



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 06:00 am BST

PDB ID : 6GX7  
Title : Tubulin-CopN-alphaRep complex  
Authors : Gigant, B.; Campanacci, V.  
Deposited on : 2018-06-26  
Resolution : 3.19 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.

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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	:	2.11
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

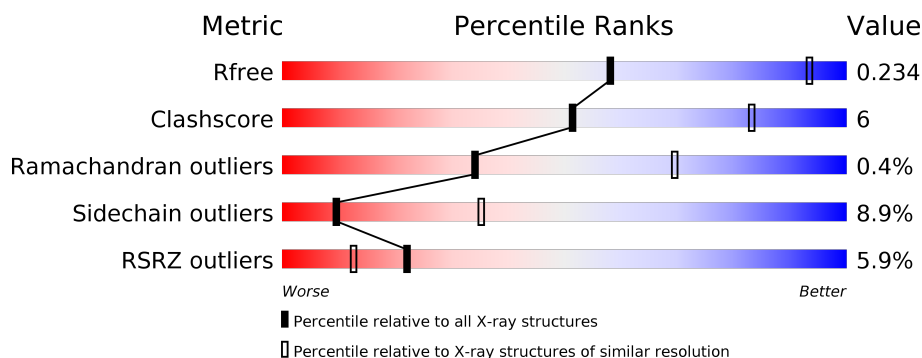
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.19 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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></div> <div>74% 19% • 5%</div> </div>
1	C	451	<div> <div></div> <div>79% 14% • 5%</div> </div>
2	B	445	<div> <div></div> <div>72% 22% • 5%</div> </div>
2	D	445	<div> <div></div> <div>72% 22% • 5%</div> </div>
3	E	201	<div> <div>4%</div> <div>76% 14% • 8%</div> </div>
3	F	201	<div> <div>2%</div> <div>80% 10% • 8%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	336	
4	H	336	

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
7	SO4	C	503	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 20365 atoms, of which 24 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3291	2079	561	630	21			
1	C	428	Total	C	N	O	S	0	0	0
			3288	2077	561	630	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	SER	GLY	conflict	UNP D0VWZ0
A	340	SER	THR	conflict	UNP D0VWZ0
C	232	SER	GLY	conflict	UNP D0VWZ0
C	340	SER	THR	conflict	UNP D0VWZ0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3296	2075	559	636	26			
2	D	423	Total	C	N	O	S	0	0	0
			3298	2076	559	637	26			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	CYS	SER	conflict	UNP D0VWY9
B	318	ILE	VAL	conflict	UNP D0VWY9
D	203	CYS	SER	conflict	UNP D0VWY9
D	318	ILE	VAL	conflict	UNP D0VWY9

- Molecule 3 is a protein called iiiA5 ALPHAREP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	184	Total	C	N	O	S	0	0	0
			1334	835	239	258	2			
3	F	184	Total	C	N	O	S	0	0	0
			1338	837	239	260	2			

- Molecule 4 is a protein called Low calcium response E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	285	Total	C	N	O	S	0	0	0
			2132	1326	358	441	7			
4	H	290	Total	C	N	O	S	0	0	0
			2146	1335	362	442	7			

There are 42 discrepancies between the modelled and reference sequences:

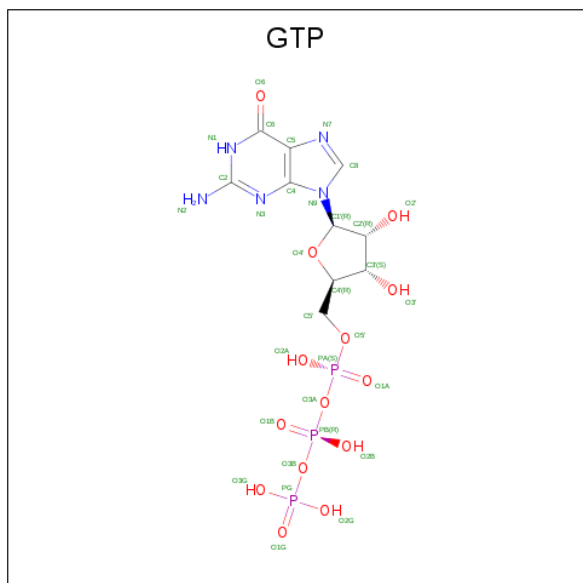
Chain	Residue	Modelled	Actual	Comment	Reference
G	64	MET	-	initiating methionine	UNP Q9Z8L4
G	65	GLY	-	expression tag	UNP Q9Z8L4
G	66	SER	-	expression tag	UNP Q9Z8L4
G	67	SER	-	expression tag	UNP Q9Z8L4
G	68	HIS	-	expression tag	UNP Q9Z8L4
G	69	HIS	-	expression tag	UNP Q9Z8L4
G	70	HIS	-	expression tag	UNP Q9Z8L4
G	71	HIS	-	expression tag	UNP Q9Z8L4
G	72	HIS	-	expression tag	UNP Q9Z8L4
G	73	HIS	-	expression tag	UNP Q9Z8L4
G	74	SER	-	expression tag	UNP Q9Z8L4
G	75	SER	-	expression tag	UNP Q9Z8L4
G	76	GLY	-	expression tag	UNP Q9Z8L4
G	77	LEU	-	expression tag	UNP Q9Z8L4
G	78	VAL	-	expression tag	UNP Q9Z8L4
G	79	PRO	-	expression tag	UNP Q9Z8L4
G	80	ARG	-	expression tag	UNP Q9Z8L4
G	81	GLY	-	expression tag	UNP Q9Z8L4
G	82	SER	-	expression tag	UNP Q9Z8L4
G	83	HIS	-	expression tag	UNP Q9Z8L4
G	84	MET	-	expression tag	UNP Q9Z8L4
H	64	MET	-	initiating methionine	UNP Q9Z8L4
H	65	GLY	-	expression tag	UNP Q9Z8L4
H	66	SER	-	expression tag	UNP Q9Z8L4
H	67	SER	-	expression tag	UNP Q9Z8L4
H	68	HIS	-	expression tag	UNP Q9Z8L4
H	69	HIS	-	expression tag	UNP Q9Z8L4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	70	HIS	-	expression tag	UNP Q9Z8L4
H	71	HIS	-	expression tag	UNP Q9Z8L4
H	72	HIS	-	expression tag	UNP Q9Z8L4
H	73	HIS	-	expression tag	UNP Q9Z8L4
H	74	SER	-	expression tag	UNP Q9Z8L4
H	75	SER	-	expression tag	UNP Q9Z8L4
H	76	GLY	-	expression tag	UNP Q9Z8L4
H	77	LEU	-	expression tag	UNP Q9Z8L4
H	78	VAL	-	expression tag	UNP Q9Z8L4
H	79	PRO	-	expression tag	UNP Q9Z8L4
H	80	ARG	-	expression tag	UNP Q9Z8L4
H	81	GLY	-	expression tag	UNP Q9Z8L4
H	82	SER	-	expression tag	UNP Q9Z8L4
H	83	HIS	-	expression tag	UNP Q9Z8L4
H	84	MET	-	expression tag	UNP Q9Z8L4

- 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	
			32	10	5	14	3	0
5	B	1	Total	C	N	O	P	
			32	10	5	14	3	0
5	C	1	Total	C	N	O	P	
			32	10	5	14	3	0

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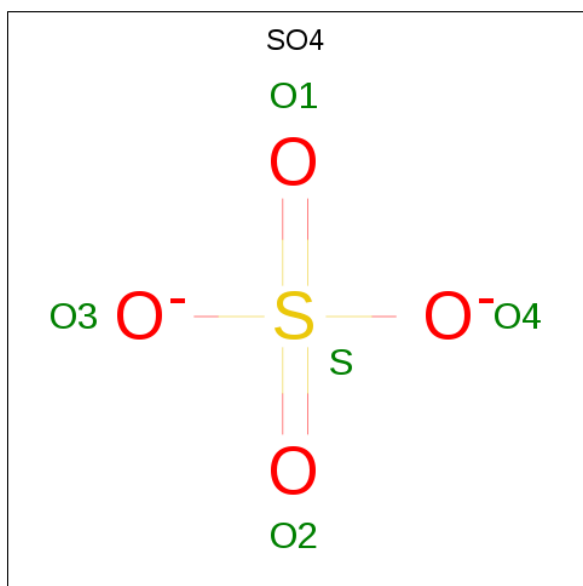
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- 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 SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



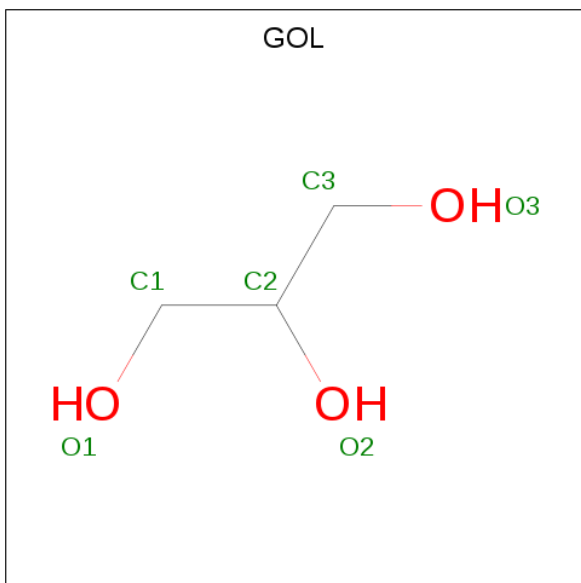
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 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
8	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
8	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
8	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
8	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

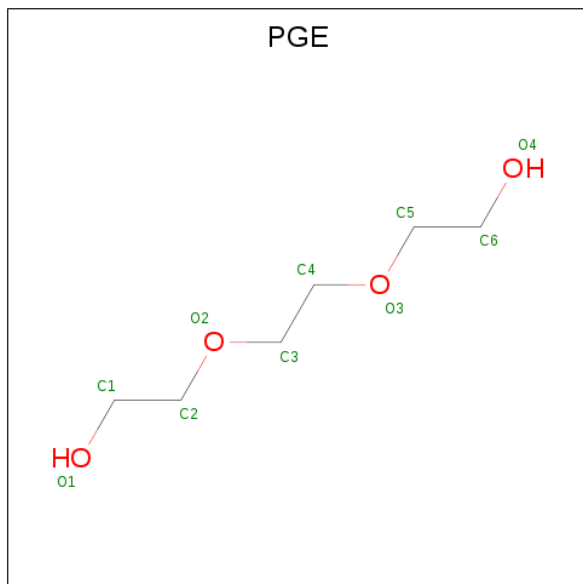
- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			14	3	8	3		
9	D	1	Total	C	H	O	0	0
			14	3	8	3		
9	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 10 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).

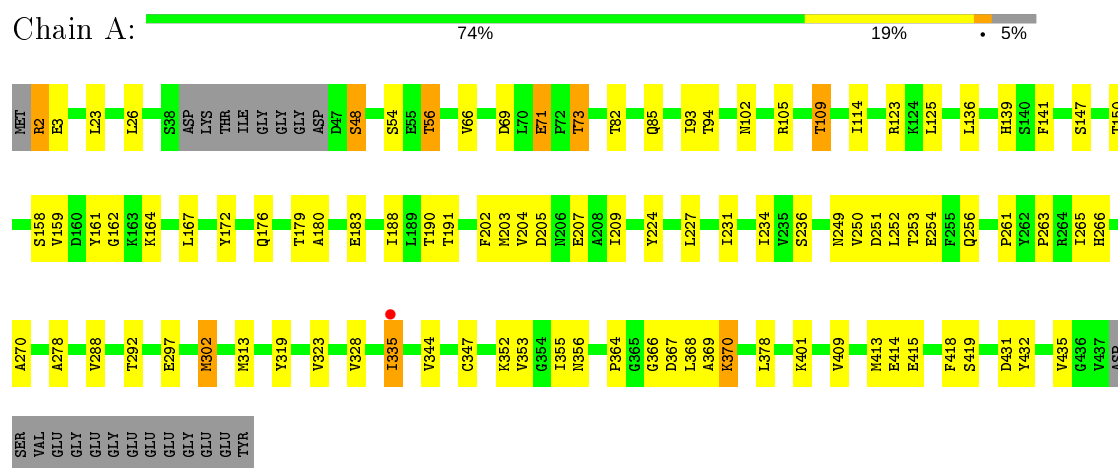


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			10	6	4		

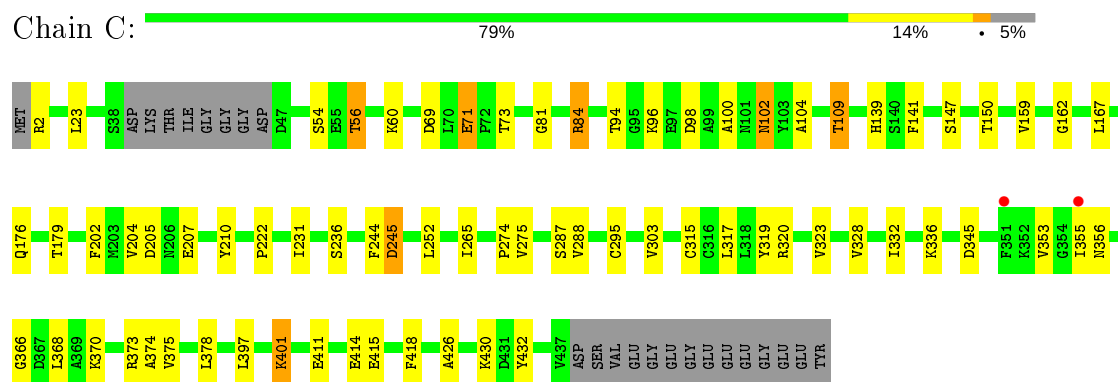
### 3 Residue-property plots [i](#)

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.

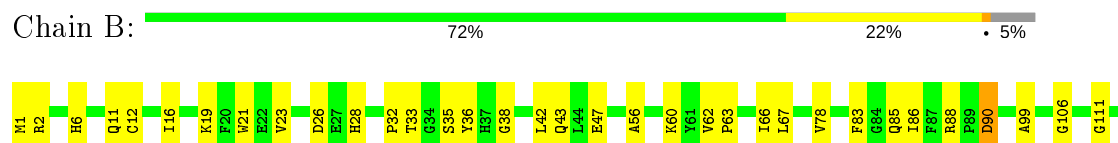
#### • Molecule 1: Tubulin alpha chain

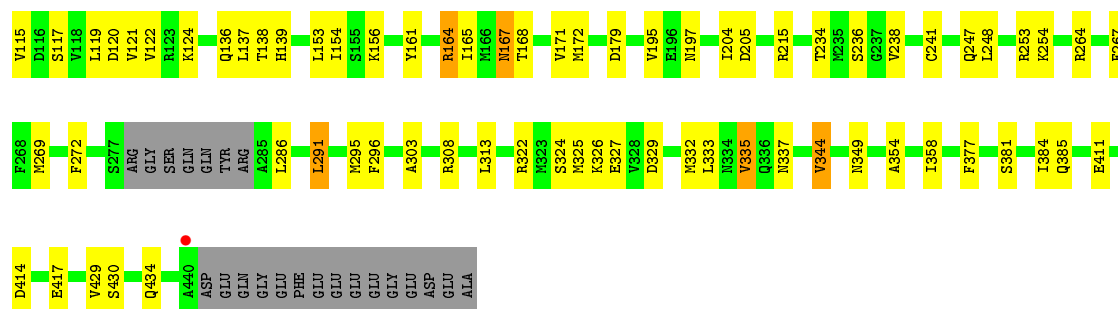


#### • Molecule 1: Tubulin alpha chain



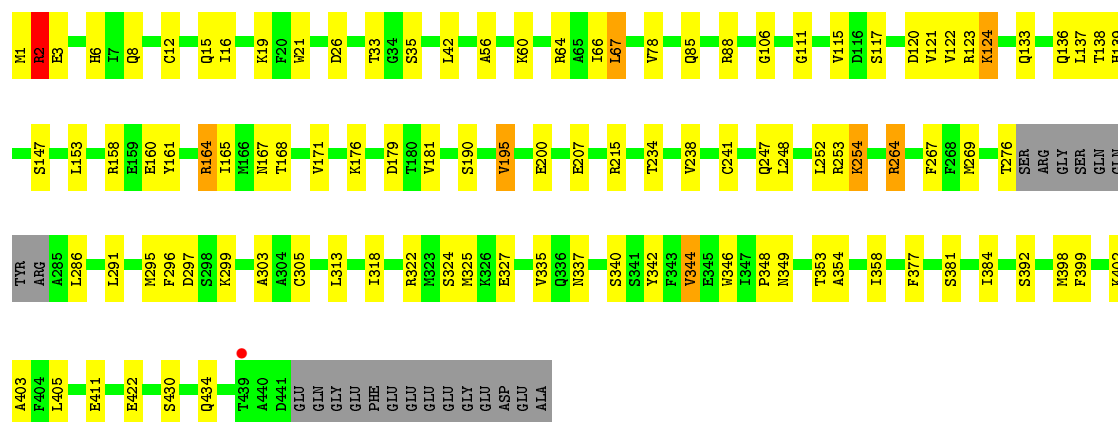
#### • Molecule 2: Tubulin beta chain





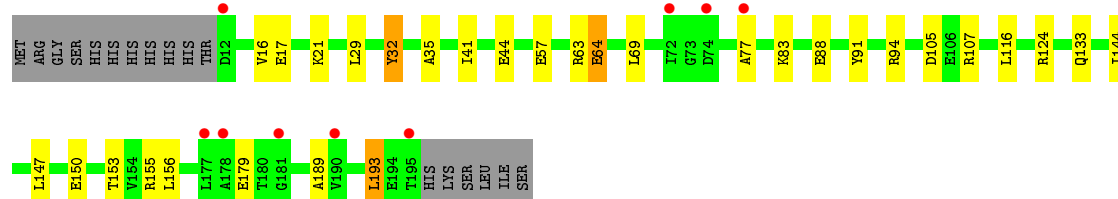
- Molecule 2: Tubulin beta chain

Chain D: 72% 22% 5%



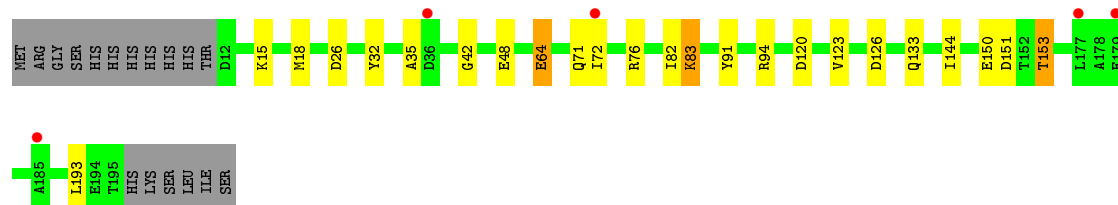
- Molecule 3: iiiA5 ALPHAREP

Chain E: 76% 14% 8%

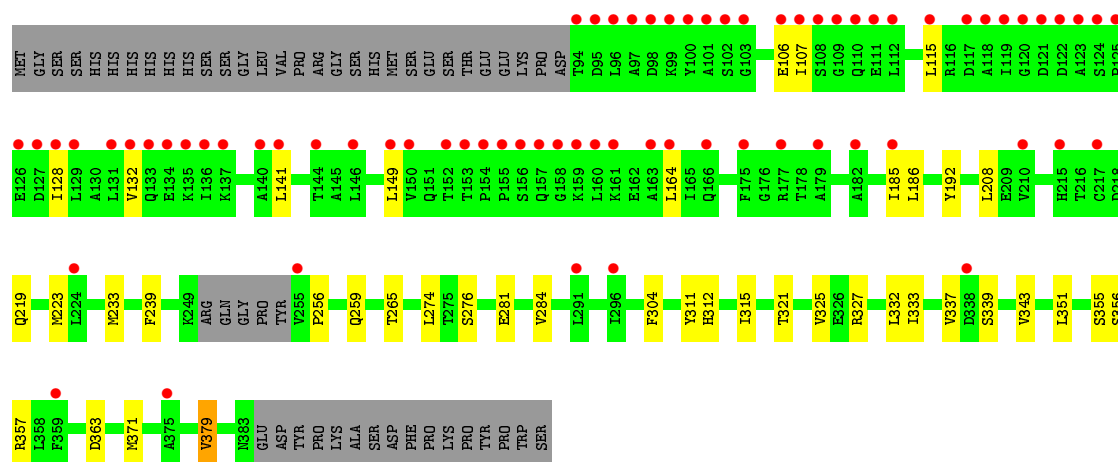
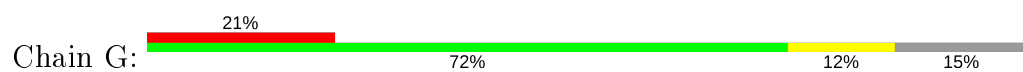


- Molecule 3: iiiA5 ALPHAREP

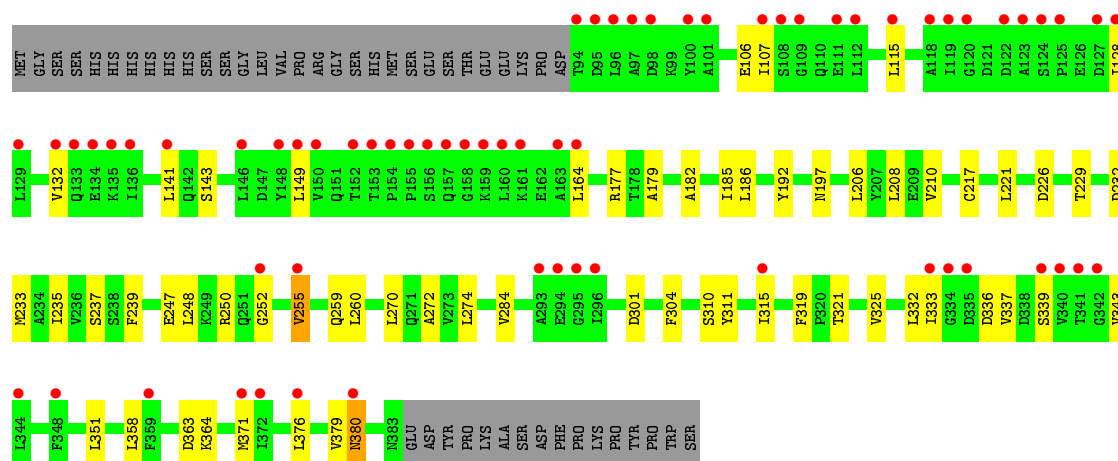
Chain F: 80% 10% 8%



- Molecule 4: Low calcium response E



• Molecule 4: Low calcium response E



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.06Å 95.85Å 158.06Å 90.00° 101.49° 90.00°	Depositor
Resolution (Å)	49.03 – 3.19 49.03 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.03-3.19) 99.2 (49.03-3.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.173 , 0.210 0.197 , 0.234	Depositor DCC
$R_{free}$ test set	3606 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 101.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	20365	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.36% 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: GOL, MG, PGE, GTP, SO4, 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	0.52	0/3364	0.75	0/4575
1	C	0.52	0/3361	0.74	0/4572
2	B	0.55	0/3369	0.74	0/4567
2	D	0.57	0/3371	0.76	0/4570
3	E	0.54	0/1348	0.67	0/1830
3	F	0.53	0/1352	0.66	0/1835
4	G	0.39	0/2158	0.57	0/2937
4	H	0.40	0/2174	0.57	0/2962
All	All	0.51	0/20497	0.70	0/27848

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	3291	0	3149	46	0
1	C	3288	0	3142	36	0
2	B	3296	0	3168	42	0
2	D	3298	0	3167	46	0
3	E	1334	0	1294	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1338	0	1298	5	0
4	G	2132	0	2055	19	0
4	H	2146	0	2053	26	0
5	A	32	0	12	0	0
5	B	32	0	12	0	0
5	C	32	0	12	0	0
5	D	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	5	0	0	0	0
7	C	5	0	0	0	0
8	B	24	0	26	2	0
8	D	24	0	26	4	0
9	B	6	8	8	0	0
9	D	12	16	16	0	0
10	D	10	0	14	0	0
All	All	20341	24	19464	222	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 6.

The worst 5 of 222 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:D:66:ILE:HD13	2:D:122:VAL:HG22	1.65	0.78
2:D:195:VAL:HG22	2:D:264:ARG:HG2	1.64	0.77
1:A:288:VAL:HG22	1:A:323:VAL:HG12	1.67	0.76
2:D:267:PHE:O	2:D:384:ILE:HD13	1.88	0.73
2:B:195:VAL:HG22	2:B:264:ARG:HG2	1.70	0.73

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/451 (94%)	402 (95%)	18 (4%)	4 (1%)	17	56
1	C	424/451 (94%)	403 (95%)	17 (4%)	4 (1%)	17	56
2	B	419/445 (94%)	403 (96%)	15 (4%)	1 (0%)	47	79
2	D	419/445 (94%)	402 (96%)	16 (4%)	1 (0%)	47	79
3	E	182/201 (90%)	180 (99%)	2 (1%)	0	100	100
3	F	182/201 (90%)	180 (99%)	2 (1%)	0	100	100
4	G	281/336 (84%)	276 (98%)	4 (1%)	1 (0%)	34	69
4	H	288/336 (86%)	282 (98%)	6 (2%)	0	100	100
All	All	2619/2866 (91%)	2528 (96%)	80 (3%)	11 (0%)	34	69

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	GLY
2	D	2	ARG
1	A	48	SER
1	A	109	THR
2	B	99	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	348/379 (92%)	317 (91%)	31 (9%)	9	35
1	C	347/379 (92%)	329 (95%)	18 (5%)	23	59
2	B	359/383 (94%)	322 (90%)	37 (10%)	7	29
2	D	359/383 (94%)	319 (89%)	40 (11%)	6	25
3	E	120/157 (76%)	103 (86%)	17 (14%)	3	15
3	F	121/157 (77%)	104 (86%)	17 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	G	230/291 (79%)	221 (96%)	9 (4%)	32 67
4	H	228/291 (78%)	209 (92%)	19 (8%)	11 40
All	All	2112/2420 (87%)	1924 (91%)	188 (9%)	9 35

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	414	GLU
2	D	215	ARG
4	H	229	THR
2	D	15	GLN
2	D	88	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	15	GLN
1	C	197	HIS
4	H	219	GLN
1	C	102	ASN
1	A	301	GLN

### 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 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	C	501	6	26,34,34	0.85	1 (3%)	33,54,54	1.99	5 (15%)
8	MES	B	504	-	12,12,12	0.66	0	14,16,16	0.33	0
7	SO4	C	503	-	4,4,4	0.13	0	6,6,6	0.29	0
7	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.29	0
8	MES	D	504	-	12,12,12	0.58	0	14,16,16	0.67	0
9	GOL	B	505	-	5,5,5	0.75	0	5,5,5	0.46	0
9	GOL	D	506	-	5,5,5	0.57	0	5,5,5	0.35	0
8	MES	B	503	-	12,12,12	0.69	0	14,16,16	0.40	0
5	GTP	B	501	6	26,34,34	1.07	2 (7%)	33,54,54	2.09	5 (15%)
5	GTP	D	501	6	26,34,34	1.05	2 (7%)	33,54,54	2.10	7 (21%)
10	PGE	D	505	-	9,9,9	0.24	0	8,8,8	0.19	0
9	GOL	D	507	-	5,5,5	0.36	0	5,5,5	0.29	0
8	MES	D	503	-	12,12,12	0.70	0	14,16,16	0.42	0
5	GTP	A	501	6	26,34,34	0.98	2 (7%)	33,54,54	1.99	5 (15%)

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	C	501	6	-	8/18/38/38	0/3/3/3
8	MES	B	504	-	-	5/6/14/14	0/1/1/1
8	MES	D	504	-	-	2/6/14/14	0/1/1/1
9	GOL	B	505	-	-	1/4/4/4	-
9	GOL	D	506	-	-	2/4/4/4	-
8	MES	B	503	-	-	2/6/14/14	0/1/1/1
5	GTP	B	501	6	-	4/18/38/38	0/3/3/3
5	GTP	D	501	6	-	7/18/38/38	0/3/3/3
10	PGE	D	505	-	-	1/7/7/7	-
9	GOL	D	507	-	-	1/4/4/4	-
8	MES	D	503	-	-	2/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	9/18/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	501	GTP	C6-N1	3.56	1.39	1.33
5	B	501	GTP	C6-N1	3.36	1.38	1.33
5	A	501	GTP	C6-N1	3.11	1.38	1.33
5	B	501	GTP	C6-C5	3.09	1.46	1.41
5	C	501	GTP	C6-N1	3.07	1.38	1.33

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	GTP	C5-C6-N1	-8.67	111.58	123.43
5	D	501	GTP	C5-C6-N1	-8.42	111.91	123.43
5	C	501	GTP	C5-C6-N1	-7.91	112.61	123.43
5	A	501	GTP	C5-C6-N1	-7.90	112.63	123.43
5	B	501	GTP	C6-N1-C2	5.99	125.45	115.93

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	504	MES	C7-C8-S-O1S
9	D	506	GOL	O1-C1-C2-C3

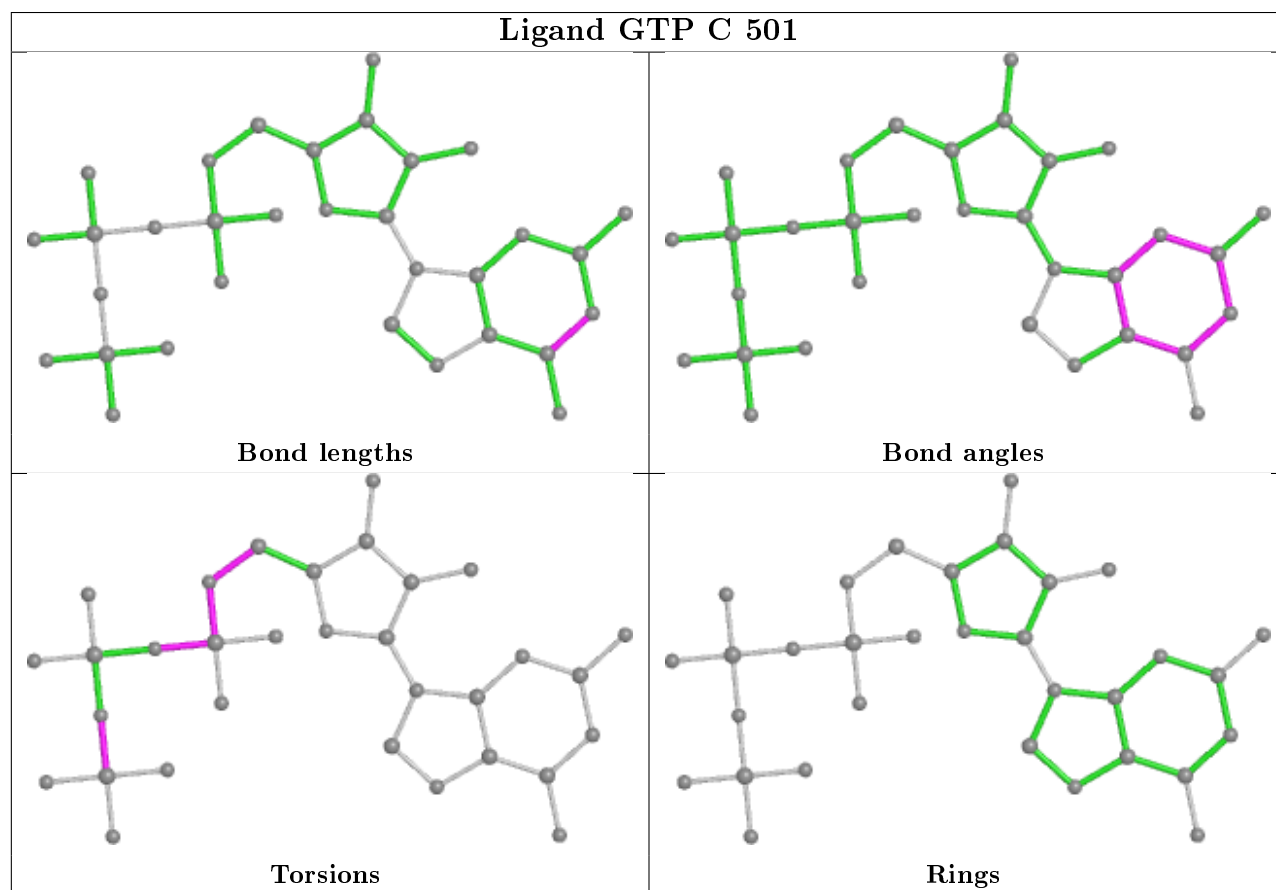
There are no ring outliers.

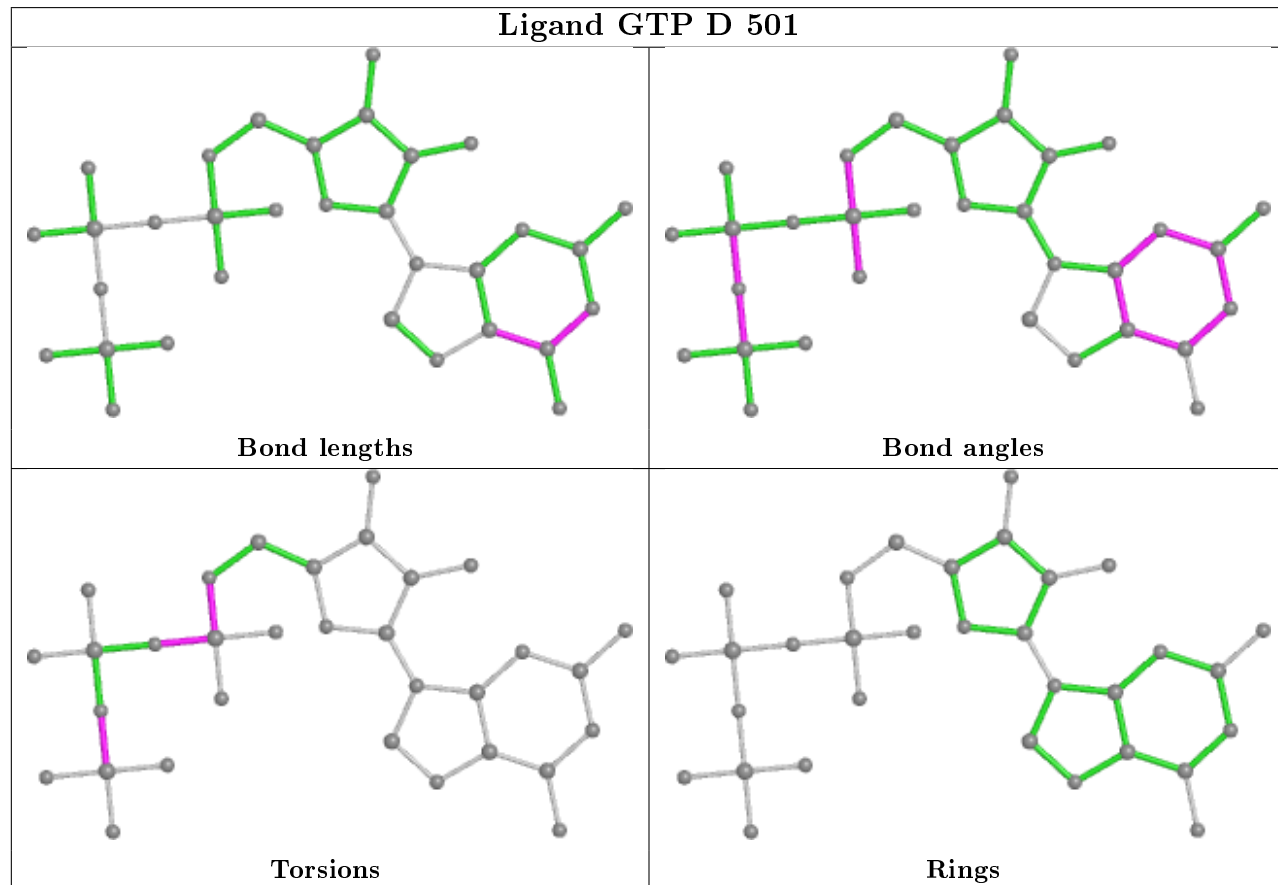
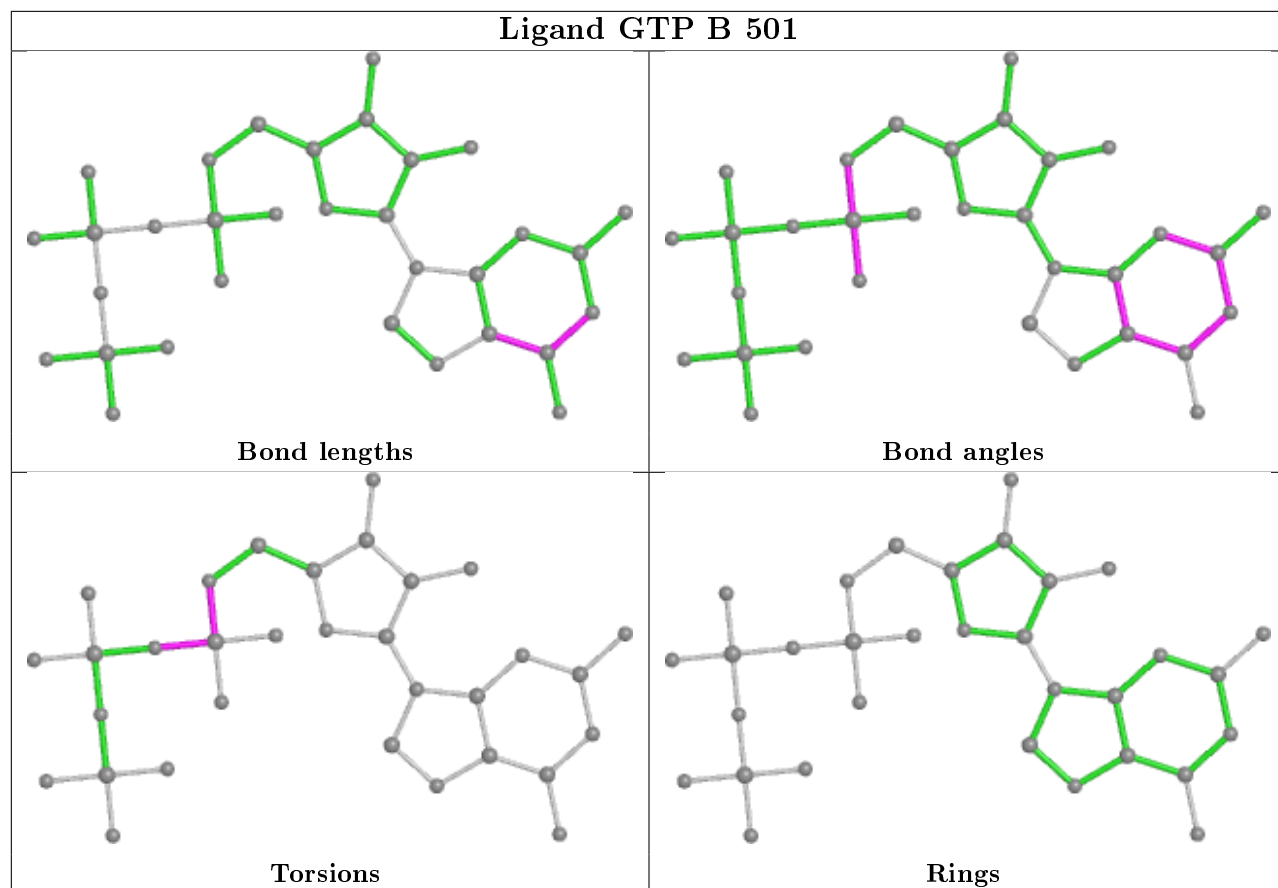
3 monomers are involved in 6 short contacts:

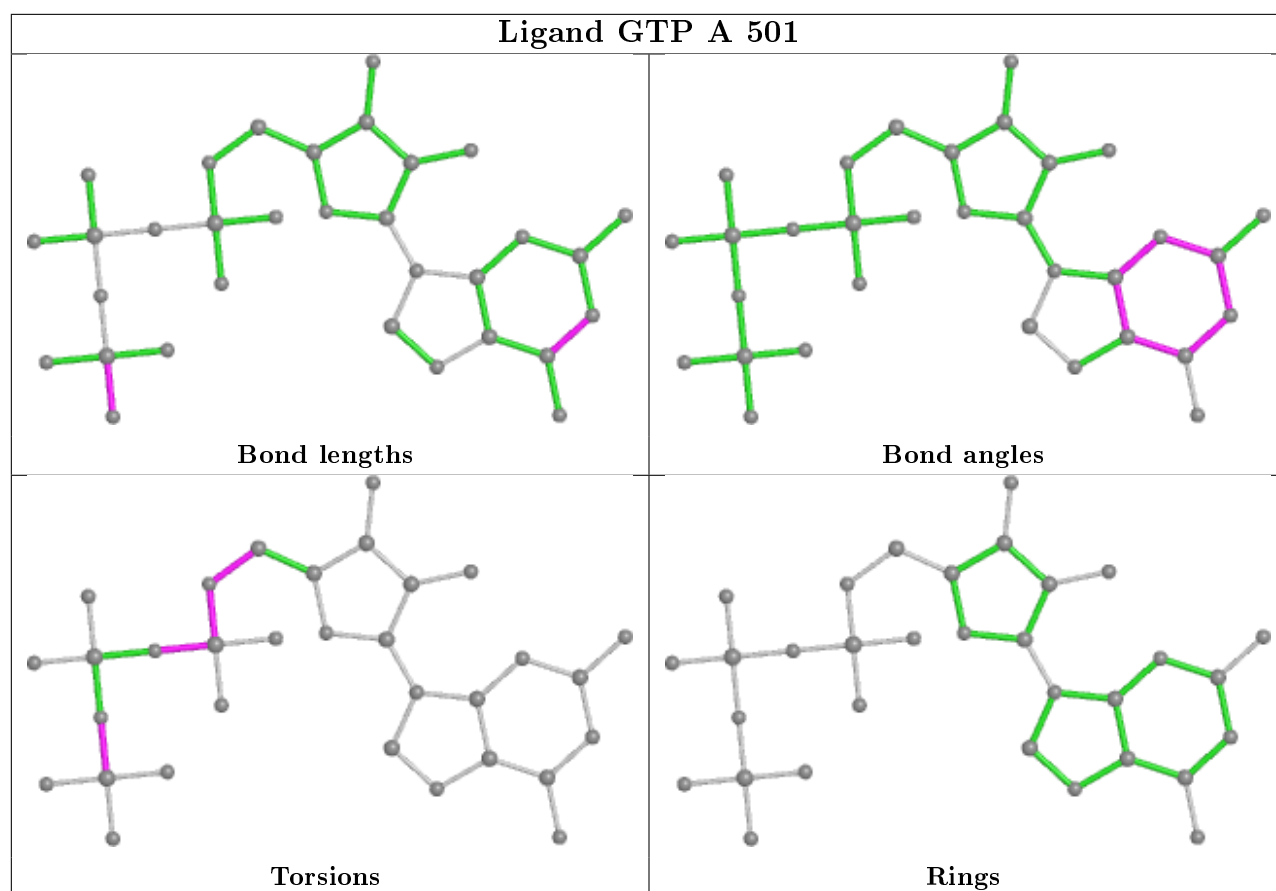
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	504	MES	2	0
8	D	504	MES	3	0
8	D	503	MES	1	0

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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	428/451 (94%)	-0.19	1 (0%) 95 94	55, 96, 156, 183	2 (0%)
1	C	428/451 (94%)	-0.14	2 (0%) 91 86	58, 95, 152, 176	2 (0%)
2	B	423/445 (95%)	-0.07	1 (0%) 95 94	64, 92, 124, 153	0
2	D	423/445 (95%)	-0.08	1 (0%) 95 94	62, 86, 121, 165	0
3	E	184/201 (91%)	0.22	9 (4%) 29 17	77, 109, 182, 191	0
3	F	184/201 (91%)	0.07	5 (2%) 54 39	77, 110, 187, 200	0
4	G	285/336 (84%)	1.22	72 (25%) 0 0	104, 164, 269, 279	0
4	H	290/336 (86%)	0.96	66 (22%) 0 0	92, 166, 250, 270	0
All	All	2645/2866 (92%)	0.18	157 (5%) 22 13	55, 103, 218, 279	4 (0%)

The worst 5 of 157 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	153	THR	13.1
4	H	153	THR	9.5
4	G	119	ILE	8.2
4	H	154	PRO	8.0
4	G	122	ASP	7.1

### 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.

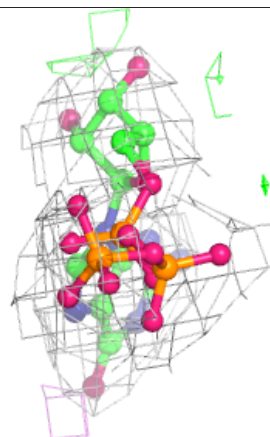
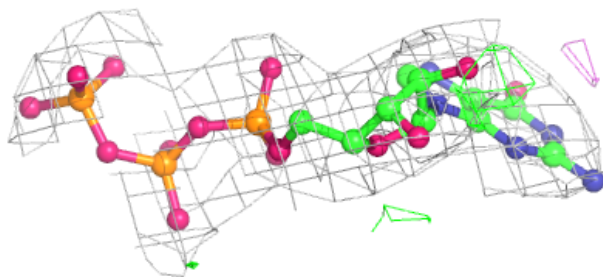
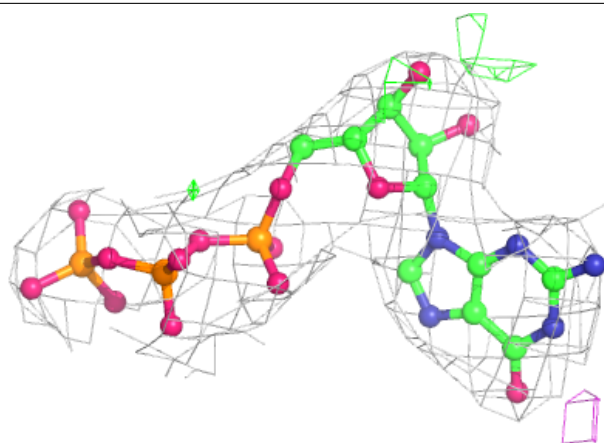
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
10	PGE	D	505	10/10	0.65	0.25	129,136,140,140	0
7	SO4	A	503	5/5	0.70	0.33	172,174,174,175	0
7	SO4	C	503	5/5	0.71	0.42	168,169,170,171	0
6	MG	B	502	1/1	0.79	0.30	85,85,85,85	0
6	MG	D	502	1/1	0.81	0.18	76,76,76,76	0
9	GOL	D	506	6/6	0.81	0.27	58,65,72,75	0
9	GOL	D	507	6/6	0.87	0.57	63,69,77,78	0
9	GOL	B	505	6/6	0.92	0.23	49,55,63,69	0
8	MES	B	503	12/12	0.94	0.22	104,107,118,118	0
8	MES	D	503	12/12	0.94	0.18	92,99,121,122	0
8	MES	D	504	12/12	0.95	0.35	88,91,111,112	0
6	MG	A	502	1/1	0.96	0.28	60,60,60,60	0
8	MES	B	504	12/12	0.96	0.33	104,107,111,112	0
5	GTP	D	501	32/32	0.97	0.23	78,88,117,121	0
6	MG	C	502	1/1	0.97	0.26	61,61,61,61	0
5	GTP	B	501	32/32	0.98	0.22	73,88,123,126	0
5	GTP	C	501	32/32	0.98	0.22	77,81,85,87	0
5	GTP	A	501	32/32	0.98	0.23	71,81,93,95	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.

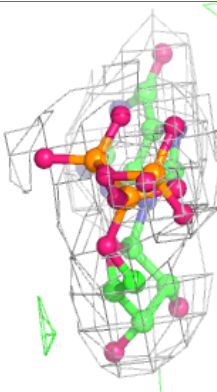
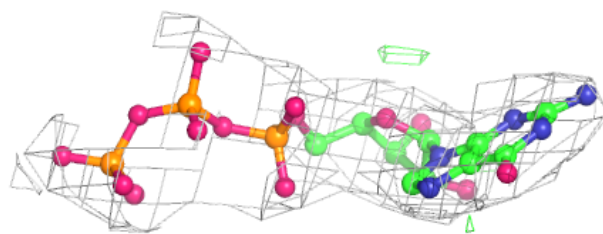
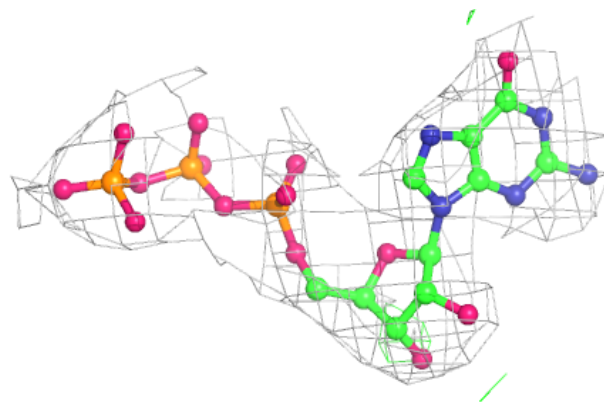


**Electron density around GTP D 501:**

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

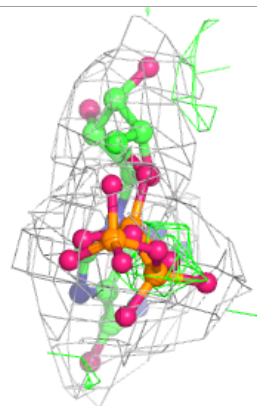
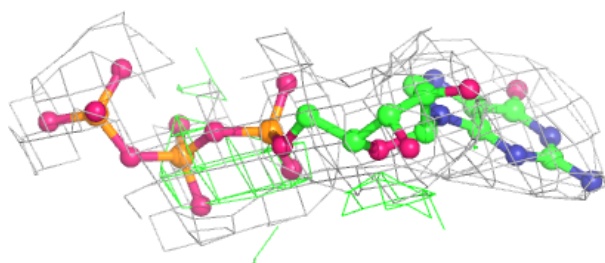
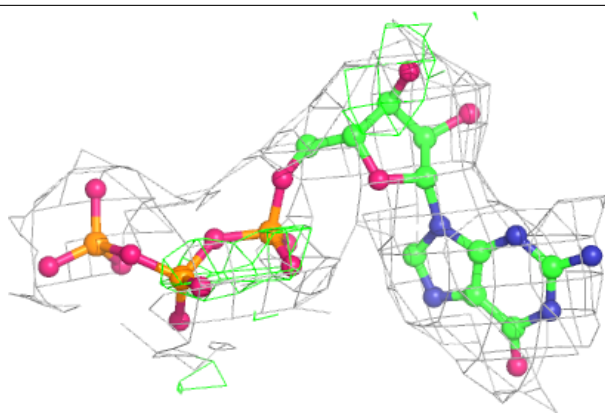
**Electron density around GTP B 501:**

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

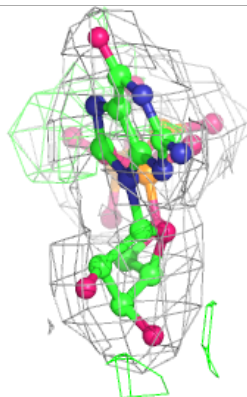
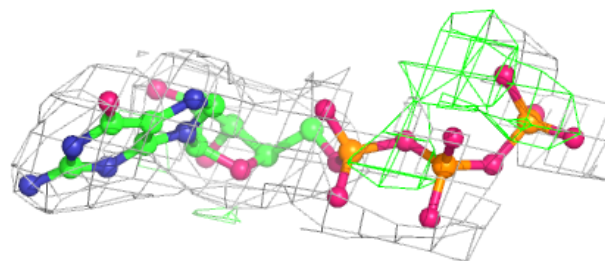
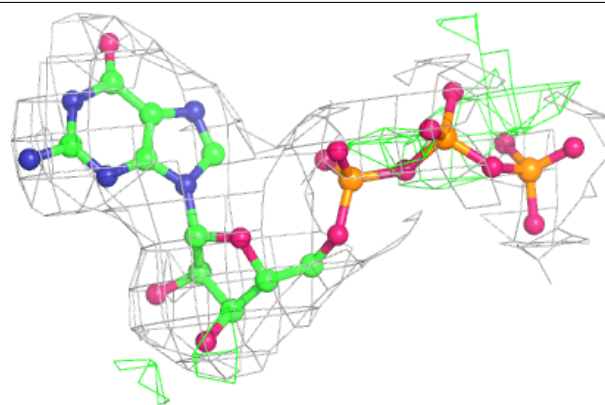


**Electron density around GTP C 501:**

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

**Electron density around GTP A 501:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.