



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 02:08 am GMT

PDB ID : 5NFZ  
Title : TUBULIN-MTC complex  
Authors : Field, J.J.; Pera, B.; Estevez Gallego, J.; Calvo, E.; Rodriguez-Salarichs, J.; Saez-Calvo, G.; Zuverra, D.; Jordi, M.; Prota, A.E.; Menchon, G.; Miller, J.H.; Altmann, K.-H.; Diaz, J.F.  
Deposited on : 2017-03-16  
Resolution : 2.10 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.

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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

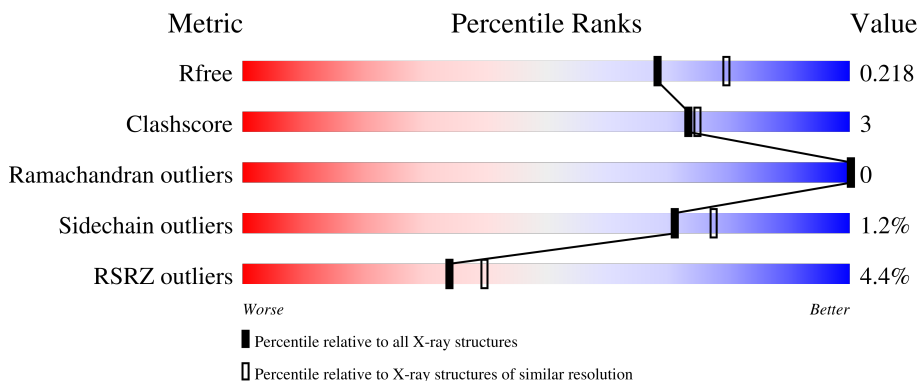
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

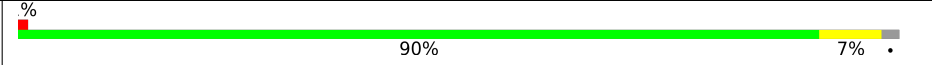

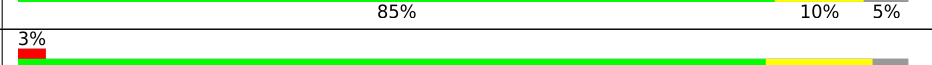

The reported resolution of this entry is 2.10 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	451	 90% 7%
1	C	451	 89% 8%
2	B	445	 85% 10% 5%
2	D	445	 84% 12%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	E	143	 <p>%</p> <p>85% 13%</p>
4	F	384	 <p>17%</p> <p>81% 9% 10%</p>

## 2 Entry composition i

There are 13 unique types of molecules in this entry. The entry contains 18133 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
			Total	C	N	O	S			
1	A	440	Total	C	N	O	S	0	3	0
			3452	2185	587	657	23			
1	C	440	Total	C	N	O	S	0	4	0
			3453	2185	585	660	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	424	Total	C	N	O	S	0	0	0
			3338	2098	569	645	26			
2	D	426	Total	C	N	O	S	0	0	0
			3344	2098	571	649	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	125	Total	C	N	O	S	0	1	0
			1038	639	190	204	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

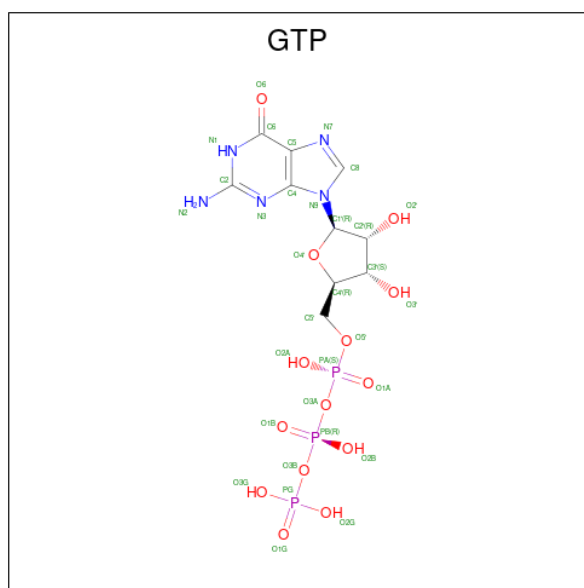
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	347	Total	C	N	O	S	0	1	0
			2837	1819	484	519	15			

There are 6 discrepancies between the modelled and reference sequences:

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
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		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

*Continued on next page...*

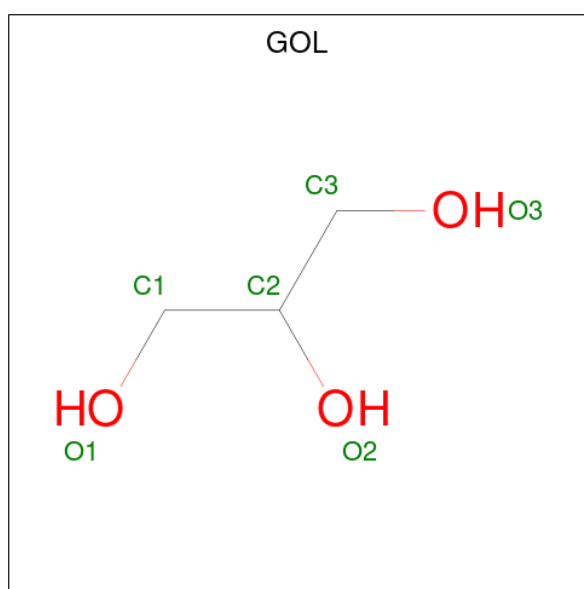
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

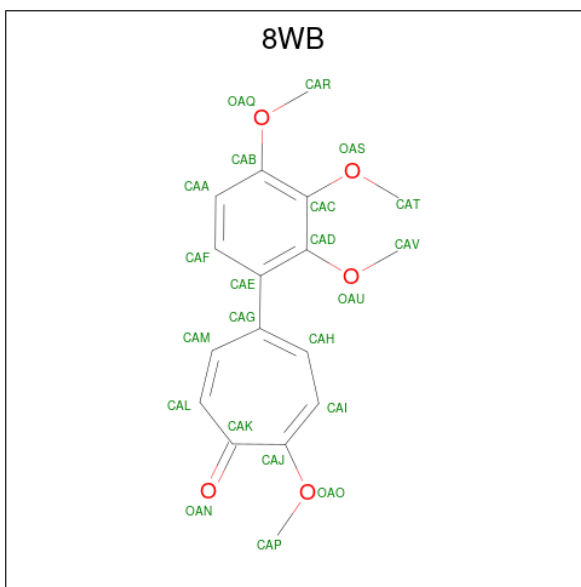
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



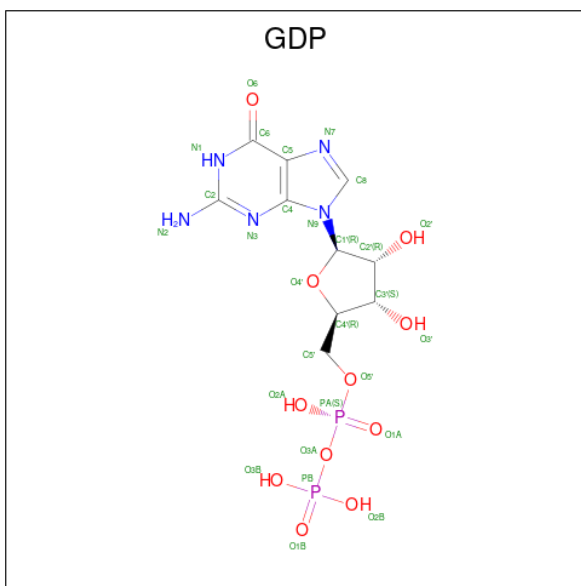
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 2-methoxy-5-(2,3,4-trimethoxyphenyl)cyclohepta-2,4,6-trien-1-one (three-letter code: 8WB) (formula: C<sub>17</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			22	17	5		
9	D	1	Total	C	O	0	0
			22	17	5		

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



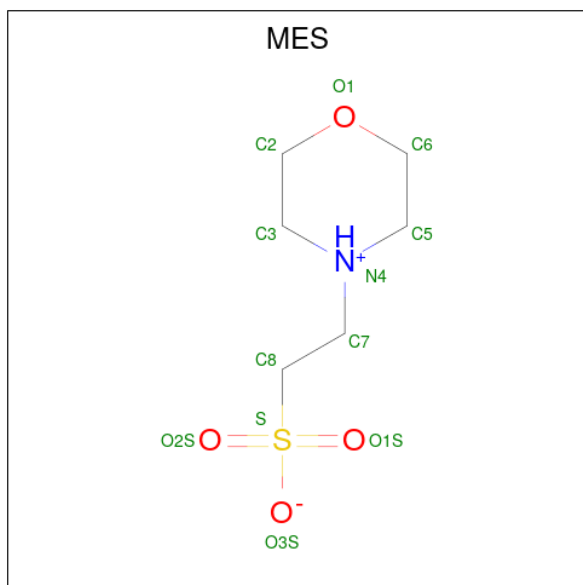
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
10	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

Continued on next page...

Continued from previous page...

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

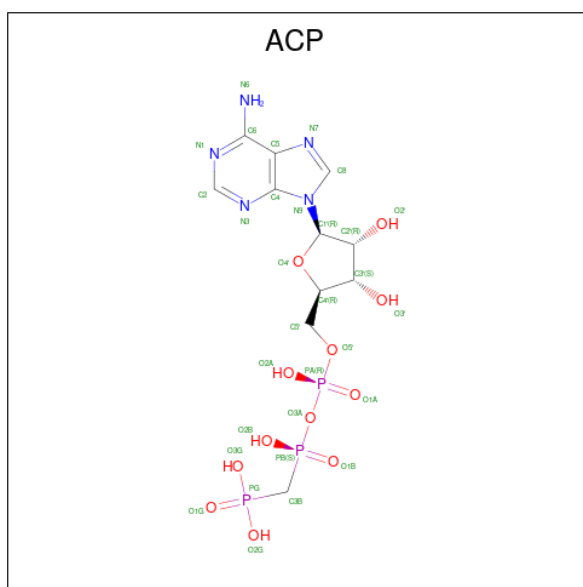
- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



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

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).





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

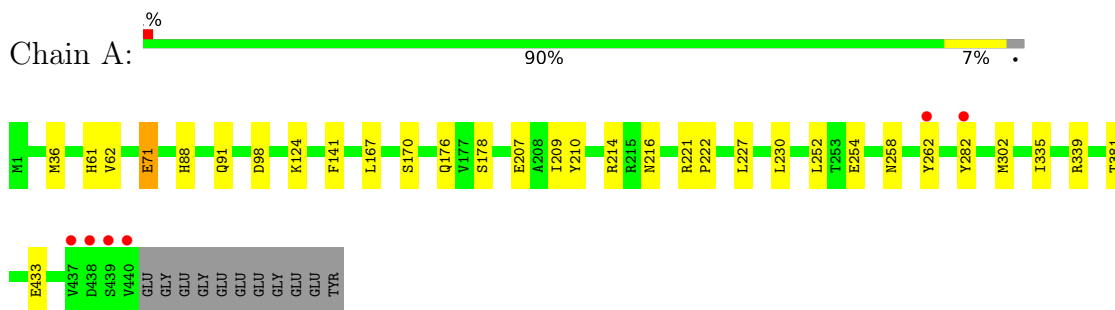
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	96	Total	O	0	0
			96	96		
13	B	92	Total	O	0	0
			92	92		
13	C	180	Total	O	0	0
			180	180		
13	D	36	Total	O	0	0
			36	36		
13	E	15	Total	O	0	0
			15	15		
13	F	30	Total	O	0	0
			30	30		

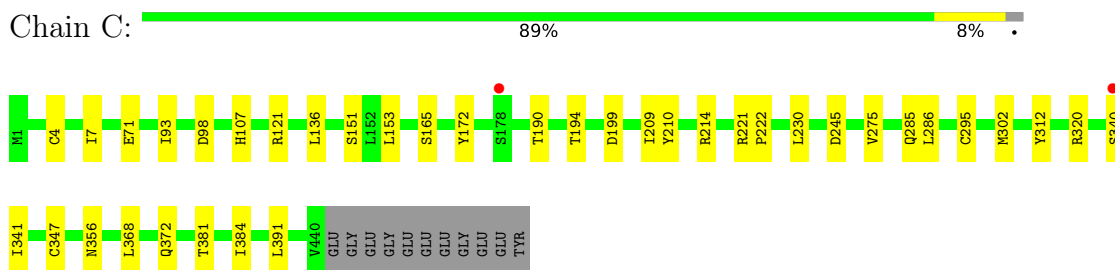
### 3 Residue-property plots [i](#)

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.

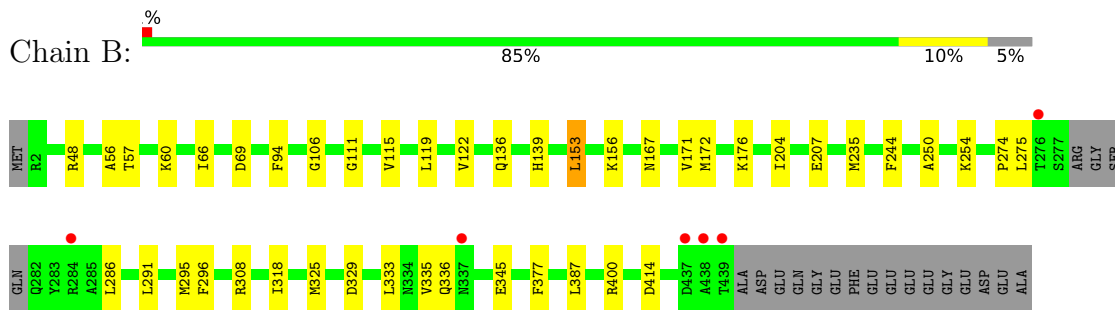
- Molecule 1: Tubulin alpha-1B chain



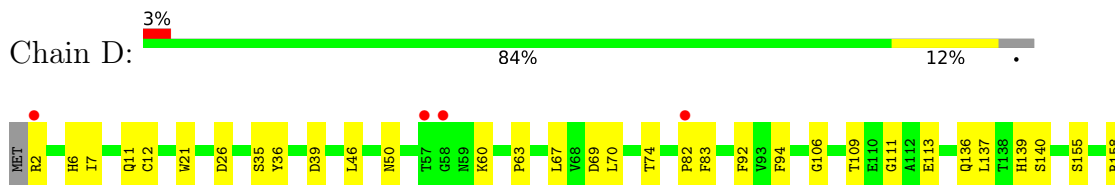
- Molecule 1: Tubulin alpha-1B chain

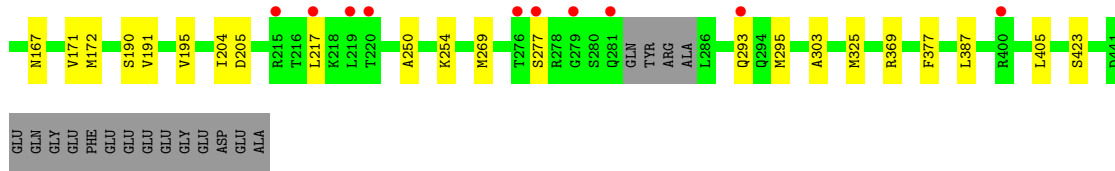


- Molecule 2: Tubulin beta-2B chain

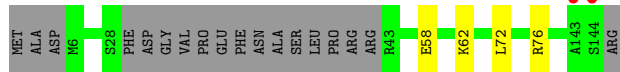
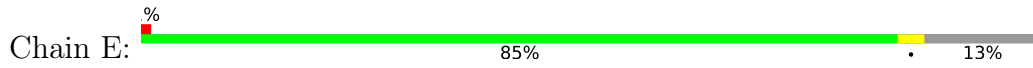


- Molecule 2: Tubulin beta-2B chain

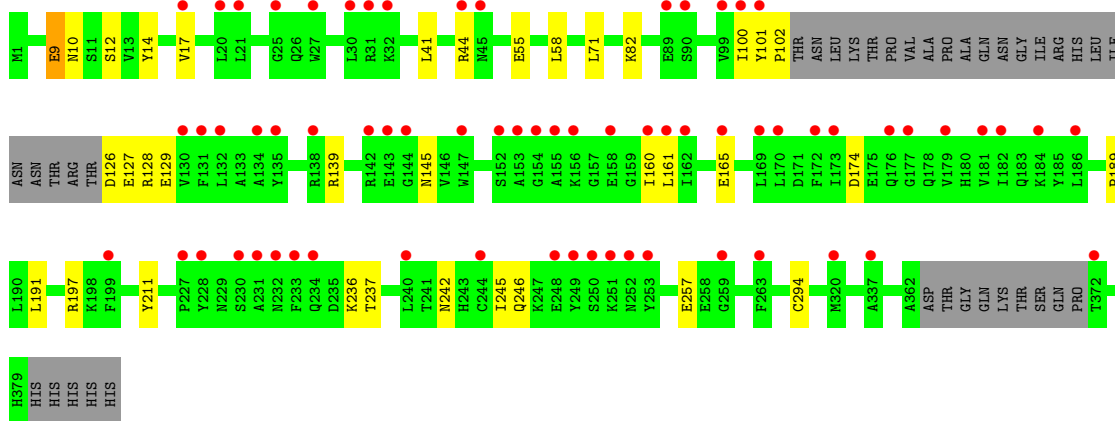
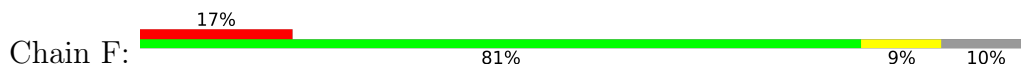




• Molecule 3: Stathmin-4



• 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, $\alpha$ , $\beta$ , $\gamma$	105.16Å 158.79Å 180.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.78 – 2.10 78.86 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (59.78-2.10) 100.0 (78.86-2.10)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.182 , 0.218 0.183 , 0.218	Depositor DCC
$R_{free}$ test set	8796 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtrriage
Anisotropy	0.120	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18133	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: 8WB, GOL, GDP, MES, MG, GTP, CA, ACP

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	0.40	0/3539	0.54	0/4804
1	C	0.51	2/3543 (0.1%)	0.60	0/4810
2	B	0.41	0/3412	0.56	0/4622
2	D	0.36	0/3417	0.52	0/4628
3	E	0.37	0/1050	0.46	0/1393
4	F	0.31	0/2904	0.48	0/3921
All	All	0.41	2/17865 (0.0%)	0.54	0/24178

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	CYS	CB-SG	-7.76	1.69	1.82
1	C	347	CYS	CB-SG	-7.20	1.70	1.82

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	3452	0	3374	19	0
1	C	3453	0	3368	20	0
2	B	3338	0	3215	27	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3344	0	3218	30	0
3	E	1038	0	1054	2	0
4	F	2837	0	2811	18	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	1	0
9	B	22	0	0	1	0
9	D	22	0	0	0	0
10	B	28	0	12	0	0
10	D	28	0	12	1	0
11	B	12	0	12	0	0
12	F	31	0	14	0	0
13	A	96	0	0	1	0
13	B	92	0	0	3	0
13	C	180	0	0	0	0
13	D	36	0	0	0	0
13	E	15	0	0	0	0
13	F	30	0	0	0	0
All	All	18133	0	17122	113	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 (113) 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:176:LYS:HD3	2:B:207:GLU:HG3	1.64	0.80
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.19	0.73
4:F:139:ARG:NH2	4:F:165:GLU:OE1	2.24	0.69
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.32	0.69
4:F:102:PRO:HB3	4:F:174:ASP:HA	1.77	0.66
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.32	0.64
1:A:221:ARG:HG2	2:B:325:MET:HG2	1.79	0.64

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.81	0.62
4:F:9:GLU:H	4:F:9:GLU:CD	2.04	0.61
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.83	0.61
2:B:329:ASP:O	2:B:333:LEU:HG	2.01	0.60
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.83	0.59
1:A:62:VAL:HG11	1:A:88:HIS:CE1	2.38	0.58
2:D:50:ASN:HD22	2:D:50:ASN:H	1.52	0.57
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.20	0.57
4:F:242:ASN:HD22	4:F:245:ILE:HD12	1.70	0.57
1:A:216:ASN:ND2	8:A:505:GOL:H2	2.20	0.57
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.87	0.55
4:F:160:ILE:O	4:F:236:LYS:NZ	2.39	0.54
2:B:136:GLN:HA	2:B:167:ASN:O	2.08	0.54
4:F:139:ARG:HB2	4:F:145:ASN:ND2	2.22	0.54
1:C:98:ASP:H	2:D:2:ARG:NH2	2.07	0.52
4:F:82:LYS:NZ	4:F:127:GLU:OE2	2.42	0.51
1:C:221:ARG:HG2	2:D:325:MET:HB3	1.92	0.51
2:B:414:ASP:OD2	13:B:601:HOH:O	2.19	0.51
2:D:171:VAL:HA	2:D:204:ILE:O	2.11	0.50
2:B:56:ALA:HB3	2:B:60:LYS:HB2	1.93	0.50
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.47	0.50
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.77	0.50
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.92	0.50
2:D:136:GLN:HA	2:D:167:ASN:O	2.13	0.49
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.93	0.49
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.47	0.49
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.47	0.48
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.95	0.48
2:B:318:ILE:HD11	9:B:501:8WB:CAT	2.43	0.48
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.95	0.48
4:F:161:LEU:HD12	4:F:236:LYS:HZ1	1.77	0.48
2:B:69:ASP:O	2:B:94:PHE:HA	2.13	0.48
4:F:237:THR:O	4:F:246:GLN:NE2	2.47	0.47
1:C:209:ILE:HD11	1:C:302:MET:SD	2.55	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.96	0.47
1:C:210:TYR:CE2	1:C:214:ARG:HD2	2.50	0.47
1:C:320:ARG:HA	1:C:356:ASN:O	2.14	0.47
2:D:11:GLN:HA	2:D:74:THR:HG21	1.97	0.47
3:E:58:GLU:HG2	3:E:62:LYS:HE3	1.96	0.47
2:B:295:MET:CG	2:B:377:PHE:HB2	2.44	0.47
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.50	0.46
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.96	0.46
1:A:209:ILE:HD11	1:A:302:MET:SD	2.55	0.46
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.98	0.46
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.34	0.46
1:A:124:LYS:HA	1:A:124:LYS:HD3	1.83	0.46
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.98	0.46
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.97	0.45
4:F:14:TYR:HA	4:F:17:VAL:HB	1.97	0.45
1:A:176:GLN:HE22	1:A:207:GLU:HG3	1.81	0.45
2:D:12:CYS:HB2	10:D:501:GDP:C8	2.52	0.45
2:B:336:GLN:NE2	13:B:605:HOH:O	2.48	0.45
2:D:50:ASN:H	2:D:50:ASN:ND2	2.13	0.45
4:F:101:TYR:N	4:F:126:ASP:OD1	2.42	0.45
4:F:189:PRO:HG2	4:F:191:LEU:HD21	1.98	0.45
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.45
1:A:88:HIS:N	1:A:91:GLN:OE1	2.42	0.45
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.43	0.44
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.53	0.44
1:C:107:HIS:HD2	1:C:151[A]:SER:OG	1.99	0.44
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.99	0.44
2:D:109:THR:O	2:D:113:GLU:HG3	2.18	0.44
2:B:106:GLY:O	2:B:111:GLY:HA3	2.18	0.44
2:B:308:ARG:NH1	13:B:608:HOH:O	2.52	0.43
3:E:72:LEU:O	3:E:76:ARG:HG2	2.18	0.43
2:B:250:ALA:HA	2:B:254:LYS:HD2	2.01	0.43
2:B:286:LEU:HD23	2:B:291:LEU:HD13	2.00	0.43
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.53	0.43
2:D:217:LEU:HA	2:D:277:SER:HB3	2.00	0.43
1:A:282:TYR:HA	13:A:644:HOH:O	2.19	0.43
2:B:235:MET:HB3	2:B:235:MET:HE2	1.83	0.42
2:D:205:ASP:HB3	2:D:303:ALA:HA	2.01	0.42
2:B:296:PHE:CE2	2:B:335:VAL:HG11	2.53	0.42
2:B:172:MET:HG3	2:B:387:LEU:HD11	2.02	0.42
2:D:35:SER:OG	2:D:60:LYS:HE2	2.19	0.42
2:B:48:ARG:NH2	2:B:244:PHE:O	2.52	0.42
1:C:151[B]:SER:HA	1:C:194:THR:HG22	2.00	0.42
2:D:69:ASP:O	2:D:94:PHE:HA	2.20	0.42
1:A:167:LEU:HD22	1:A:252:LEU:HD22	2.02	0.42
1:C:165:SER:HA	1:C:199:ASP:OD2	2.20	0.42
2:D:191:VAL:O	2:D:195:VAL:HG23	2.20	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.55	0.41
2:B:115:VAL:HG23	2:B:153:LEU:HD13	2.01	0.41
1:A:209:ILE:HG22	1:A:227:LEU:HD22	2.03	0.41
2:B:171:VAL:HA	2:B:204:ILE:O	2.20	0.41
2:B:400:ARG:HE	2:B:400:ARG:HB3	1.55	0.41
4:F:55:GLU:HB3	4:F:58:LEU:HD12	2.03	0.41
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.02	0.41
1:C:190:THR:O	1:C:194:THR:HG23	2.20	0.41
2:D:172:MET:HG3	2:D:387:LEU:HD11	2.02	0.41
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.56	0.41
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.21	0.41
2:D:250:ALA:HA	2:D:254:LYS:HD2	2.03	0.41
2:D:405:LEU:HD23	2:D:405:LEU:HA	1.91	0.41
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.56	0.41
2:B:66:ILE:HD12	2:B:122:VAL:HG22	2.03	0.41
1:C:286:LEU:HD23	1:C:286:LEU:HA	1.94	0.40
2:D:106:GLY:O	2:D:111:GLY:HA3	2.21	0.40
2:B:345:GLU:H	2:B:345:GLU:CD	2.22	0.40
2:D:7:ILE:O	2:D:137:LEU:HA	2.20	0.40
1:A:176:GLN:NE2	1:A:207:GLU:HG3	2.36	0.40
2:B:345:GLU:OE1	2:B:345:GLU:N	2.47	0.40
2:D:39:ASP:OD1	2:D:39:ASP:N	2.53	0.40
2:D:82:PRO:O	2:D:83:PHE:HB2	2.21	0.40
2:D:69:ASP:OD1	2:D:70:LEU:N	2.54	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	441/451 (98%)	430 (98%)	11 (2%)	0	<a href="#">100</a> <a href="#">100</a>

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	442/451 (98%)	430 (97%)	12 (3%)	0	100	100
2	B	420/445 (94%)	412 (98%)	8 (2%)	0	100	100
2	D	422/445 (95%)	414 (98%)	8 (2%)	0	100	100
3	E	122/143 (85%)	122 (100%)	0	0	100	100
4	F	342/384 (89%)	337 (98%)	5 (2%)	0	100	100
All	All	2189/2319 (94%)	2145 (98%)	44 (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	374/379 (99%)	369 (99%)	5 (1%)	69	75
1	C	375/379 (99%)	371 (99%)	4 (1%)	73	79
2	B	367/383 (96%)	363 (99%)	4 (1%)	73	79
2	D	368/383 (96%)	362 (98%)	6 (2%)	62	69
3	E	113/127 (89%)	113 (100%)	0	100	100
4	F	310/342 (91%)	306 (99%)	4 (1%)	69	75
All	All	1907/1993 (96%)	1884 (99%)	23 (1%)	71	77

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	178	SER
1	A	262	TYR
1	A	381	THR
1	A	433	GLU
2	B	57	THR
2	B	139	HIS
2	B	153	LEU

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	275	LEU
1	C	245	ASP
1	C	340	SER
1	C	381	THR
1	C	384	ILE
2	D	139	HIS
2	D	155	SER
2	D	158	ARG
2	D	190	SER
2	D	293	GLN
2	D	423	SER
4	F	9	GLU
4	F	12	SER
4	F	129	GLU
4	F	211	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
2	B	192	HIS
1	C	356	ASN
2	D	50	ASN
2	D	406	HIS
4	F	242	ASN
4	F	260	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 18 ligands modelled in this entry, 9 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	GDP	D	501	6	24,30,30	1.42	3 (12%)	30,47,47	0.95	1 (3%)
9	8WB	D	500	-	22,23,23	2.10	3 (13%)	29,31,31	1.64	5 (17%)
8	GOL	A	505	-	5,5,5	0.32	0	5,5,5	0.50	0
5	GTP	C	501	6	26,34,34	1.70	5 (19%)	32,54,54	0.83	1 (3%)
5	GTP	A	501	6	26,34,34	1.70	4 (15%)	32,54,54	0.94	2 (6%)
10	GDP	B	502	6	24,30,30	1.37	3 (12%)	30,47,47	1.15	4 (13%)
11	MES	B	505	-	12,12,12	1.95	1 (8%)	14,16,16	1.82	4 (28%)
9	8WB	B	501	-	22,23,23	2.17	4 (18%)	29,31,31	1.52	6 (20%)
12	ACP	F	402	6	27,33,33	1.61	5 (18%)	32,52,52	1.29	3 (9%)

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	GDP	D	501	6	-	5/12/32/32	0/3/3/3
9	8WB	D	500	-	-	1/11/12/12	0/2/2/2
8	GOL	A	505	-	-	2/4/4/4	-
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
10	GDP	B	502	6	-	5/12/32/32	0/3/3/3
11	MES	B	505	-	-	1/6/14/14	0/1/1/1
9	8WB	B	501	-	-	1/11/12/12	0/2/2/2
12	ACP	F	402	6	-	3/15/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	8WB	CAE-CAG	-7.70	1.39	1.48
9	D	500	8WB	CAE-CAG	-7.68	1.39	1.48
11	B	505	MES	C8-S	-6.42	1.68	1.77
5	C	501	GTP	C6-N1	-5.04	1.30	1.37
5	A	501	GTP	C6-N1	-4.64	1.31	1.37
9	B	501	8WB	CAJ-CAK	-4.31	1.40	1.47
9	D	500	8WB	CAJ-CAK	-3.95	1.41	1.47
10	D	501	GDP	C6-N1	-3.77	1.32	1.37
12	F	402	ACP	PB-O1B	3.50	1.60	1.51
12	F	402	ACP	PB-O2B	-3.44	1.48	1.56
12	F	402	ACP	C2'-C1'	-3.34	1.48	1.53
5	C	501	GTP	PG-O3G	-3.32	1.42	1.54
10	B	502	GDP	C6-N1	-3.26	1.33	1.37
5	A	501	GTP	C2'-C1'	-3.24	1.48	1.53
10	B	502	GDP	C2'-C1'	-3.10	1.49	1.53
5	A	501	GTP	PG-O3G	-2.91	1.43	1.54
5	C	501	GTP	C2'-C1'	-2.73	1.49	1.53
10	D	501	GDP	C2-N1	-2.69	1.31	1.37
5	A	501	GTP	C2-N1	-2.67	1.31	1.37
10	D	501	GDP	C2'-C1'	-2.66	1.49	1.53
12	F	402	ACP	PG-O2G	2.56	1.60	1.54
12	F	402	ACP	PG-O3G	2.45	1.60	1.54
10	B	502	GDP	C2-N1	-2.34	1.31	1.37
9	B	501	8WB	OAU-CAD	-2.24	1.34	1.38
9	D	500	8WB	CAM-CAG	-2.20	1.39	1.45
5	C	501	GTP	PA-O2A	-2.18	1.45	1.55
9	B	501	8WB	CAL-CAK	-2.07	1.40	1.44
5	C	501	GTP	C2-N1	-2.03	1.32	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	500	8WB	OAO-CAJ-CAK	4.67	114.11	109.56
11	B	505	MES	C5-N4-C3	4.11	118.08	108.83
9	B	501	8WB	OAO-CAJ-CAK	3.87	113.33	109.56
12	F	402	ACP	N3-C2-N1	-3.84	122.67	128.68
11	B	505	MES	O1S-S-C8	3.44	111.06	106.92
12	F	402	ACP	PB-O3A-PA	-3.37	121.89	132.56
9	D	500	8WB	CAL-CAK-CAJ	3.31	126.77	121.64
9	B	501	8WB	CAL-CAK-CAJ	3.30	126.75	121.64
9	D	500	8WB	CAR-OAQ-CAB	-2.97	113.05	117.53
10	B	502	GDP	O6-C6-C5	-2.92	118.66	124.37
11	B	505	MES	O2S-S-C8	2.91	110.42	106.92

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	500	8WB	OAN-CAK-CAL	-2.73	114.65	119.44
10	D	501	GDP	C8-N7-C5	2.49	107.73	102.99
10	B	502	GDP	C5-C6-N1	2.45	118.28	113.95
9	B	501	8WB	CAP-OAO-CAJ	2.39	121.38	116.96
9	B	501	8WB	OAN-CAK-CAL	-2.34	115.33	119.44
9	B	501	8WB	CAE-CAG-CAM	2.25	119.02	117.22
5	C	501	GTP	C8-N7-C5	2.25	107.28	102.99
9	D	500	8WB	CAP-OAO-CAJ	2.25	121.11	116.96
5	A	501	GTP	C8-N7-C5	2.23	107.24	102.99
11	B	505	MES	C7-N4-C5	2.17	116.77	111.23
10	B	502	GDP	C8-N7-C5	2.13	107.04	102.99
9	B	501	8WB	CAR-OAQ-CAB	-2.06	114.42	117.53
12	F	402	ACP	N6-C6-N1	2.05	122.82	118.57
10	B	502	GDP	O6-C6-N1	2.04	123.06	120.65
5	A	501	GTP	C5-C6-N1	2.01	117.49	113.95

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	A	505	GOL	O1-C1-C2-C3
9	B	501	8WB	CAD-CAE-CAG-CAH
9	D	500	8WB	CAD-CAE-CAG-CAH
10	B	502	GDP	C5'-O5'-PA-O1A
10	B	502	GDP	C5'-O5'-PA-O2A
10	D	501	GDP	C5'-O5'-PA-O1A
11	B	505	MES	C8-C7-N4-C5
12	F	402	ACP	C5'-O5'-PA-O3A
8	A	505	GOL	O1-C1-C2-O2
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
10	D	501	GDP	C5'-O5'-PA-O3A
10	D	501	GDP	C5'-O5'-PA-O2A
12	F	402	ACP	C5'-O5'-PA-O1A
12	F	402	ACP	C5'-O5'-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G

Continued on next page...

*Continued from previous page...*

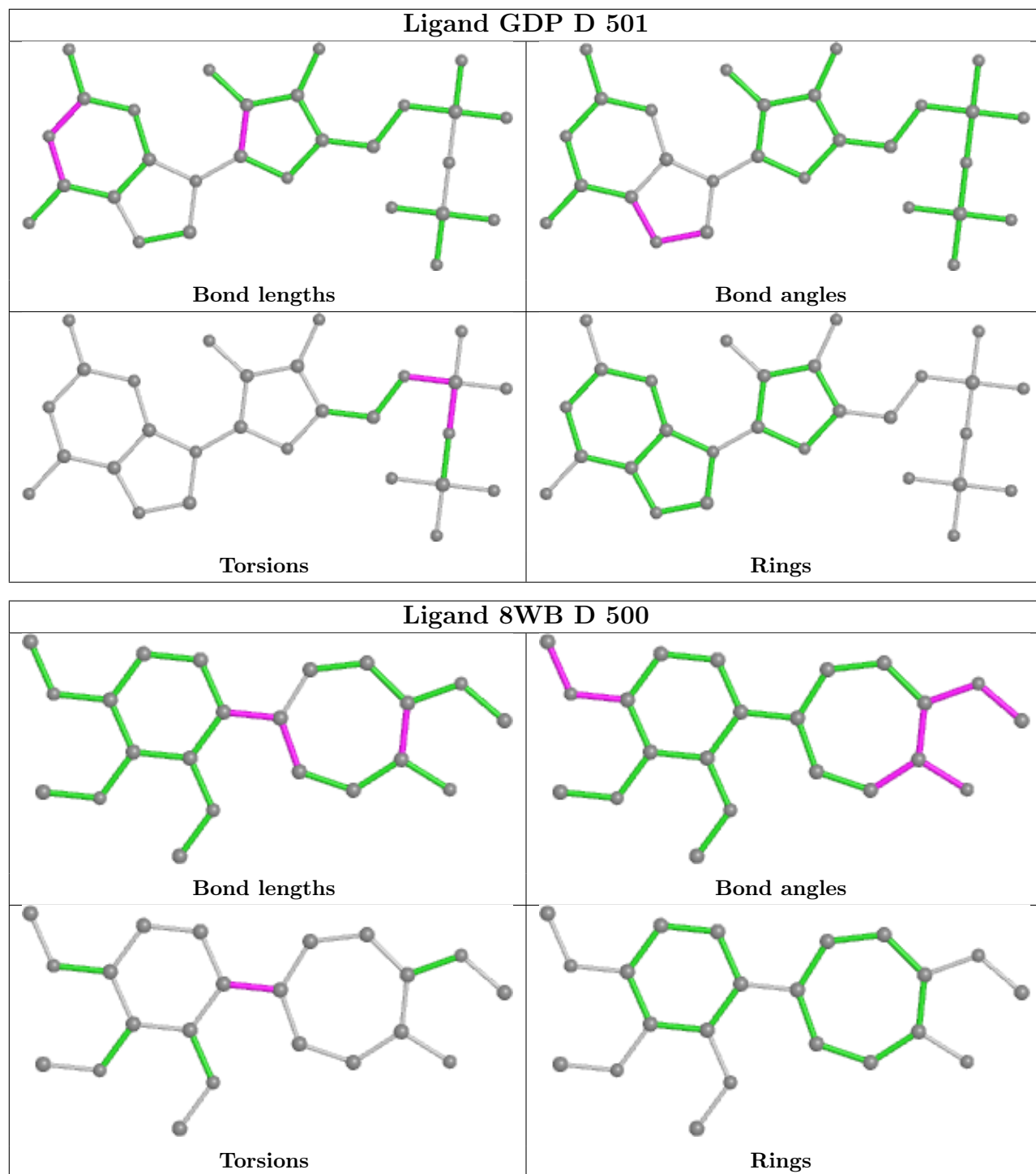
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
10	B	502	GDP	C5'-O5'-PA-O3A
10	B	502	GDP	PB-O3A-PA-O1A
10	B	502	GDP	PB-O3A-PA-O2A
10	D	501	GDP	PB-O3A-PA-O1A
10	D	501	GDP	PB-O3A-PA-O2A

There are no ring outliers.

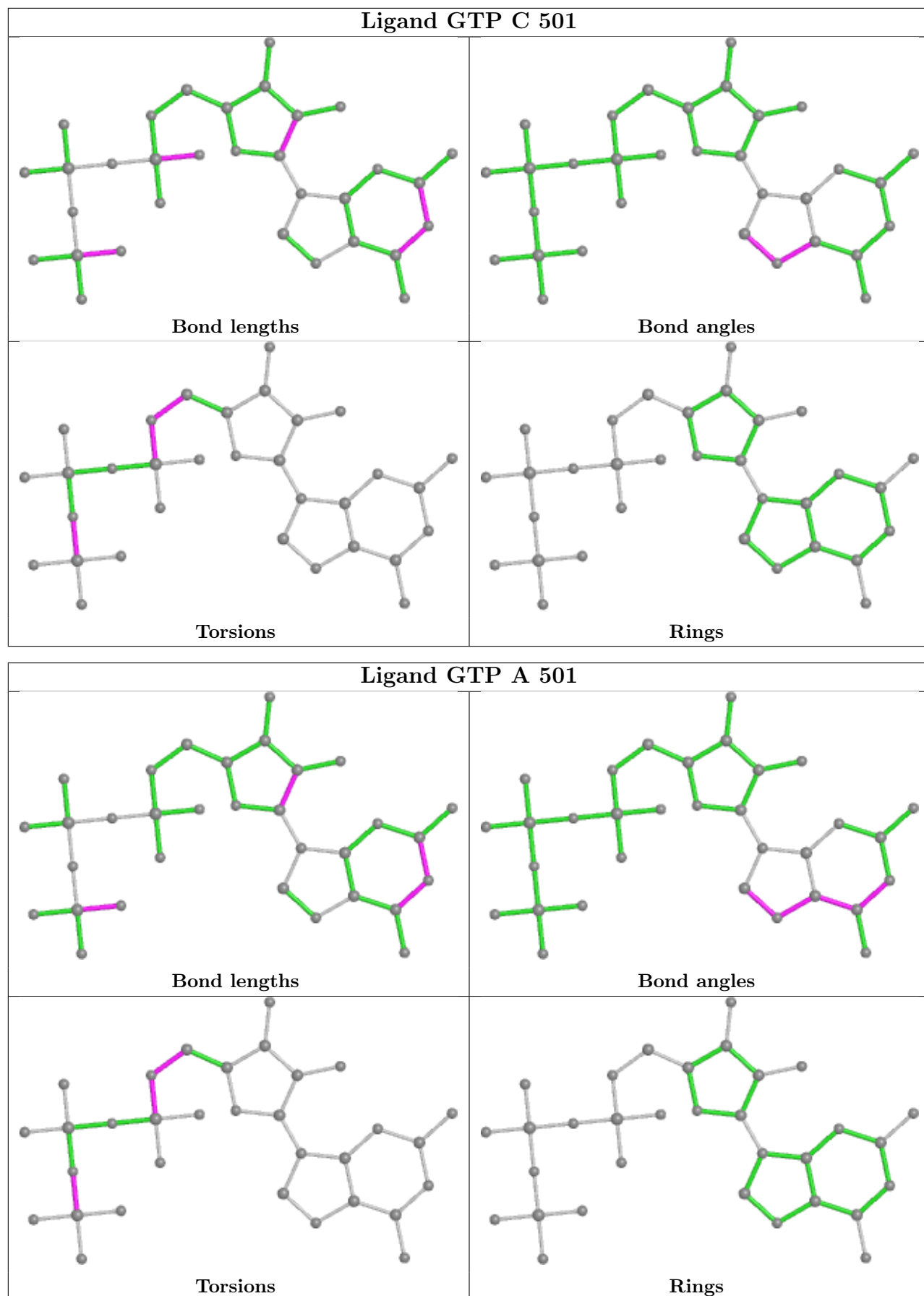
3 monomers are involved in 3 short contacts:

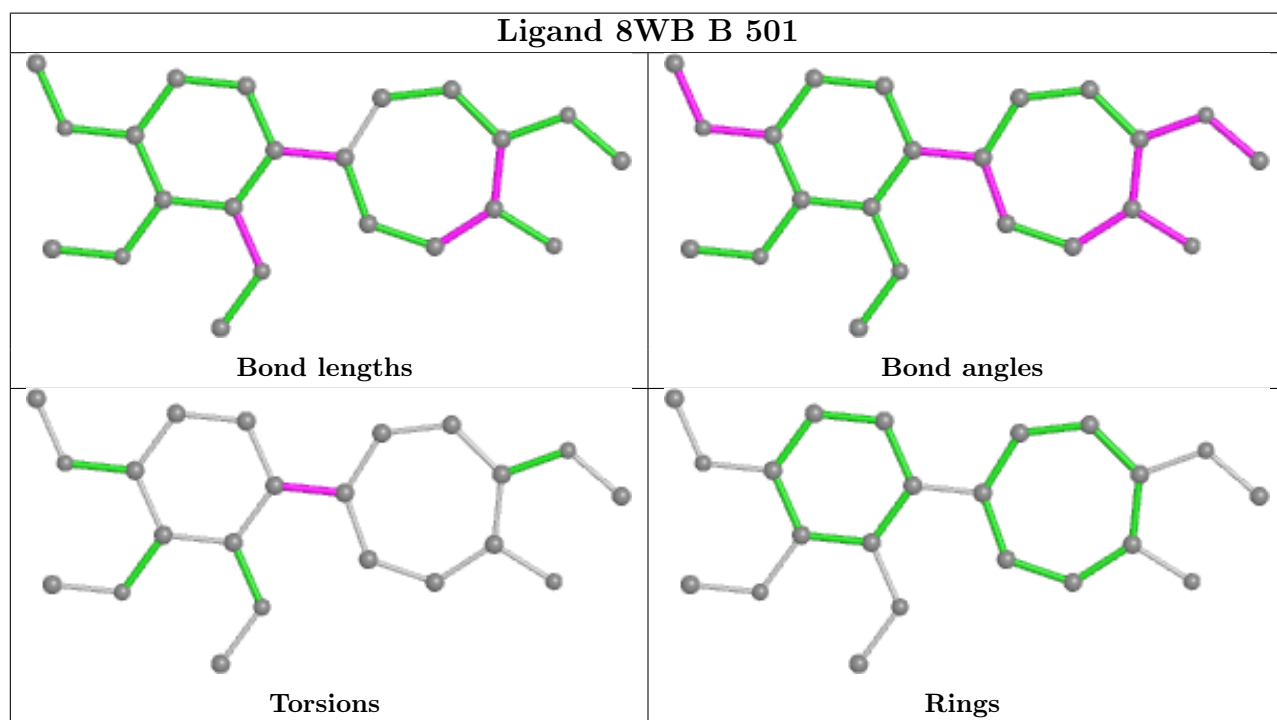
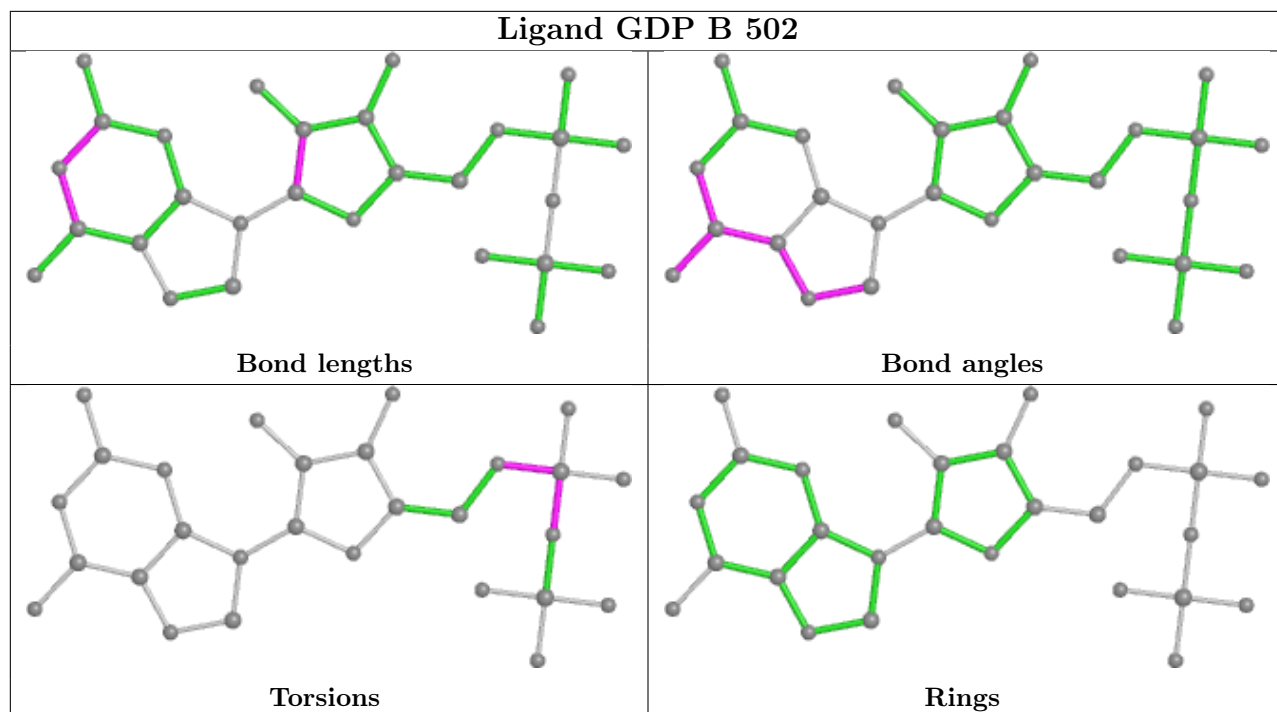
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	501	GDP	1	0
8	A	505	GOL	1	0
9	B	501	8WB	1	0

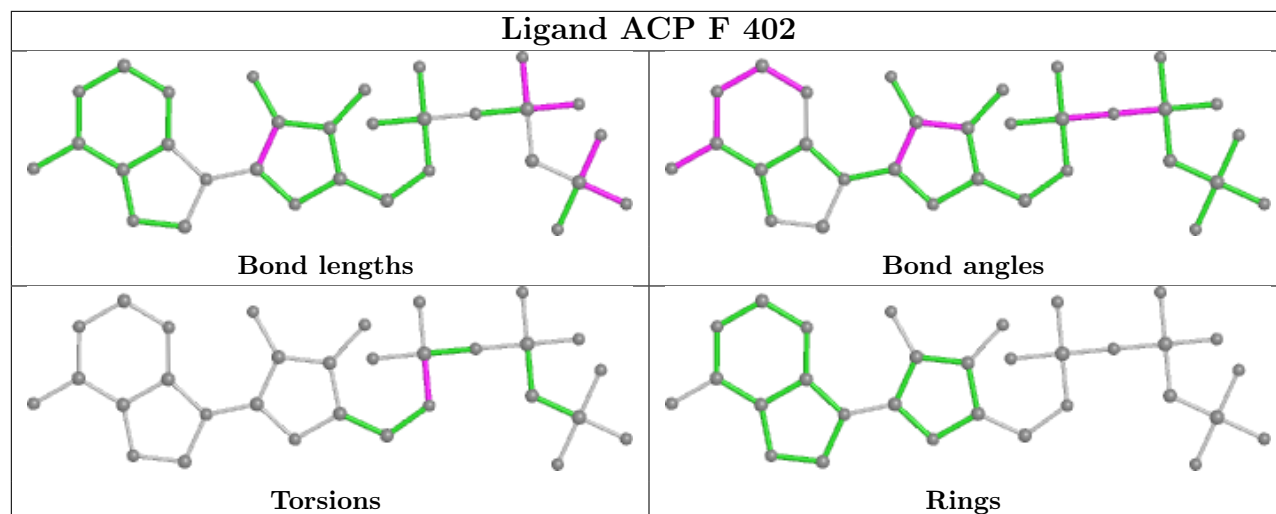
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 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	440/451 (97%)	-0.12	6 (1%) 75 78	34, 52, 85, 127	0
1	C	440/451 (97%)	-0.15	2 (0%) 91 92	27, 39, 67, 113	0
2	B	424/445 (95%)	0.00	6 (1%) 75 78	28, 49, 85, 132	2 (0%)
2	D	426/445 (95%)	-0.02	14 (3%) 46 53	36, 62, 98, 131	3 (0%)
3	E	125/143 (87%)	0.08	2 (1%) 72 75	40, 66, 109, 126	0
4	F	347/384 (90%)	0.89	67 (19%) 1 1	42, 80, 146, 172	0
All	All	2202/2319 (94%)	0.09	97 (4%) 34 40	27, 55, 109, 172	5 (0%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	438	ALA	8.5
4	F	153	ALA	7.8
4	F	173	ILE	6.8
2	B	439	THR	6.7
1	A	440	VAL	5.8
4	F	182	ILE	5.6
4	F	179	VAL	5.3
4	F	244	CYS	5.3
4	F	90	SER	5.0
4	F	132	LEU	4.7
4	F	154	GLY	4.6
4	F	134	ALA	4.6
1	A	282	TYR	4.5
4	F	233	PHE	4.5
4	F	250	SER	4.4
4	F	142	ARG	4.3
4	F	249	TYR	4.2
4	F	177	GLY	4.1
4	F	169	LEU	4.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	F	234	GLN	4.1
1	A	439	SER	4.0
2	D	276	THR	3.9
4	F	144	GLY	3.8
4	F	186	LEU	3.8
4	F	89	GLU	3.8
4	F	161	LEU	3.7
4	F	131	PHE	3.7
2	B	276	THR	3.7
4	F	231	ALA	3.7
4	F	17	VAL	3.6
4	F	181	VAL	3.5
2	B	437	ASP	3.5
4	F	32	LYS	3.4
4	F	143	GLU	3.4
4	F	155	ALA	3.4
4	F	259	GLY	3.3
4	F	176	GLN	3.3
1	A	262	TYR	3.2
2	B	284	ARG	3.2
4	F	320	MET	3.2
2	D	57	THR	3.2
2	D	281	GLN	3.1
2	D	400	ARG	3.1
3	E	144	SER	3.0
4	F	232	ASN	3.0
4	F	138	ARG	3.0
4	F	248	GLU	3.0
3	E	143	ALA	3.0
4	F	20	LEU	2.9
4	F	152	SER	2.9
4	F	165	GLU	2.9
2	B	337	ASN	2.9
2	D	220	THR	2.9
4	F	130	VAL	2.8
4	F	227	PRO	2.8
2	D	215	ARG	2.7
4	F	44	ARG	2.7
4	F	99	VAL	2.7
2	D	219	LEU	2.7
2	D	82	PRO	2.7
4	F	101	TYR	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	340	SER	2.6
2	D	217	LEU	2.6
1	C	178	SER	2.6
2	D	279	GLY	2.6
4	F	253	TYR	2.6
4	F	27	TRP	2.6
4	F	135	TYR	2.5
2	D	293	GLN	2.5
4	F	156	LYS	2.5
4	F	251	LYS	2.5
4	F	170	LEU	2.4
4	F	158	GLU	2.4
4	F	147	TRP	2.4
4	F	240	LEU	2.3
4	F	252	ASN	2.3
1	A	437	VAL	2.3
4	F	230	SER	2.3
2	D	277	SER	2.3
4	F	372	THR	2.3
4	F	184	LYS	2.2
4	F	228	TYR	2.2
2	D	58	GLY	2.2
4	F	25	GLY	2.2
4	F	45	ASN	2.2
1	A	438	ASP	2.2
4	F	162	ILE	2.2
4	F	21	LEU	2.2
4	F	30	LEU	2.1
4	F	172	PHE	2.1
4	F	263	PHE	2.1
4	F	160	ILE	2.1
2	D	2	ARG	2.1
4	F	31	ARG	2.0
4	F	199	PHE	2.0
4	F	337	ALA	2.0
4	F	100	ILE	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 [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

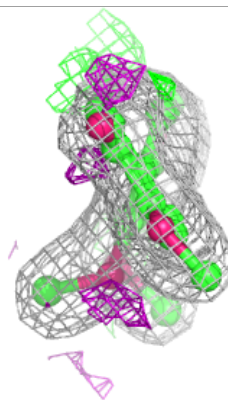
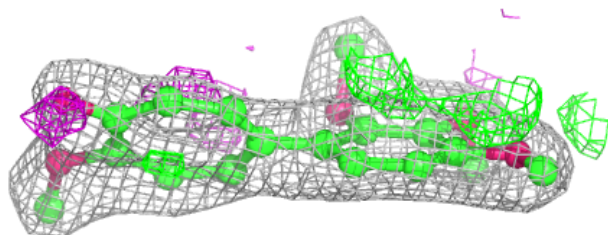
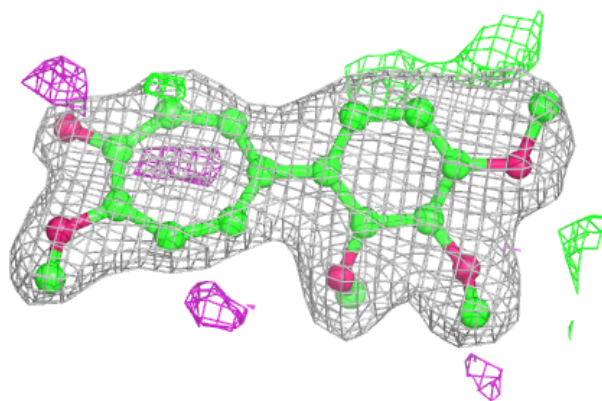
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	F	401	1/1	0.80	0.04	72,72,72,72	0
8	GOL	A	505	6/6	0.90	0.17	72,73,75,76	0
9	8WB	D	500	22/22	0.91	0.18	33,44,48,50	22
6	MG	D	502	1/1	0.92	0.04	58,58,58,58	0
7	CA	B	504	1/1	0.93	0.04	86,86,86,86	0
11	MES	B	505	12/12	0.94	0.11	55,61,71,82	0
7	CA	A	503	1/1	0.95	0.08	69,69,69,69	0
7	CA	A	504	1/1	0.95	0.12	96,96,96,96	0
12	ACP	F	402	31/31	0.95	0.12	83,90,105,118	0
9	8WB	B	501	22/22	0.96	0.10	33,41,48,49	0
10	GDP	D	501	28/28	0.96	0.09	46,53,61,63	0
6	MG	A	502	1/1	0.97	0.15	34,34,34,34	0
6	MG	C	502	1/1	0.98	0.14	32,32,32,32	0
6	MG	B	503	1/1	0.99	0.18	27,27,27,27	0
10	GDP	B	502	28/28	0.99	0.12	29,34,38,40	0
7	CA	C	503	1/1	0.99	0.10	54,54,54,54	0
5	GTP	C	501	32/32	0.99	0.11	27,30,34,34	0
5	GTP	A	501	32/32	0.99	0.12	26,35,38,42	0

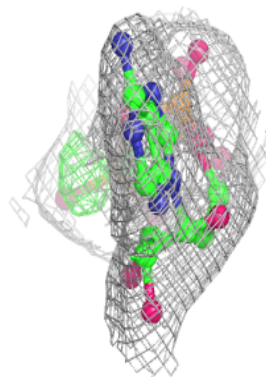
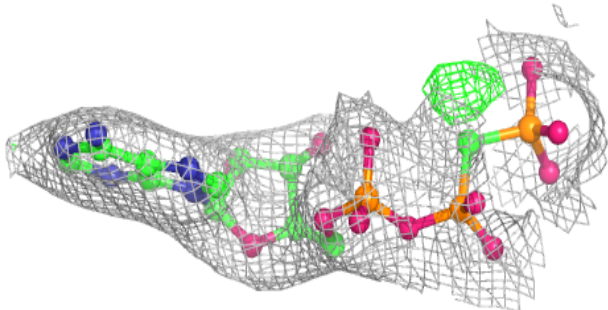
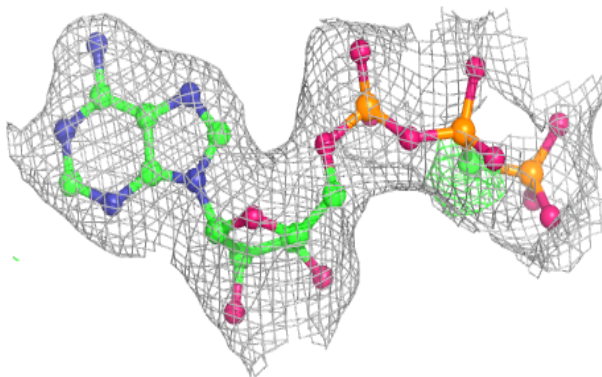
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 8WB D 500:**

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

**Electron density around ACP F 402:**

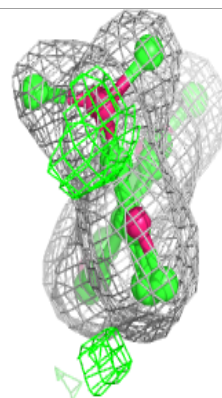
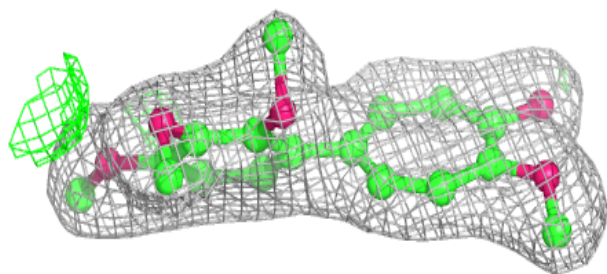
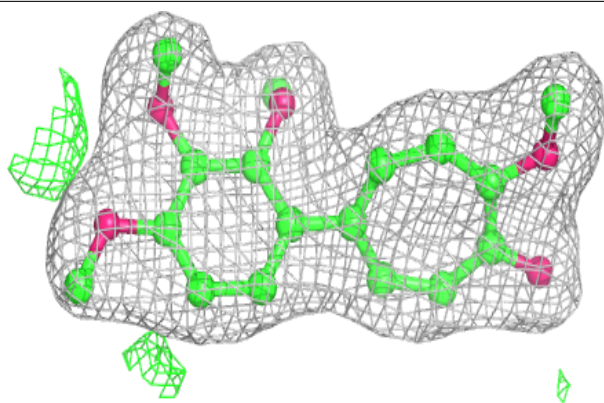
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



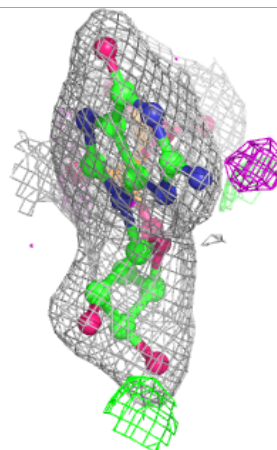
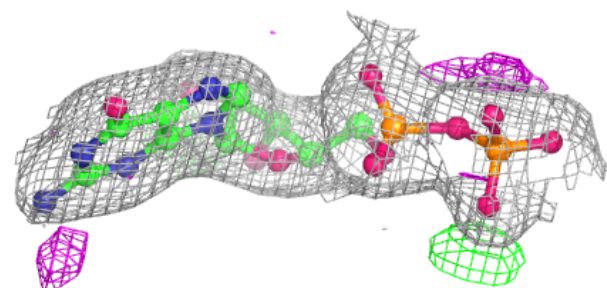
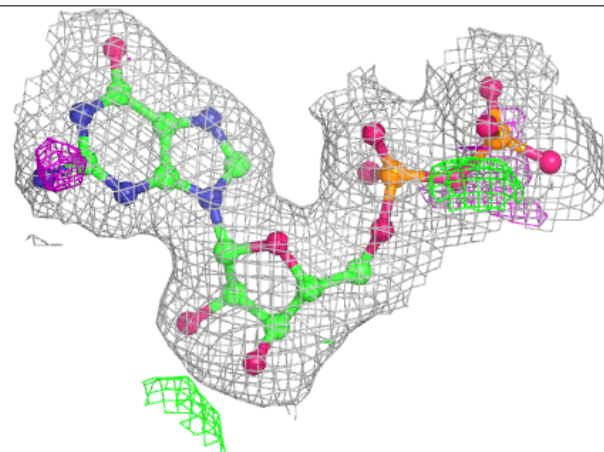


**Electron density around 8WB B 501:**

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

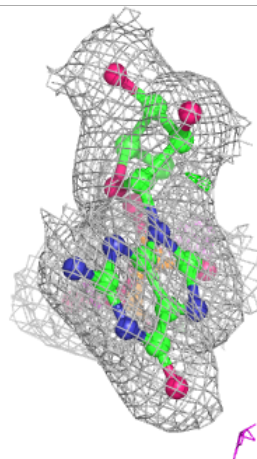
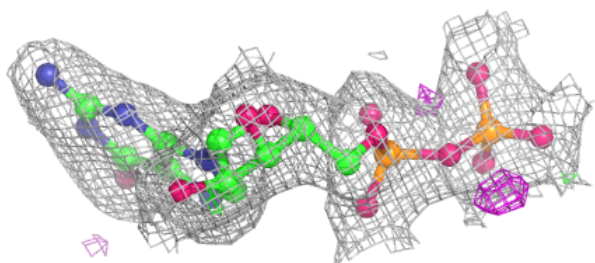
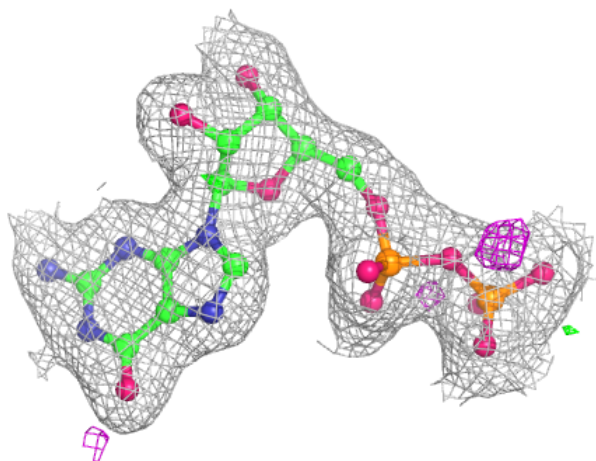
**Electron density around GDP D 501:**

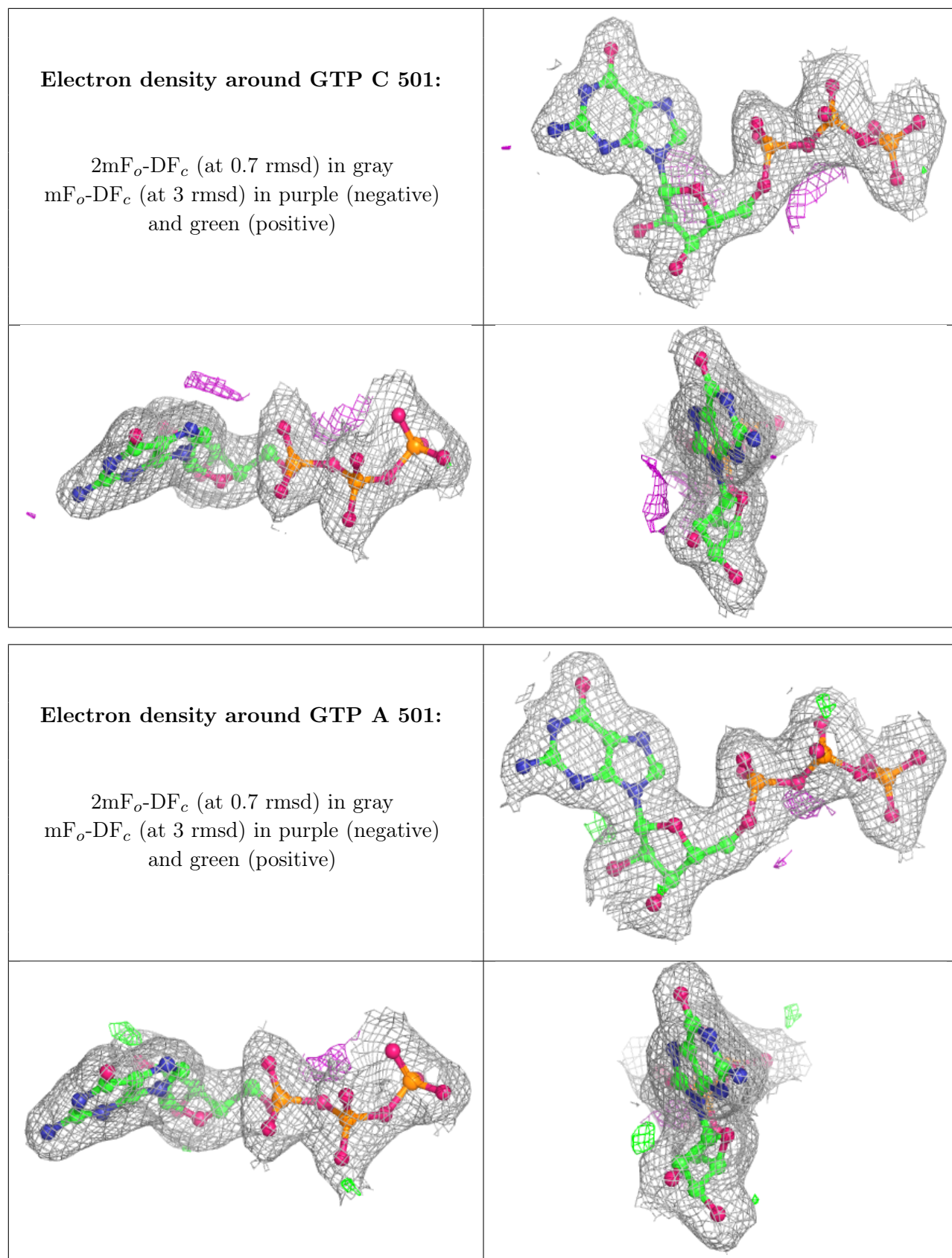
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 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.