61,61,61,61	0
11	ACP	F	401	31/31	0.92	0.18	61,85,116,121	0
9	MES	B	503	12/12	0.95	0.15	53,69,80,81	0
6	CA	C	502	1/1	0.96	0.05	43,43,43,43	0
9	MES	B	502	12/12	0.96	0.16	41,53,73,86	0
7	MG	C	503	1/1	0.96	0.12	32,32,32,32	0
5	GTP	D	501	32/32	0.96	0.13	44,56,106,109	0
10	Y5J	D	502	23/23	0.97	0.16	32,38,57,78	0
7	MG	A	503	1/1	0.97	0.10	32,32,32,32	0
5	GTP	A	501	32/32	0.98	0.16	16,25,36,38	0
10	Y5J	B	505	23/23	0.98	0.14	19,26,39,56	0
8	GDP	B	501	28/28	0.98	0.16	11,28,37,43	0
7	MG	B	504	1/1	0.98	0.15	37,37,37,37	0
5	GTP	C	501	32/32	0.99	0.15	13,24,30,36	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.

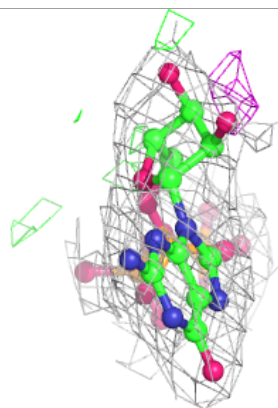
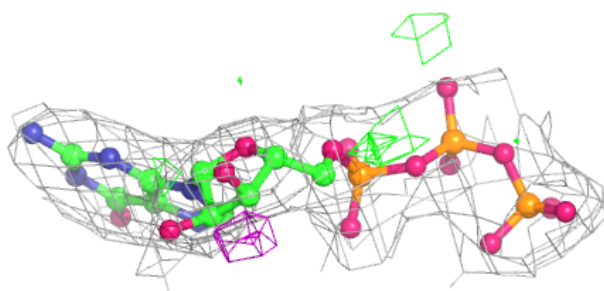
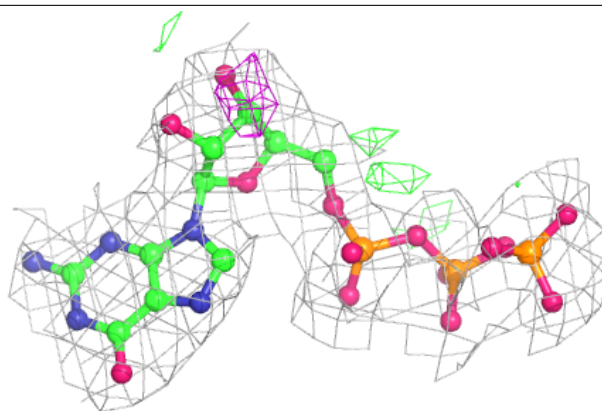
#### Electron density around ACP F 401:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
 mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
 and green (positive)

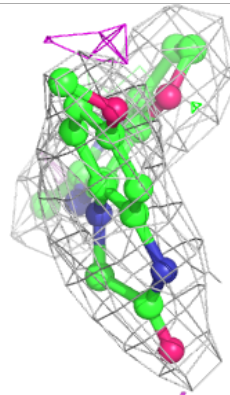
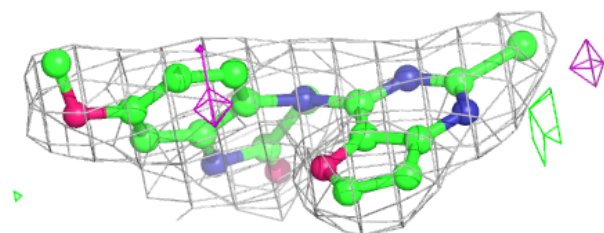
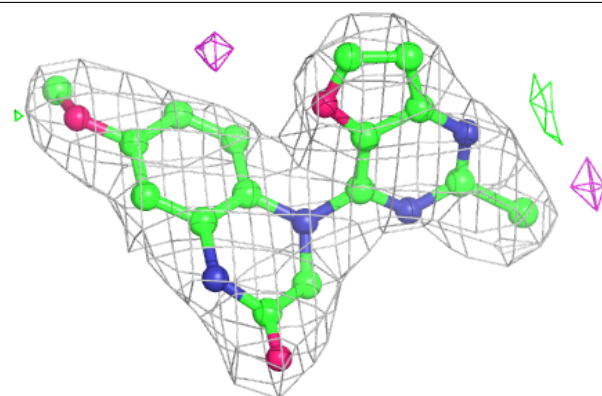


**Electron density around GTP D 501:**

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

**Electron density around Y5J D 502:**

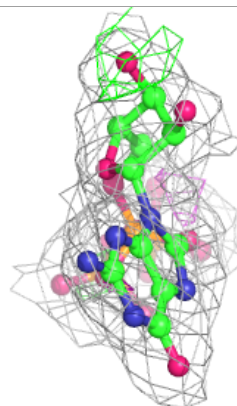
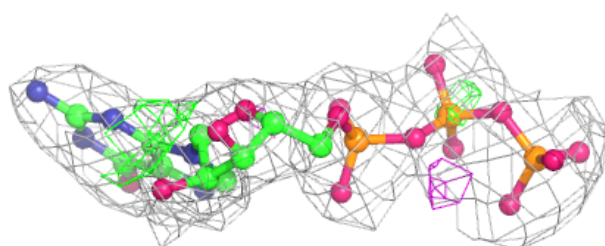
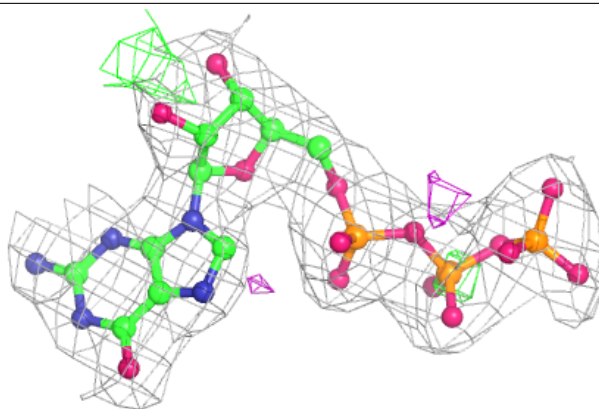
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



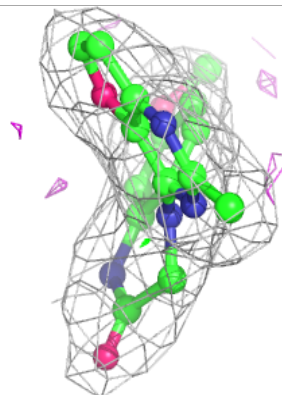
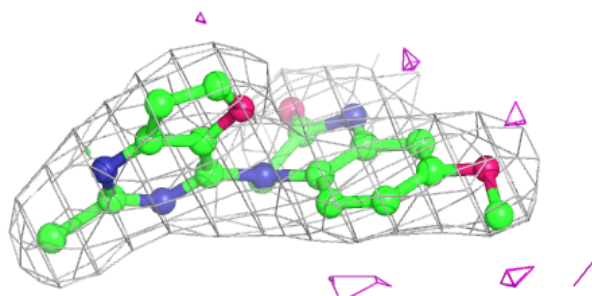
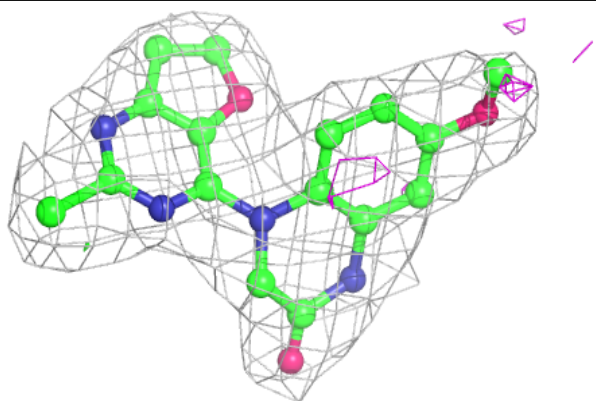


**Electron density around GTP A 501:**

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

**Electron density around Y5J B 505:**

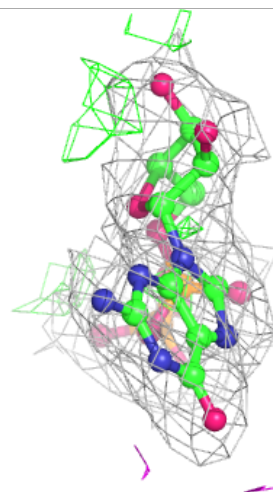
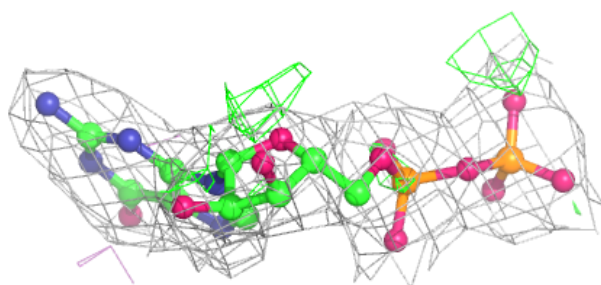
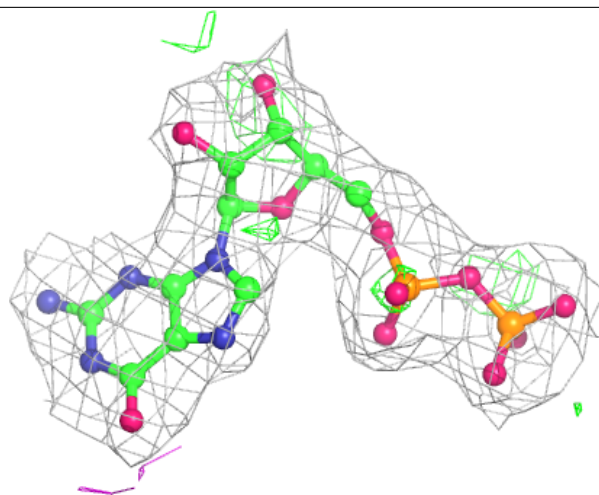
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

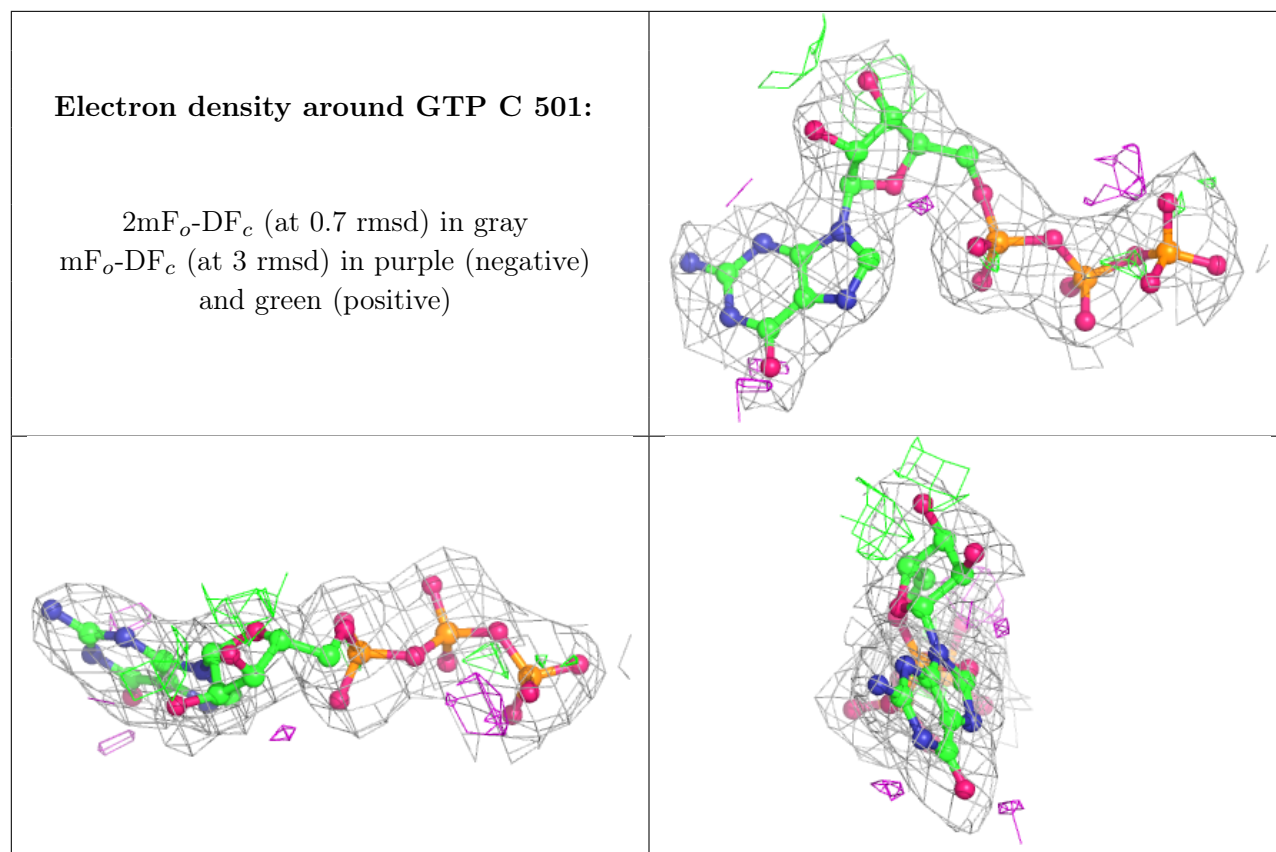




**Electron density around GDP B 501:**

$2mF_o-DF_c$  (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.