



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 10:27 am BST

PDB ID : 4ZOL  
Title : Crystal Structure of Tubulin-Stathmin-TTL-Tubulysin M Complex  
Authors : Wang, Y.; Zhang, R.  
Deposited on : 2015-05-06  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 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 : 2.11  
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) : 2.11

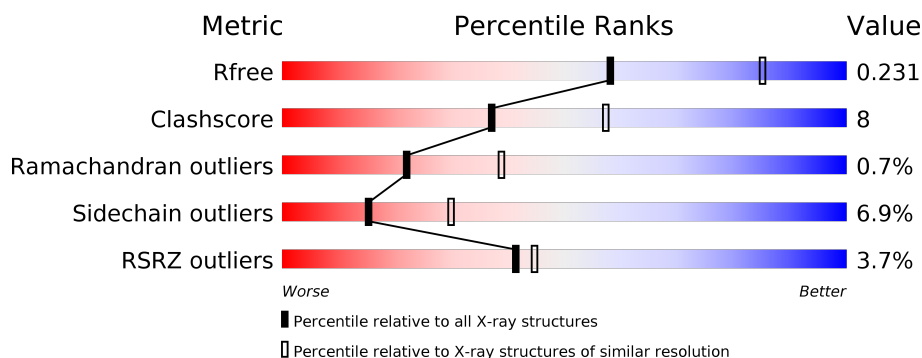
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>••</div> </div> </div>
1	C	451	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>••</div> </div> </div>
2	B	445	<div> <div></div> <div> <div></div> <div>81%</div> <div>14%</div> <div>••</div> </div> </div>
2	D	445	<div> <div>6%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>••</div> </div> </div>
3	E	143	<div> <div>6%</div> <div> <div></div> <div>66%</div> <div>16%</div> <div>•</div> <div>15%</div> </div> </div>
4	F	384	<div> <div>9%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>•</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	GOL	A	506	-	-	X	-

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18159 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	439	Total	C	N	O	S	0	0	0
			3430	2170	583	655	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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	0	0
			3376	2120	579	651	26			
2	D	427	Total	C	N	O	S	0	0	0
			3343	2099	571	647	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	3	0
			1033	637	190	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	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	348	Total	C	N	O	S	0	0	0
			2862	1832	494	522	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		

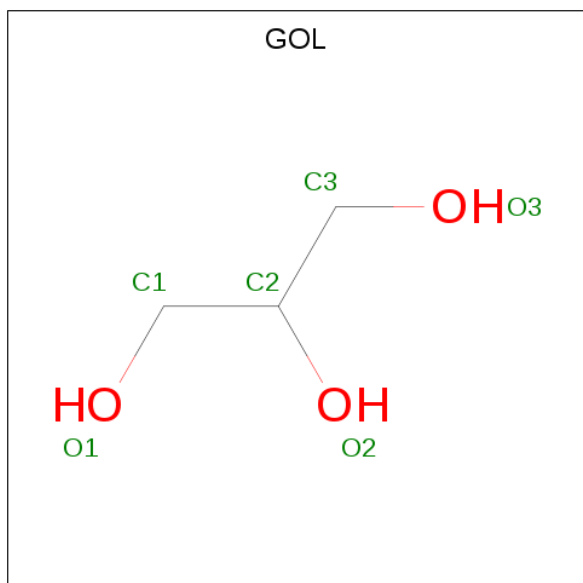
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

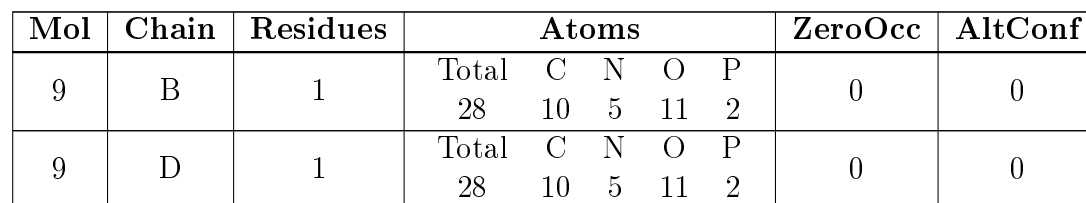
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- 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		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	C	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



- 
- Chemical structure of MES (3-(S-mesyloxy)propylamine) is shown. The structure consists of a pyridinium ring (labeled C2, C3, C5, C6, O1, N4) connected to a propyl chain (labeled C7, C8) which is further connected to a sulfonate group (labeled S, O2S, O1S, O3S).

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

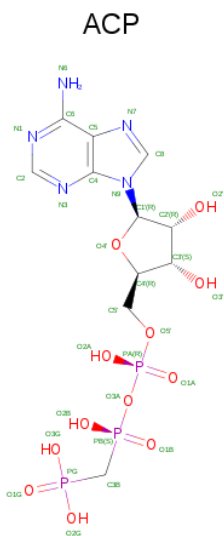
*Continued on next page...*

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

- # 55Q

- Molecule 12 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
12	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

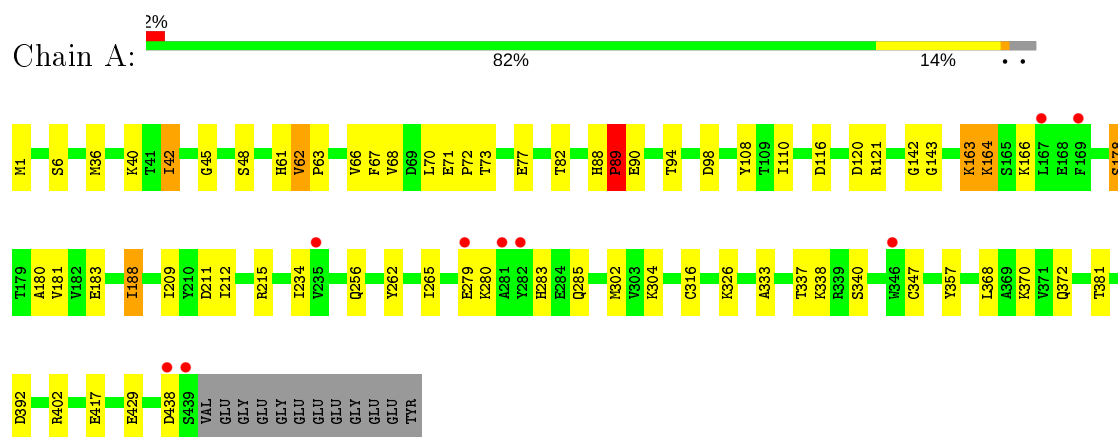
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	80	Total O 80 80	0	0
13	B	63	Total O 63 63	0	0
13	C	123	Total O 123 123	0	0
13	D	34	Total O 34 34	0	0
13	E	9	Total O 9 9	0	0
13	F	44	Total O 44 44	0	0

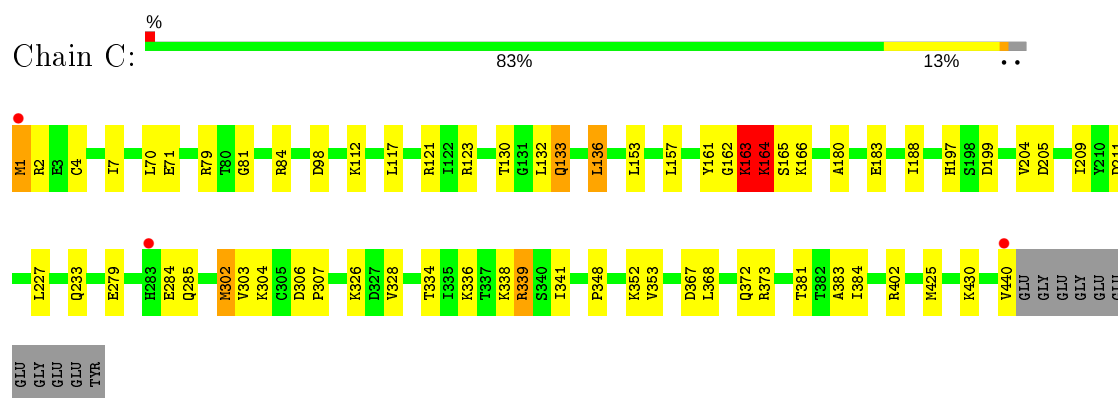
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

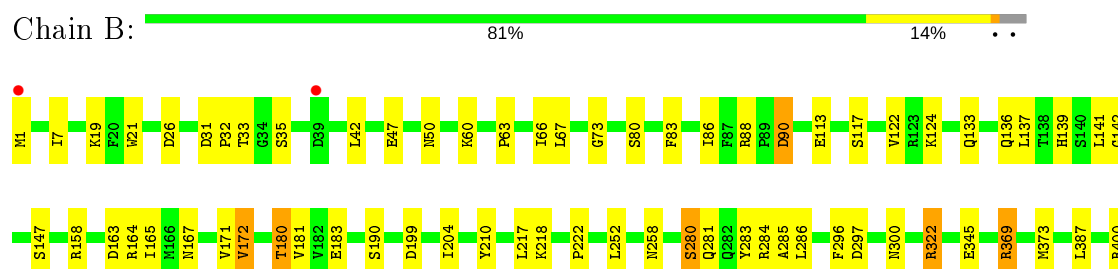
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.13Å 154.82Å 186.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.63 – 2.50 40.14 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.63-2.50) 99.9 (40.14-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.30 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.174 , 0.232 0.176 , 0.231	Depositor DCC
$R_{free}$ test set	5201 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.8	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18159	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: GDP, GOL, MG, CA, 55Q, GTP, 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	0.79	0/3508	0.89	2/4762 (0.0%)
1	C	0.86	0/3515	0.95	6/4772 (0.1%)
2	B	0.85	0/3451	0.90	2/4676 (0.0%)
2	D	0.76	1/3416 (0.0%)	0.87	5/4628 (0.1%)
3	E	0.78	0/1049	0.87	2/1393 (0.1%)
4	F	0.67	0/2929	0.84	2/3958 (0.1%)
All	All	0.79	1/17868 (0.0%)	0.89	19/24189 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	173	PRO	N-CD	5.06	1.54	1.47

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	LEU	CA-CB-CG	7.19	131.83	115.30
1	A	402	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	316	CYS	CB-CA-C	-6.11	98.18	110.40
2	D	359	PRO	C-N-CD	6.06	141.12	128.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	402	ARG	NE-CZ-NH2	5.93	123.26	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	280	SER	Peptide
3	E	115[B]	HIS	Mainchain

## 5.2 Too-close contacts ⓘ

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	3430	0	3340	45	0
1	C	3437	0	3348	54	0
2	B	3376	0	3258	40	0
2	D	3343	0	3223	75	0
3	E	1033	0	1048	12	0
4	F	2862	0	2808	49	0
5	A	32	0	12	1	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
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	18	0	24	13	0
8	B	12	0	16	1	0
8	C	6	0	8	0	0
8	F	6	0	8	0	0
9	B	28	0	12	1	0
9	D	28	0	12	1	0
10	B	24	0	26	4	0
11	B	51	0	0	0	0
11	D	51	0	0	0	0
12	F	31	0	14	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	80	0	0	4	0
13	B	63	0	0	4	0
13	C	123	0	0	6	0
13	D	34	0	0	1	0
13	E	9	0	0	0	0
13	F	44	0	0	3	0
All	All	18159	0	17169	271	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 8.

The worst 5 of 271 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:4:CYS:HB3	13:C:719:HOH:O	1.12	1.24
1:C:161:TYR:O	1:C:163:LYS:CD	1.86	1.23
2:D:57:ALA:O	2:D:60:LYS:HD2	1.33	1.22
1:C:1:MET:CE	1:C:130:THR:OG1	1.87	1.22
4:F:296:MET:HE1	13:F:540:HOH:O	1.47	1.15

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	437/451 (97%)	416 (95%)	20 (5%)	1 (0%)	47 68
1	C	438/451 (97%)	419 (96%)	15 (3%)	4 (1%)	17 31
2	B	428/445 (96%)	415 (97%)	12 (3%)	1 (0%)	47 68
2	D	423/445 (95%)	401 (95%)	18 (4%)	4 (1%)	17 31
3	E	121/143 (85%)	114 (94%)	6 (5%)	1 (1%)	19 35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	338/384 (88%)	313 (93%)	21 (6%)	4 (1%)	13	24
All	All	2185/2319 (94%)	2078 (95%)	92 (4%)	15 (1%)	22	39

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	162	GLY
1	C	339	ARG
2	D	399	PHE
2	D	402	LYS
4	F	32	LYS

### 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	370/379 (98%)	344 (93%)	26 (7%)	15	29
1	C	371/379 (98%)	357 (96%)	14 (4%)	33	58
2	B	369/381 (97%)	353 (96%)	16 (4%)	29	53
2	D	366/381 (96%)	336 (92%)	30 (8%)	11	22
3	E	113/127 (89%)	95 (84%)	18 (16%)	2	4
4	F	314/342 (92%)	286 (91%)	28 (9%)	9	19
All	All	1903/1989 (96%)	1771 (93%)	132 (7%)	15	30

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	50	ASN
2	D	181	VAL
4	F	234	GLN
2	D	60	LYS
2	D	128	SER



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	285	GLN
1	C	293	ASN
4	F	234	GLN
1	C	11	GLN
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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	GOL	A	506	-	5,5,5	0.47	0	5,5,5	0.55	0
5	GTP	A	501	6	26,34,34	1.45	4 (15%)	33,54,54	1.93	9 (27%)
9	GDP	B	501	6	24,30,30	1.37	3 (12%)	31,47,47	1.85	7 (22%)
5	GTP	C	501	6	26,34,34	1.20	2 (7%)	33,54,54	2.55	11 (33%)
10	MES	B	503	-	12,12,12	2.04	1 (8%)	14,16,16	2.31	7 (50%)
11	55Q	B	507	-	48,53,53	1.96	12 (25%)	54,73,73	2.46	15 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	55Q	D	503	-	48,53,53	1.97	10 (20%)	54,73,73	2.42	16 (29%)
8	GOL	A	504	-	5,5,5	0.37	0	5,5,5	0.48	0
8	GOL	C	504	-	5,5,5	0.41	0	5,5,5	1.18	0
8	GOL	B	506	-	5,5,5	0.38	0	5,5,5	0.40	0
8	GOL	B	505	-	5,5,5	0.33	0	5,5,5	0.48	0
10	MES	B	504	-	12,12,12	2.06	1 (8%)	14,16,16	6.49	10 (71%)
8	GOL	A	505	-	5,5,5	0.17	0	5,5,5	0.89	0
12	ACP	F	401	-	27,33,33	1.97	8 (29%)	32,52,52	1.26	5 (15%)
8	GOL	F	402	-	5,5,5	0.59	0	5,5,5	1.05	0
9	GDP	D	501	6	24,30,30	1.00	2 (8%)	31,47,47	2.24	11 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	A	506	-	-	2/4/4/4	-
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3
9	GDP	B	501	6	-	5/12/32/32	0/3/3/3
5	GTP	C	501	6	-	4/18/38/38	0/3/3/3
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
11	55Q	B	507	-	-	15/50/73/73	0/3/3/3
11	55Q	D	503	-	-	21/50/73/73	0/3/3/3
8	GOL	A	504	-	-	3/4/4/4	-
8	GOL	C	504	-	-	4/4/4/4	-
8	GOL	B	506	-	-	4/4/4/4	-
8	GOL	B	505	-	-	2/4/4/4	-
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
8	GOL	A	505	-	-	4/4/4/4	-
12	ACP	F	401	-	-	6/15/38/38	0/3/3/3
8	GOL	F	402	-	-	0/4/4/4	-
9	GDP	D	501	6	-	5/12/32/32	0/3/3/3

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	55Q	CBF-CBH	-7.33	1.32	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	507	55Q	CBF-CBH	-6.56	1.34	1.50
10	B	504	MES	C8-S	-6.46	1.68	1.77
10	B	503	MES	C8-S	-6.44	1.68	1.77
12	F	401	ACP	PG-O1G	5.64	1.62	1.50

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	MES	O1S-S-C8	-13.76	90.34	106.92
10	B	504	MES	O3S-S-O1S	-11.62	82.88	111.27
11	D	503	55Q	CAS-OAZ-CBB	11.26	127.19	117.37
10	B	504	MES	O2S-S-O1S	-9.81	79.99	113.95
11	B	507	55Q	CAS-OAZ-CBB	9.50	125.65	117.37

There are no chirality outliers.

5 of 86 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	506	GOL	C1-C2-C3-O3
5	A	501	GTP	C5'-O5'-PA-O1A
10	B	503	MES	C8-C7-N4-C3
9	B	501	GDP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A

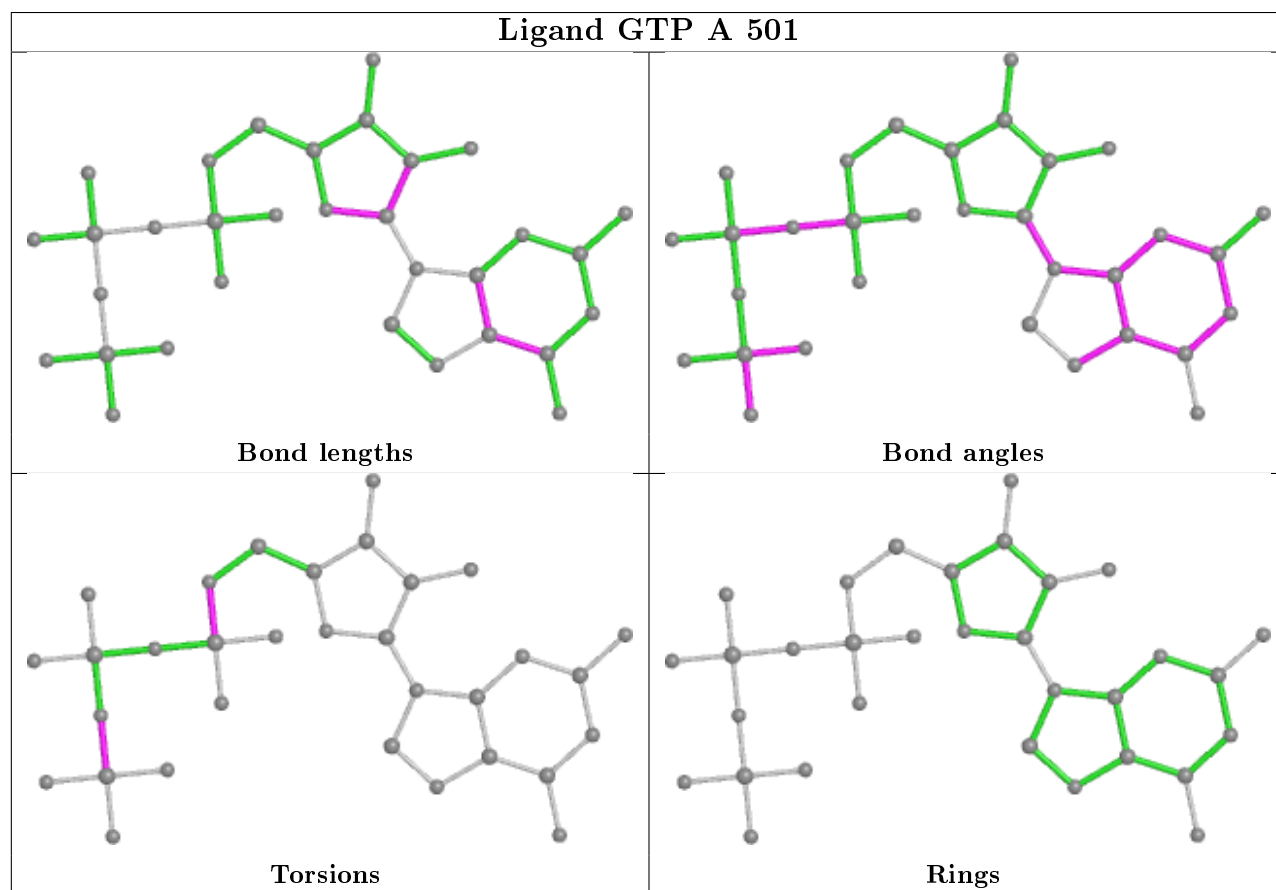
There are no ring outliers.

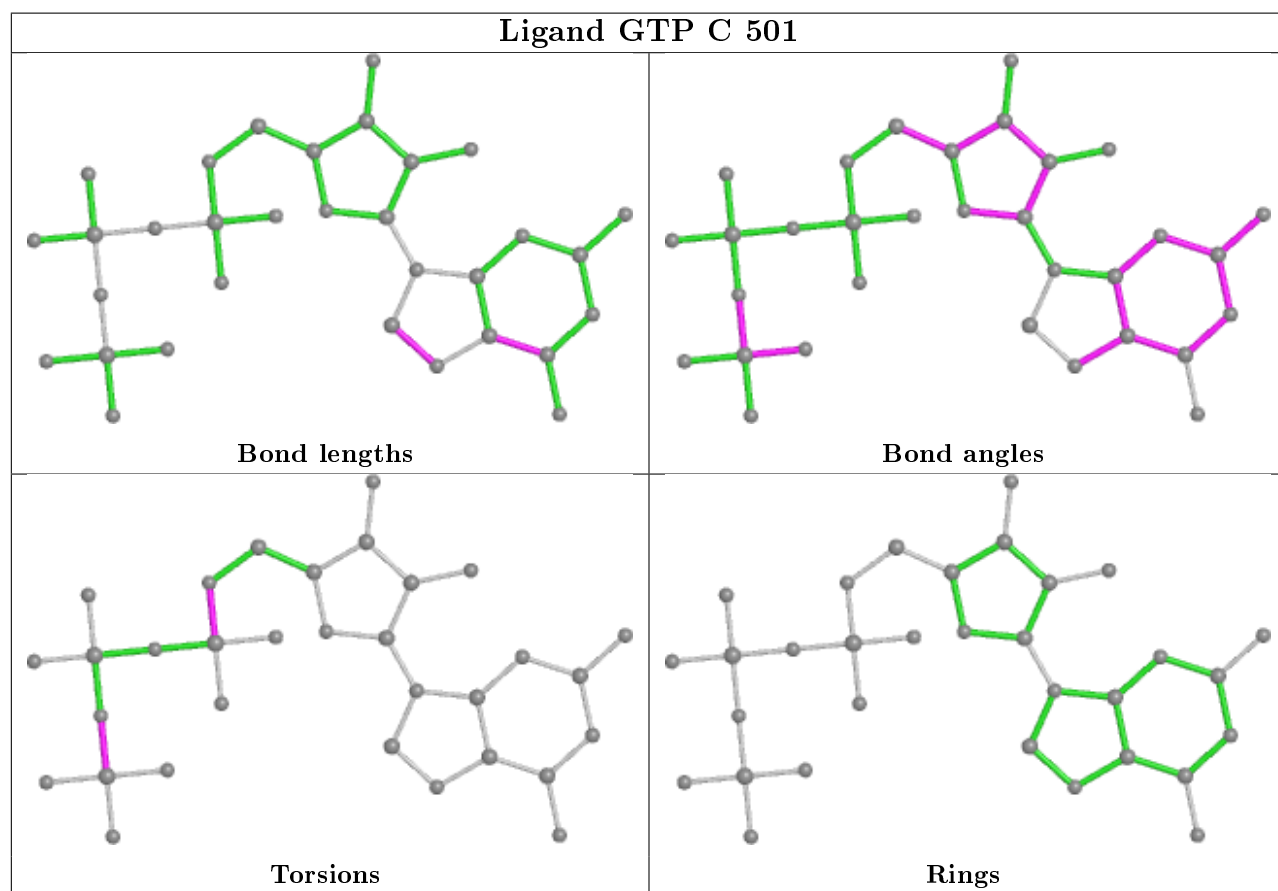
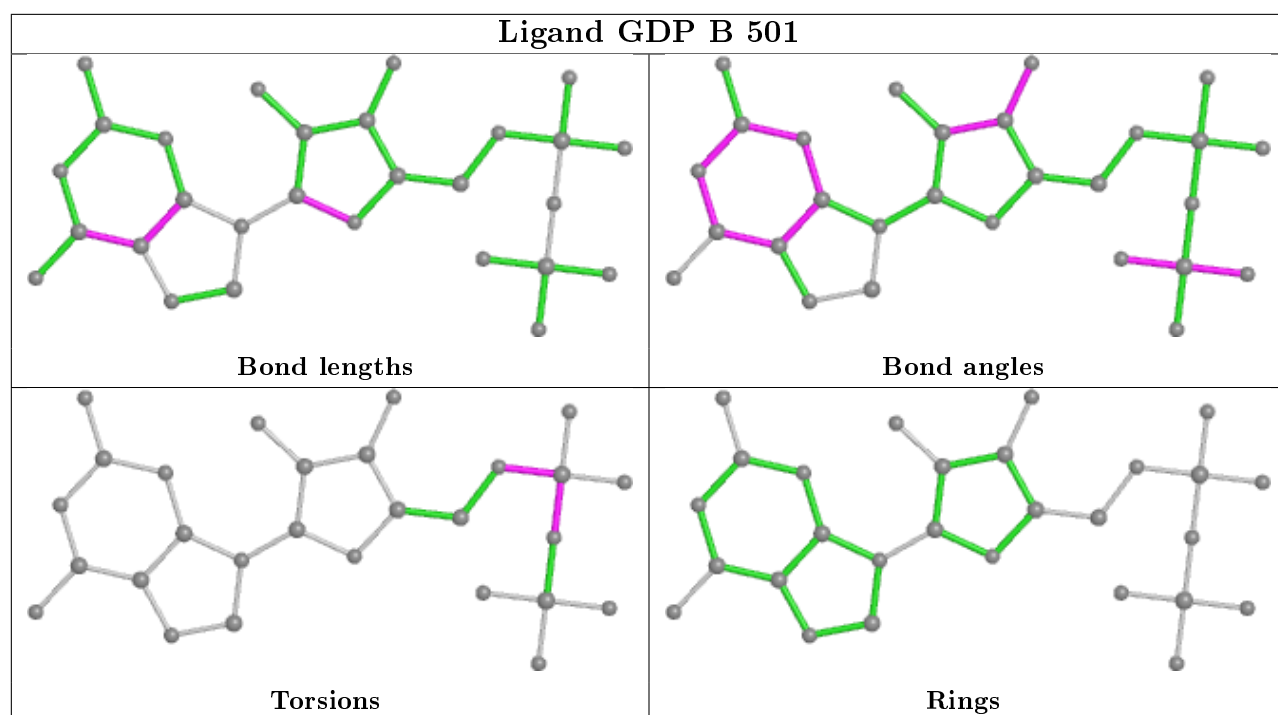
9 monomers are involved in 25 short contacts:

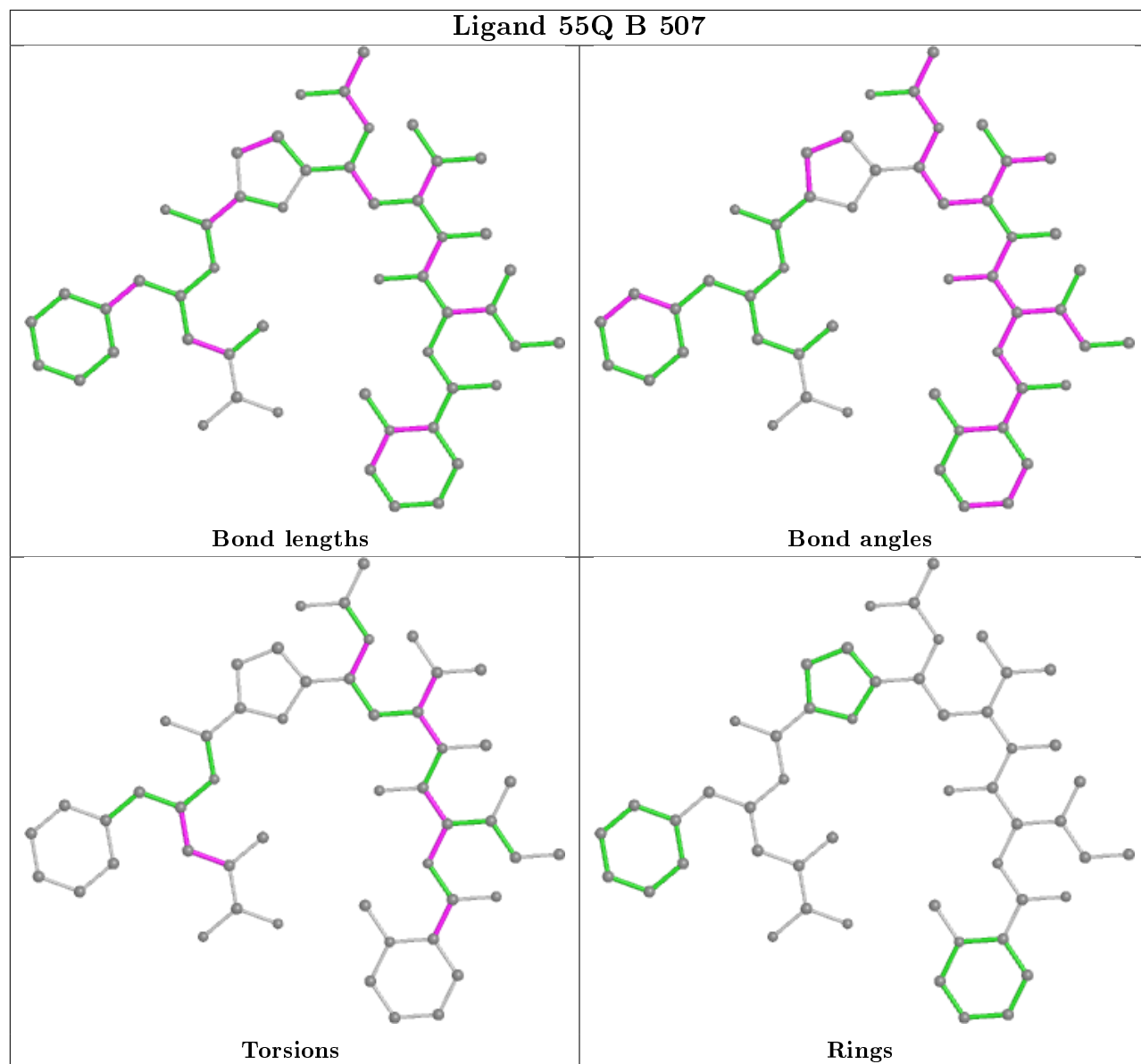
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	506	GOL	12	0
5	A	501	GTP	1	0
9	B	501	GDP	1	0
10	B	503	MES	1	0
8	A	504	GOL	1	0
8	B	506	GOL	1	0
10	B	504	MES	3	0
12	F	401	ACP	4	0
9	D	501	GDP	1	0

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

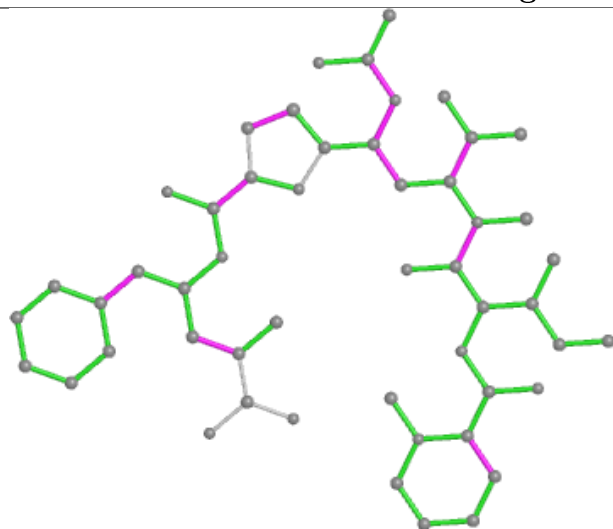
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.



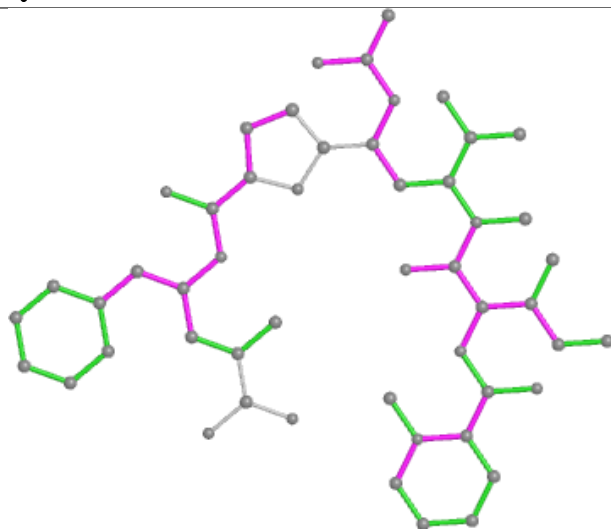




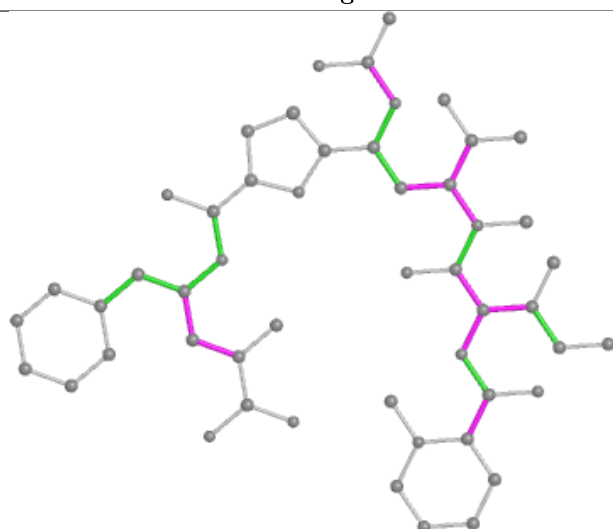
## Ligand 55Q D 503



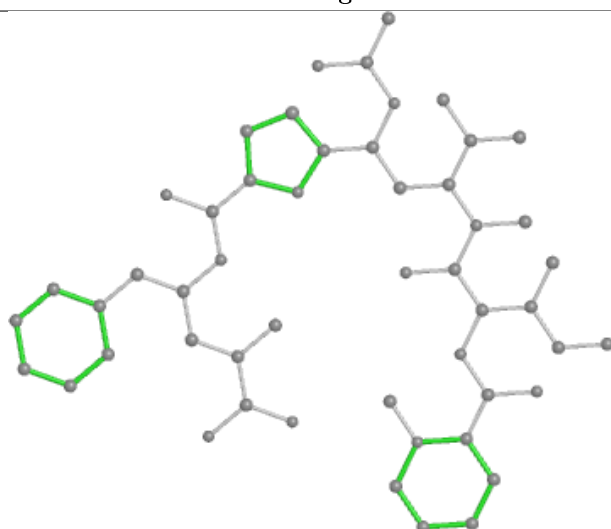
Bond lengths



Bond angles

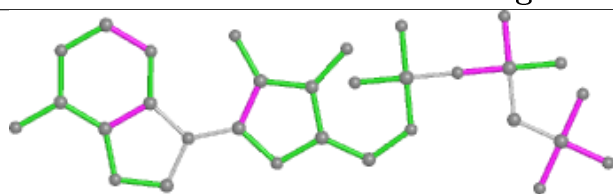


Torsions

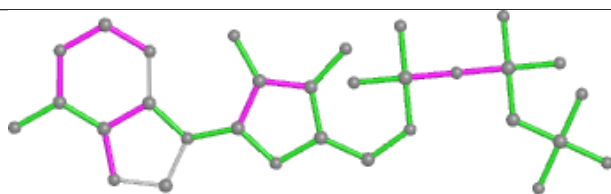


Rings

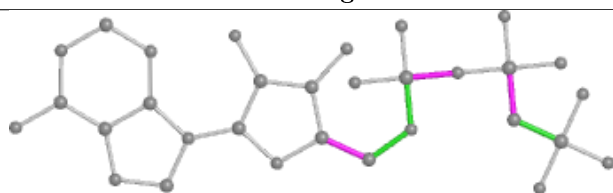
## Ligand ACP F 401



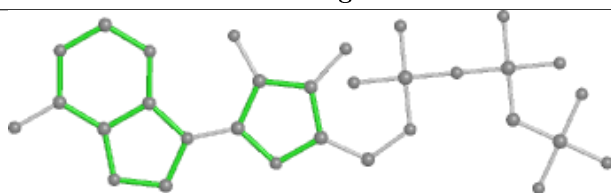
Bond lengths



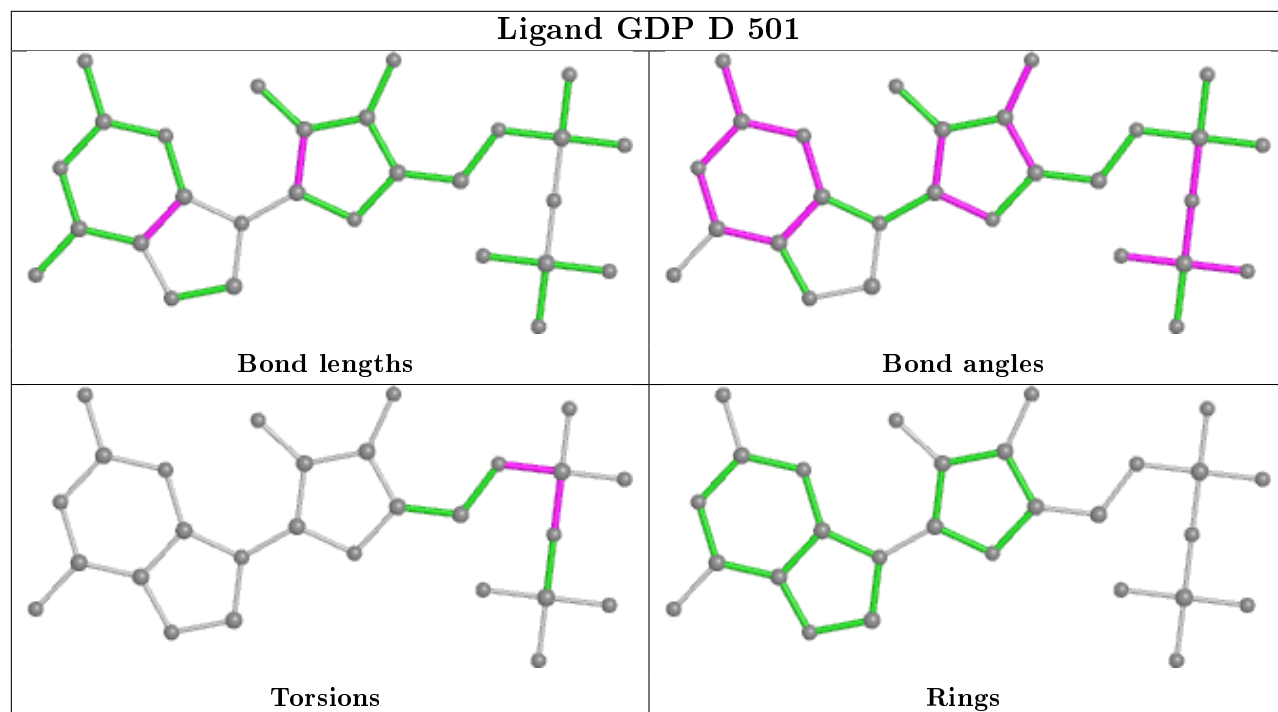
Bond angles



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	439/451 (97%)	-0.18	9 (2%) 63 66	23, 39, 66, 116	0
1	C	440/451 (97%)	-0.46	3 (0%) 87 89	21, 33, 62, 91	0
2	B	430/445 (96%)	-0.29	2 (0%) 91 91	20, 36, 71, 107	0
2	D	427/445 (95%)	0.06	26 (6%) 21 22	28, 50, 86, 124	0
3	E	122/143 (85%)	0.24	8 (6%) 18 19	30, 55, 87, 114	0
4	F	348/384 (90%)	0.13	34 (9%) 7 7	25, 56, 108, 138	0
All	All	2206/2319 (95%)	-0.14	82 (3%) 41 45	20, 42, 85, 138	0

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	177	GLY	5.7
1	A	282	TYR	4.9
4	F	372	THR	4.6
1	C	440	VAL	4.3
4	F	166	ALA	4.2

### 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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

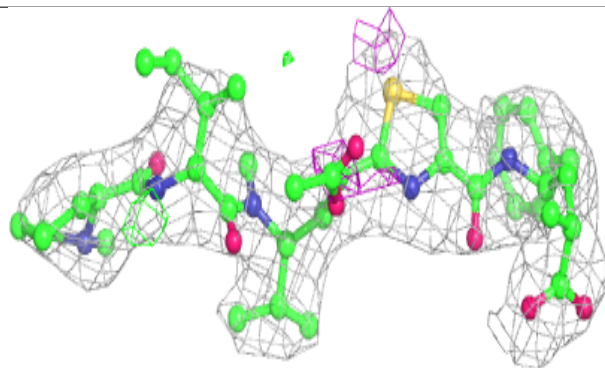
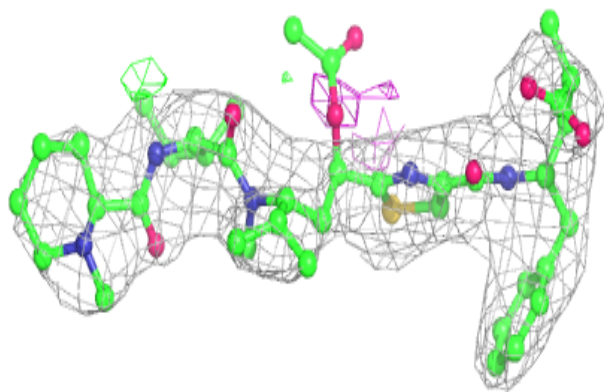
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
8	GOL	F	402	6/6	0.82	0.22	77,80,83,84	0
8	GOL	B	506	6/6	0.86	0.18	60,76,80,93	0
8	GOL	A	504	6/6	0.88	0.18	61,72,78,87	0
8	GOL	A	506	6/6	0.88	0.46	39,67,99,101	0
11	55Q	D	503	51/51	0.89	0.25	54,70,113,127	0
8	GOL	C	504	6/6	0.92	0.15	54,58,62,76	0
8	GOL	B	505	6/6	0.92	0.08	66,72,74,75	0
6	MG	D	502	1/1	0.93	0.16	36,36,36,36	0
12	ACP	F	401	31/31	0.94	0.14	58,72,124,137	0
10	MES	B	504	12/12	0.95	0.14	57,64,73,74	0
8	GOL	A	505	6/6	0.96	0.11	50,51,55,58	0
6	MG	B	502	1/1	0.96	0.12	44,44,44,44	0
10	MES	B	503	12/12	0.96	0.15	50,54,59,60	0
11	55Q	B	507	51/51	0.96	0.15	21,36,74,103	0
6	MG	C	502	1/1	0.97	0.04	30,30,30,30	0
9	GDP	D	501	28/28	0.98	0.13	33,39,47,52	0
7	CA	A	503	1/1	0.99	0.04	50,50,50,50	0
6	MG	A	502	1/1	0.99	0.08	37,37,37,37	0
7	CA	C	503	1/1	0.99	0.02	38,38,38,38	0
9	GDP	B	501	28/28	0.99	0.14	20,27,31,32	0
5	GTP	C	501	32/32	0.99	0.11	19,22,26,28	0
5	GTP	A	501	32/32	0.99	0.15	24,27,30,31	0

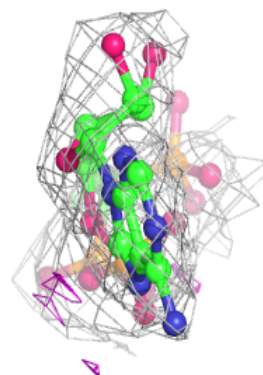
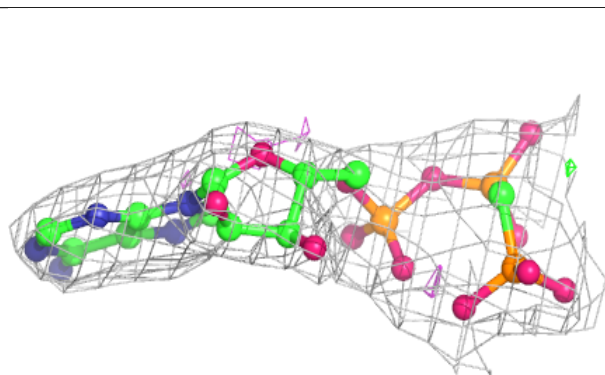
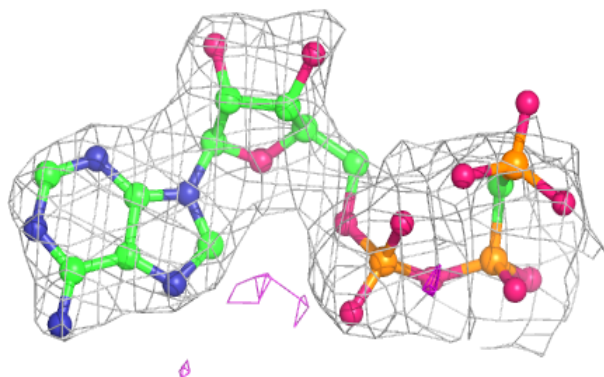
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 55Q D 503:**

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

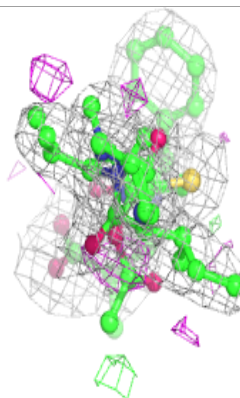
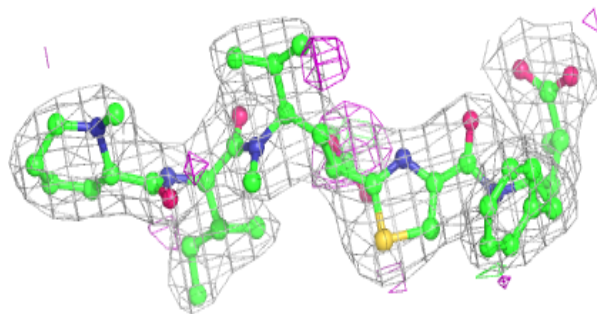
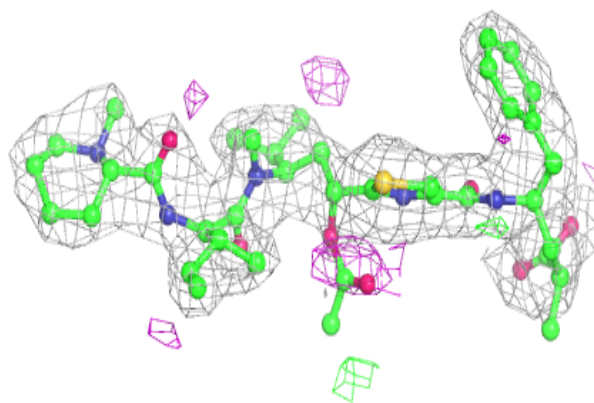
**Electron density around ACP F 401:**

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

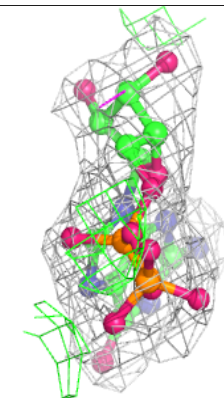
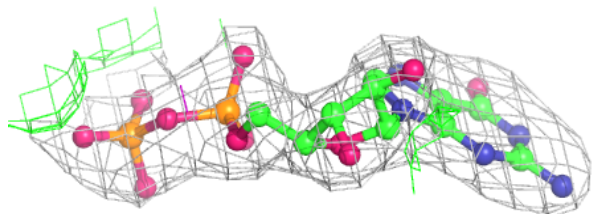
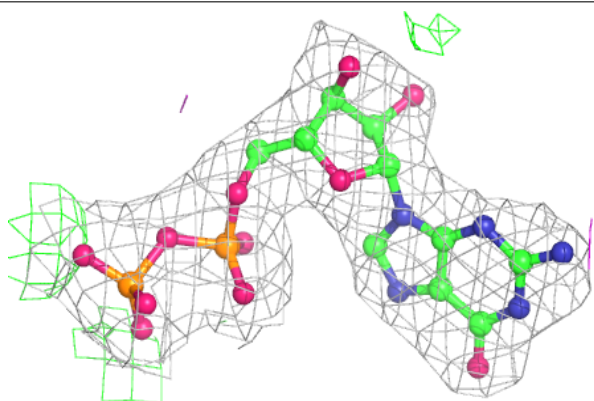


**Electron density around 55Q B 507:**

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

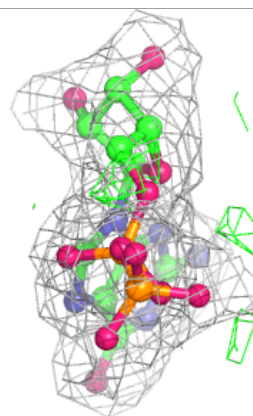
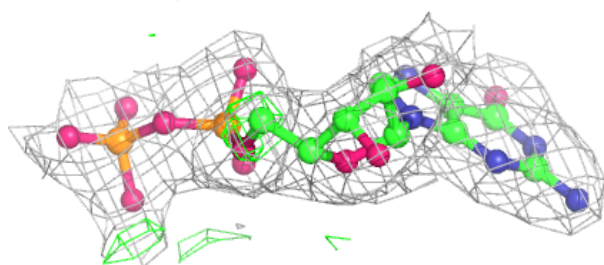
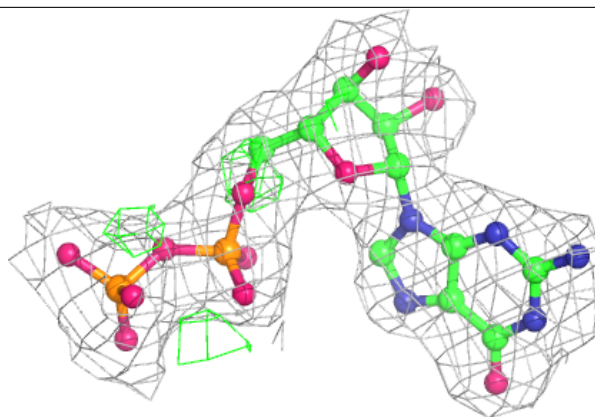
**Electron density around GDP D 501:**

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

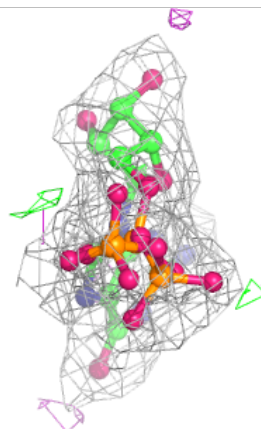
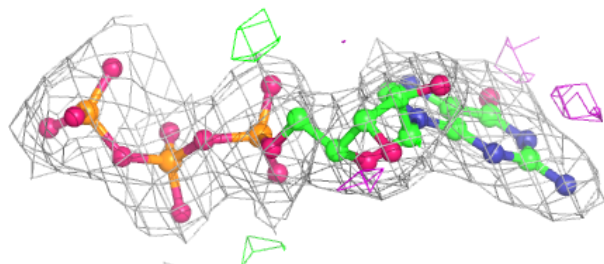
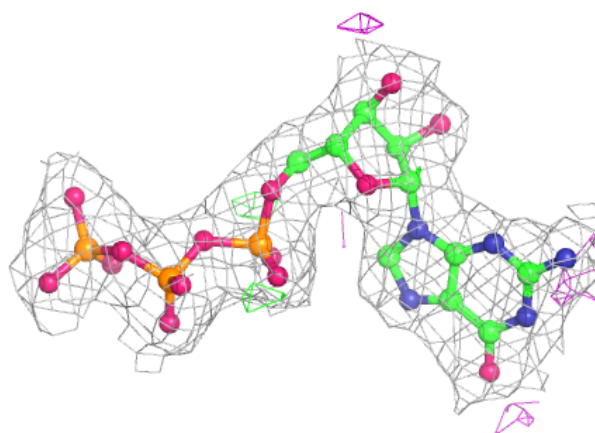


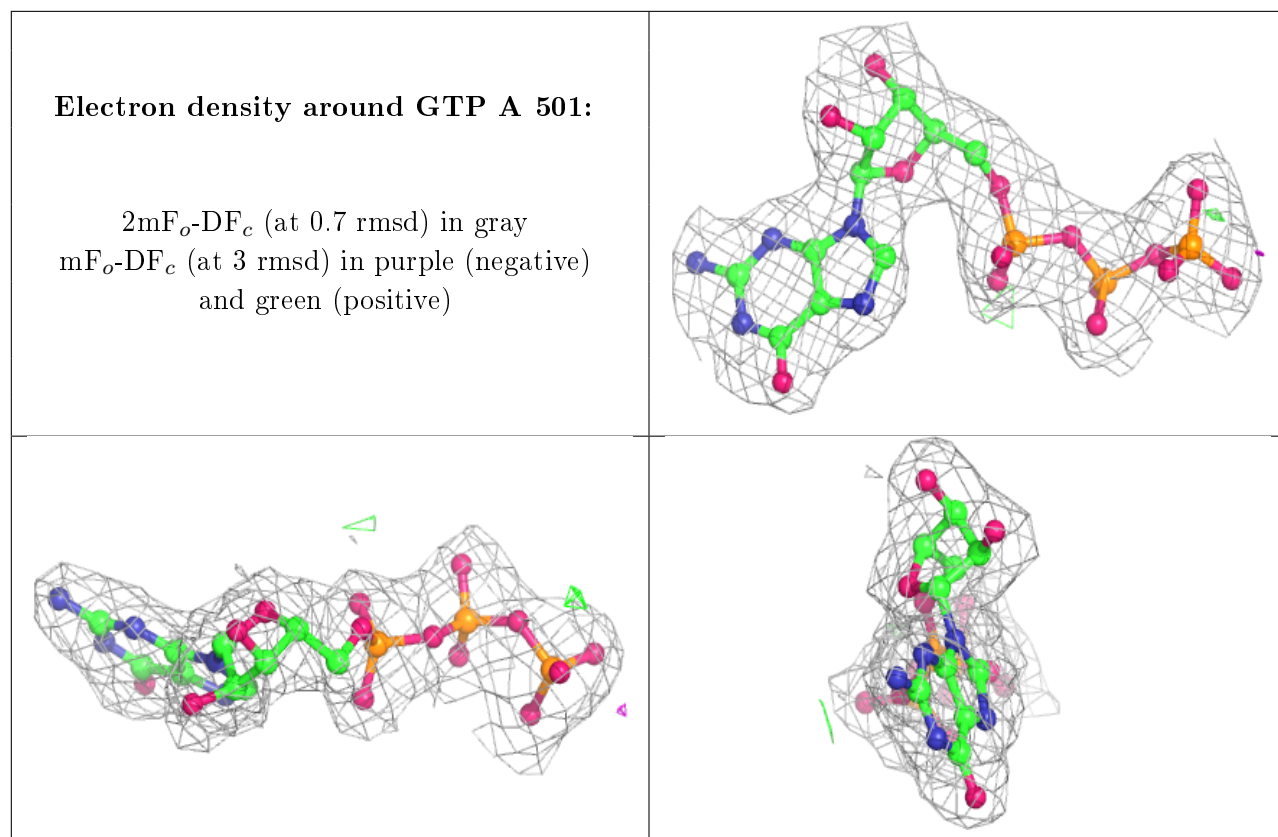
**Electron density around GDP B 501:**

$2mF_o-DF_c$  (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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.