



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:52 PM UTC

PDB ID : 9F07 / pdb_00009f07
Title : TUBULIN:STATHMIN:DARPIN:TAU MTBR3 COMPLEX
Authors : Ammar Khodja, L.; Campanacci, V.; Gigant, b.
Deposited on : 2024-04-15
Resolution : 2.21 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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

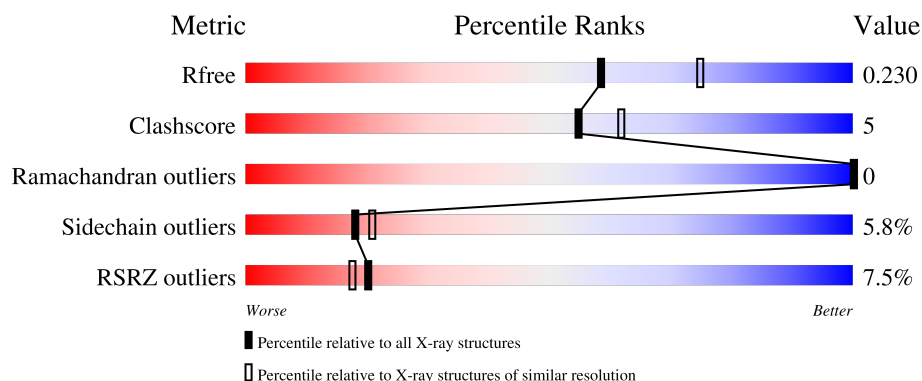
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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.



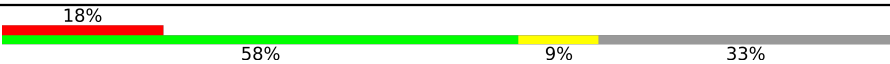
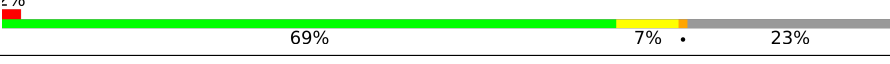
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	13% 76% 17% • 6%
1	E	451	8% 80% 13% • 6%
2	B	445	• 82% 13% • •
2	F	445	2% 81% 15% • •
3	C	121	19% 60% 7% • 31%

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Mol	Chain	Length	Quality of chain
3	G	121	
4	D	190	
4	H	190	

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
12	PGE	D	401	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17447 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 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	1	0
			3283	2082	556	624	21			
1	E	426	Total	C	N	O	S	0	1	0
			3310	2097	563	628	22			

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
E	232	SER	GLY	conflict	UNP D0VWZ0
E	340	SER	THR	conflict	UNP D0VWZ0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	431	Total	C	N	O	S	0	1	0
			3385	2126	579	653	27			
2	F	431	Total	C	N	O	S	0	4	0
			3408	2143	580	658	27			

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
F	203	CYS	SER	conflict	UNP D0VWY9
F	318	ILE	VAL	conflict	UNP D0VWY9

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	83	Total 637	C 399	N 114	O 122	S 2	0	0	0
3	G	81	Total 629	C 397	N 113	O 118	S 1	0	0	0

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	204	MET	-	initiating methionine	UNP Q9H169
C	205	ALA	-	expression tag	UNP Q9H169
C	215	ALA	CYS	engineered mutation	UNP Q9H169
C	221	TRP	PHE	engineered mutation	UNP Q9H169
C	266	PHE	LEU	engineered mutation	UNP Q9H169
C	292	GLY	-	expression tag	UNP Q9H169
C	293	GLY	-	expression tag	UNP Q9H169
C	294	GLY	-	expression tag	UNP Q9H169
C	295	GLY	-	expression tag	UNP Q9H169
C	296	SER	-	expression tag	UNP Q9H169
C	297	GLY	-	expression tag	UNP Q9H169
C	298	GLY	-	expression tag	UNP Q9H169
C	299	GLY	-	expression tag	UNP Q9H169
C	300	GLY	-	expression tag	UNP Q9H169
C	301	SER	-	expression tag	UNP Q9H169
C	302	GLY	-	expression tag	UNP Q9H169
C	303	GLY	-	expression tag	UNP Q9H169
C	304	GLY	-	expression tag	UNP Q9H169
C	305	SER	-	expression tag	UNP Q9H169
C	306	VAL	-	expression tag	UNP Q9H169
C	307	GLN	-	expression tag	UNP Q9H169
C	308	ILE	-	expression tag	UNP Q9H169
C	309	VAL	-	expression tag	UNP Q9H169
C	310	TYR	-	expression tag	UNP Q9H169
C	311	LYS	-	expression tag	UNP Q9H169
C	312	PRO	-	expression tag	UNP Q9H169
C	313	VAL	-	expression tag	UNP Q9H169
C	314	ASP	-	expression tag	UNP Q9H169
C	315	LEU	-	expression tag	UNP Q9H169
C	316	SER	-	expression tag	UNP Q9H169
C	317	LYS	-	expression tag	UNP Q9H169
C	318	VAL	-	expression tag	UNP Q9H169
C	319	THR	-	expression tag	UNP Q9H169
C	320	SER	-	expression tag	UNP Q9H169
C	321	LYS	-	expression tag	UNP Q9H169

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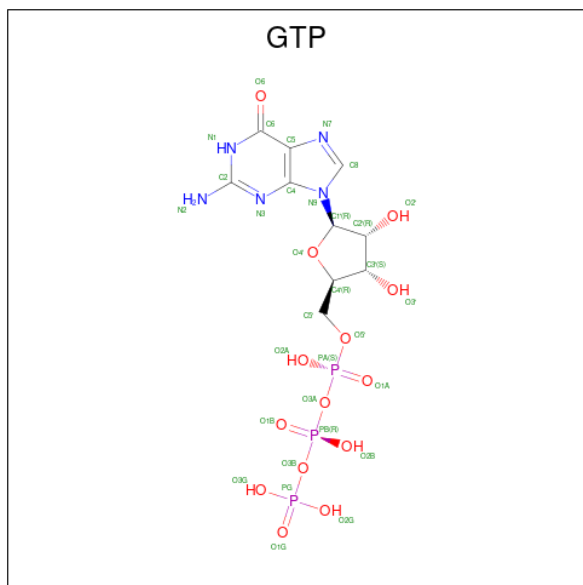
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Chain	Residue	Modelled	Actual	Comment	Reference
C	322	SER	-	expression tag	UNP Q9H169
C	323	GLY	-	expression tag	UNP Q9H169
C	324	SER	-	expression tag	UNP Q9H169
G	204	MET	-	initiating methionine	UNP Q9H169
G	205	ALA	-	expression tag	UNP Q9H169
G	215	ALA	CYS	engineered mutation	UNP Q9H169
G	221	TRP	PHE	engineered mutation	UNP Q9H169
G	266	PHE	LEU	engineered mutation	UNP Q9H169
G	292	GLY	-	expression tag	UNP Q9H169
G	293	GLY	-	expression tag	UNP Q9H169
G	294	GLY	-	expression tag	UNP Q9H169
G	295	GLY	-	expression tag	UNP Q9H169
G	296	SER	-	expression tag	UNP Q9H169
G	297	GLY	-	expression tag	UNP Q9H169
G	298	GLY	-	expression tag	UNP Q9H169
G	299	GLY	-	expression tag	UNP Q9H169
G	300	GLY	-	expression tag	UNP Q9H169
G	301	SER	-	expression tag	UNP Q9H169
G	302	GLY	-	expression tag	UNP Q9H169
G	303	GLY	-	expression tag	UNP Q9H169
G	304	GLY	-	expression tag	UNP Q9H169
G	305	SER	-	expression tag	UNP Q9H169
G	306	VAL	-	expression tag	UNP Q9H169
G	307	GLN	-	expression tag	UNP Q9H169
G	308	ILE	-	expression tag	UNP Q9H169
G	309	VAL	-	expression tag	UNP Q9H169
G	310	TYR	-	expression tag	UNP Q9H169
G	311	LYS	-	expression tag	UNP Q9H169
G	312	PRO	-	expression tag	UNP Q9H169
G	313	VAL	-	expression tag	UNP Q9H169
G	314	ASP	-	expression tag	UNP Q9H169
G	315	LEU	-	expression tag	UNP Q9H169
G	316	SER	-	expression tag	UNP Q9H169
G	317	LYS	-	expression tag	UNP Q9H169
G	318	VAL	-	expression tag	UNP Q9H169
G	319	THR	-	expression tag	UNP Q9H169
G	320	SER	-	expression tag	UNP Q9H169
G	321	LYS	-	expression tag	UNP Q9H169
G	322	SER	-	expression tag	UNP Q9H169
G	323	GLY	-	expression tag	UNP Q9H169
G	324	SER	-	expression tag	UNP Q9H169

- Molecule 4 is a protein called D2-R3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	155	Total	C	N	O	S	0	0	0
			1132	715	191	224	2			
4	H	146	Total	C	N	O	S	0	0	0
			1072	673	183	214	2			

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

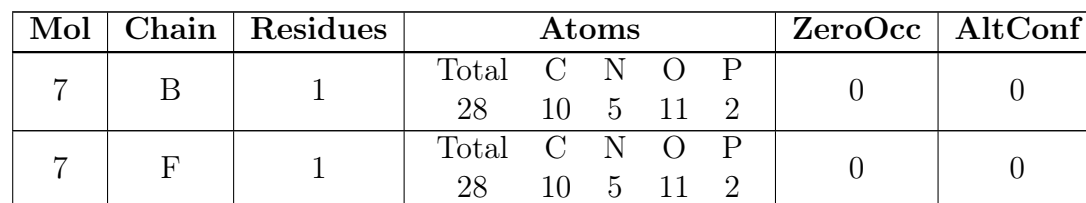


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	E	1	Total	Mg	0	0
			1	1		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



- GOL
-
- The diagram shows the skeletal structure of 1,2,3-propanetriol (glycerol). The carbon chain is represented by a zigzag line with three vertices labeled C1, C2, and C3 in green. C1 is at the left, C2 is in the middle, and C3 is at the right. Each carbon is bonded to a hydroxyl group (OH) in red. The OH group on C1 is labeled O1 in green below it. The OH group on C2 is labeled O2 in green below it. The OH group on C3 is labeled O3 in green to its right. The entire structure is enclosed in a black rectangular box.

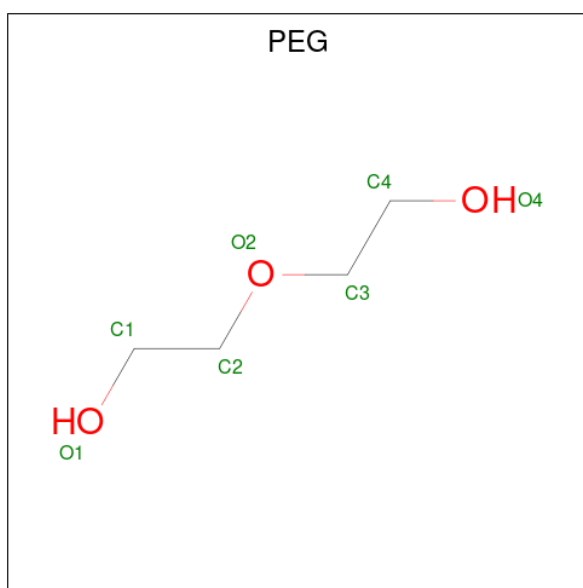
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total 6	C 3	O 3	0	0
8	B	1	Total 6	C 3	O 3	0	0



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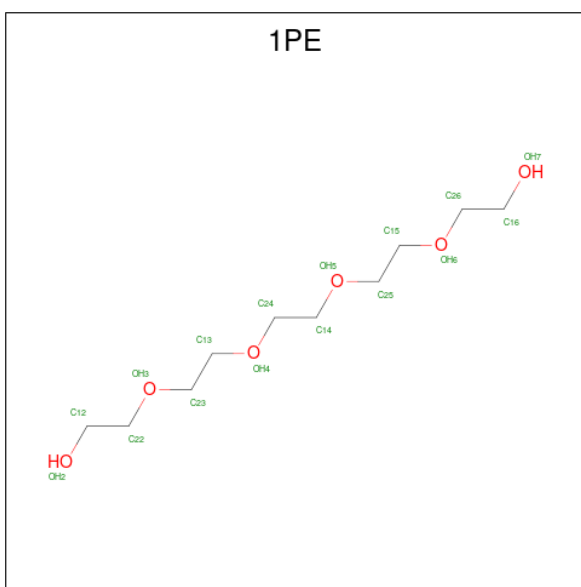
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		
8	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



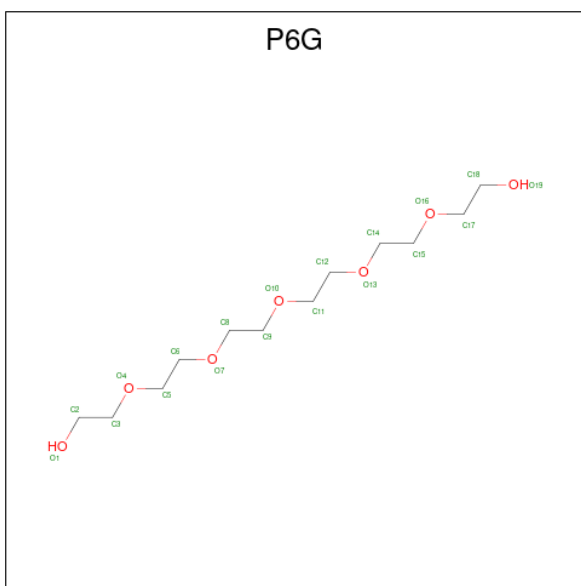
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			7	4	3		
9	F	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



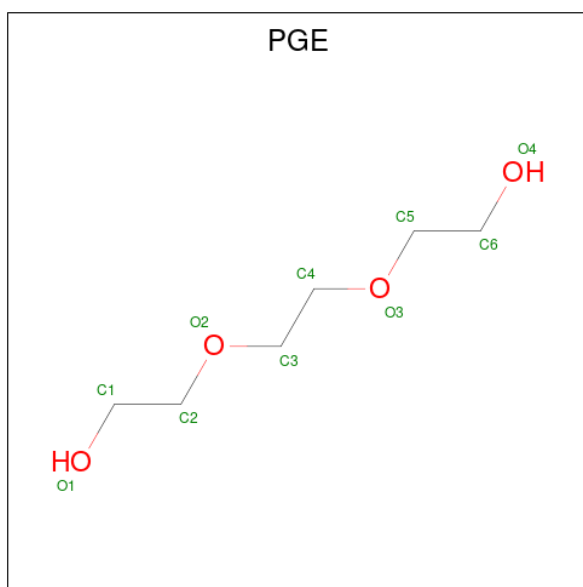
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 11 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 12 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			10	6	4		
12	D	1	Total	C	O	0	0
			10	6	4		
12	F	1	Total	C	O	0	0
			10	6	4		
12	F	1	Total	C	O	0	0
			10	6	4		
12	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	36	Total	O	0	0
			36	36		
13	B	110	Total	O	0	0
			110	110		
13	C	2	Total	O	0	0
			2	2		
13	D	15	Total	O	0	0
			15	15		
13	E	51	Total	O	0	0
			51	51		
13	F	99	Total	O	0	0
			99	99		
13	G	4	Total	O	0	0
			4	4		

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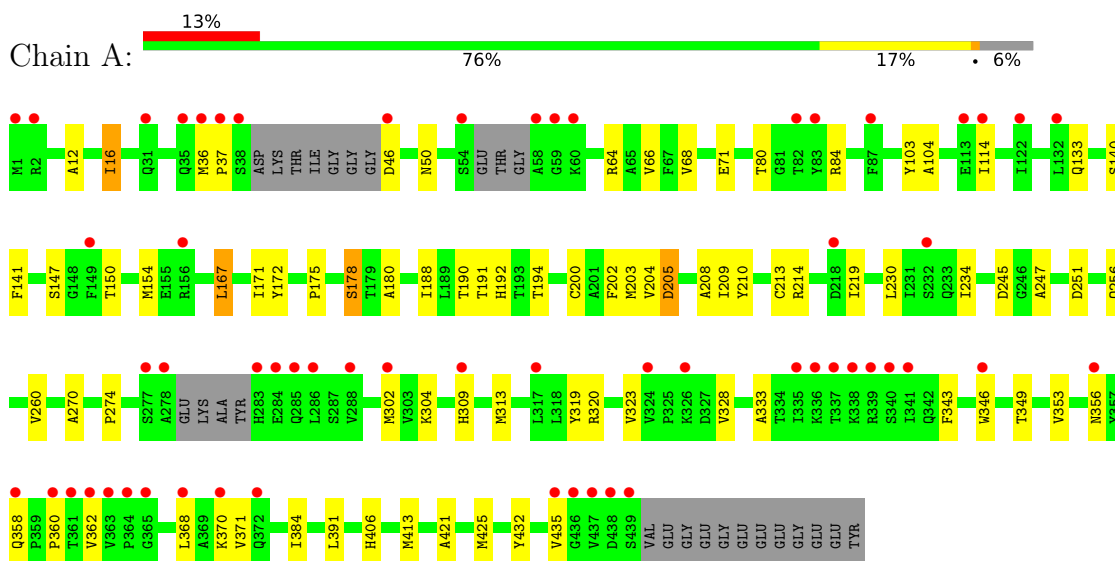
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	H	11	Total	O	0	0
			11	11		

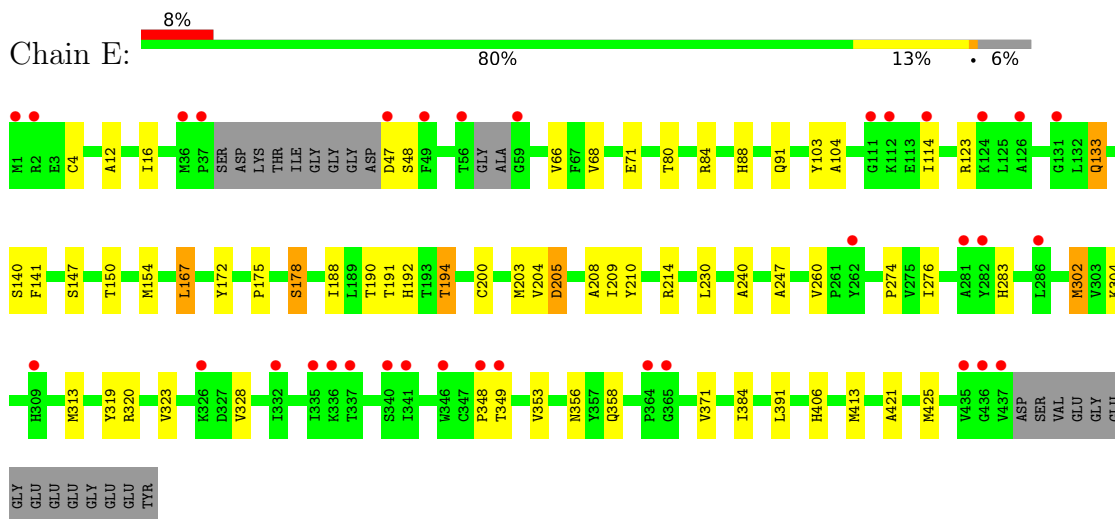
3 Residue-property plots [i](#)

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.

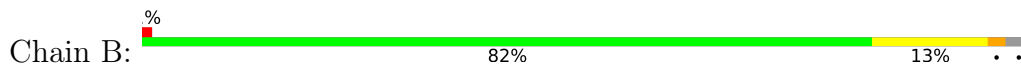
• Molecule 1: Tubulin alpha chain

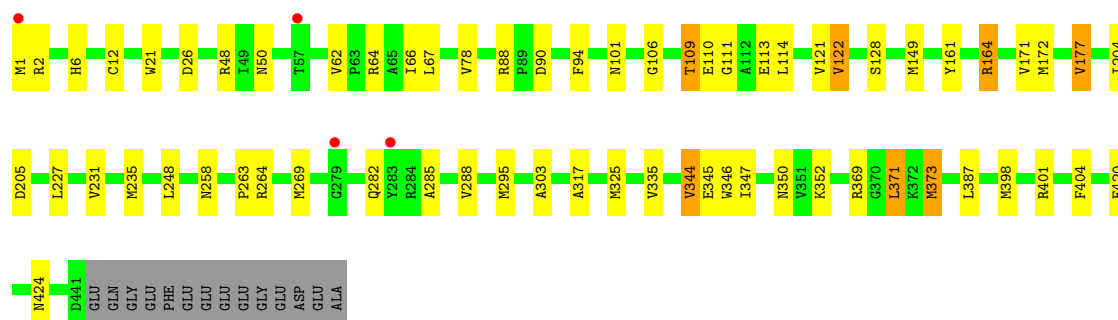


• Molecule 1: Tubulin alpha chain

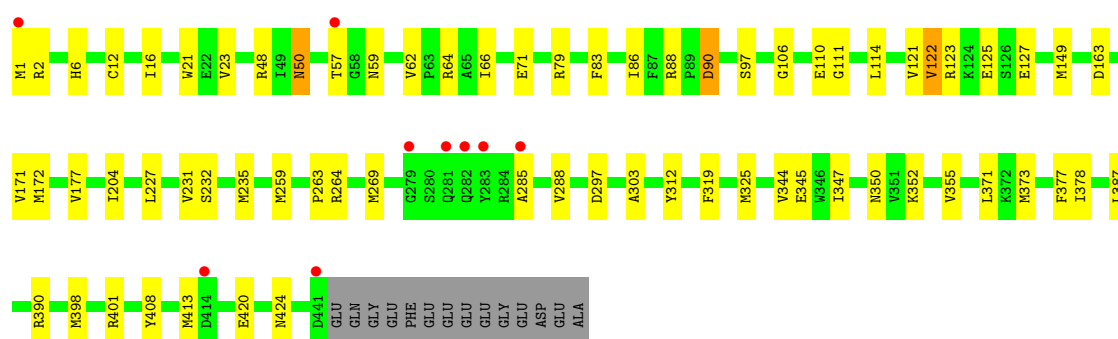
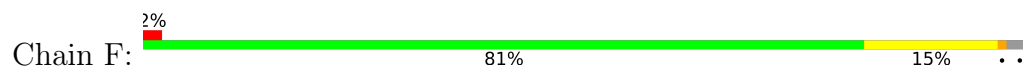


• Molecule 2: Tubulin beta chain

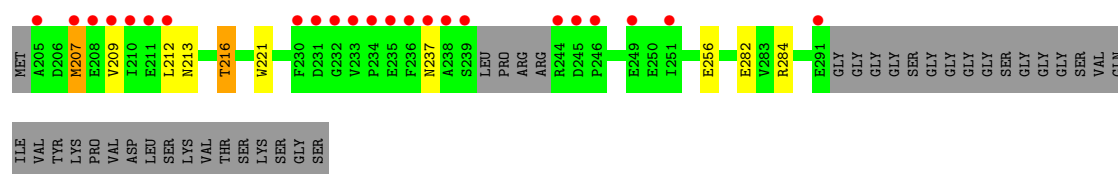




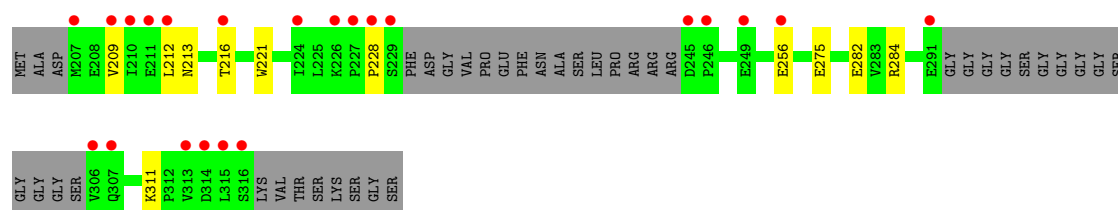
● Molecule 2: Tubulin beta chain



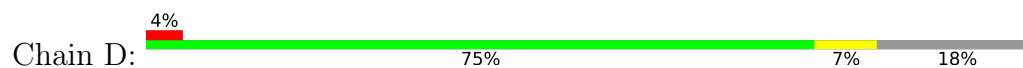
● Molecule 3: Stathmin-4

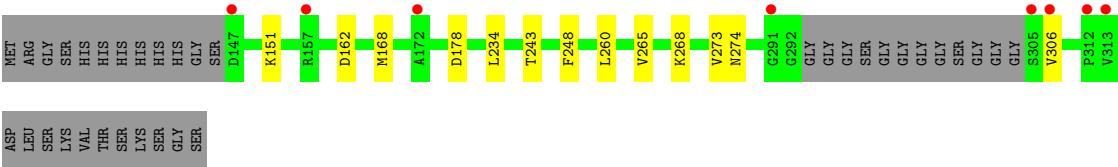


● Molecule 3: Stathmin-4



● Molecule 4: D2-R3





● Molecule 4: D2-R3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.30Å 222.25Å 227.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	159.03 – 2.21 159.03 – 2.21	Depositor EDS
% Data completeness (in resolution range)	60.6 (159.03-2.21) 60.6 (159.03-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.200 , 0.234 0.194 , 0.230	Depositor DCC
R_{free} test set	4073 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17447	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, GTP, GOL, PGE, PEG, P6G, 1PE

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	0.65	0/3357	1.05	3/4561 (0.1%)
1	E	0.66	0/3385	1.07	3/4596 (0.1%)
2	B	0.78	0/3463	1.09	3/4690 (0.1%)
2	F	0.76	0/3493	1.07	1/4732 (0.0%)
3	C	0.66	0/646	1.10	0/867
3	G	0.66	0/636	1.09	0/852
4	D	0.67	0/1148	1.09	2/1560 (0.1%)
4	H	0.69	0/1087	1.13	1/1476 (0.1%)
All	All	0.71	0/17215	1.08	13/23334 (0.1%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	ASP	CA-CB-CG	5.92	118.52	112.60
2	B	109	THR	CA-C-O	-5.71	115.62	119.68
1	A	251	ASP	CA-CB-CG	5.70	118.30	112.60
1	E	240	ALA	CA-C-N	5.64	127.84	120.28
1	E	240	ALA	C-N-CA	5.64	127.84	120.28

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	3283	0	3174	37	0
1	E	3310	0	3216	30	0
2	B	3385	0	3259	46	0
2	F	3408	0	3285	36	0
3	C	637	0	608	6	0
3	G	629	0	621	6	0
4	D	1132	0	1104	2	0
4	H	1072	0	1047	7	0
5	A	32	0	12	0	0
5	E	32	0	12	0	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	B	28	0	12	1	0
7	F	28	0	12	1	0
8	B	24	0	32	1	0
8	F	18	0	24	2	0
9	B	7	0	10	0	0
9	F	7	0	10	1	0
10	B	16	0	22	5	0
11	B	19	0	26	1	0
12	B	10	0	14	1	0
12	D	10	0	14	7	0
12	F	20	0	28	3	0
12	H	10	0	14	3	0
13	A	36	0	0	0	0
13	B	110	0	0	0	0
13	C	2	0	0	0	0
13	D	15	0	0	1	0
13	E	51	0	0	0	0
13	F	99	0	0	1	0
13	G	4	0	0	0	0
13	H	11	0	0	0	0
All	All	17447	0	16556	160	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 5.

The worst 5 of 160 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)
4:H:249:THR:HG22	4:H:252:HIS:ND1	1.92	0.83
4:H:195:GLU:H	4:H:195:GLU:CD	1.90	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:163:ASP:HA	8:F:504:GOL:H31	1.66	0.77
4:H:259:HIS:NE2	12:H:401:PGE:H3	2.04	0.72
2:B:401:ARG:HD2	12:D:401:PGE:H5	1.72	0.69

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	418/451 (93%)	404 (97%)	14 (3%)	0	100	100
1	E	421/451 (93%)	410 (97%)	11 (3%)	0	100	100
2	B	430/445 (97%)	422 (98%)	8 (2%)	0	100	100
2	F	433/445 (97%)	425 (98%)	8 (2%)	0	100	100
3	C	79/121 (65%)	74 (94%)	5 (6%)	0	100	100
3	G	75/121 (62%)	72 (96%)	3 (4%)	0	100	100
4	D	151/190 (80%)	150 (99%)	1 (1%)	0	100	100
4	H	144/190 (76%)	143 (99%)	1 (1%)	0	100	100
All	All	2151/2414 (89%)	2100 (98%)	51 (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	350/379 (92%)	326 (93%)	24 (7%)	14	15
1	E	355/379 (94%)	330 (93%)	25 (7%)	14	15
2	B	370/383 (97%)	356 (96%)	14 (4%)	29	38
2	F	374/383 (98%)	357 (96%)	17 (4%)	24	31
3	C	62/98 (63%)	56 (90%)	6 (10%)	8	7
3	G	63/98 (64%)	58 (92%)	5 (8%)	11	12
4	D	113/141 (80%)	105 (93%)	8 (7%)	13	14
4	H	107/141 (76%)	100 (94%)	7 (6%)	15	17
All	All	1794/2002 (90%)	1688 (94%)	106 (6%)	18	20

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	71	GLU
1	E	313	MET
4	H	195	GLU
1	E	84	ARG
1	E	188	ILE

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

Mol	Chain	Res	Type
4	H	226	HIS
3	G	219	GLN
1	E	11	GLN
2	F	37	HIS
4	D	241	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	1PE	B	507	-	15,15,15	0.21	0	14,14,14	0.20	0
12	PGE	F	505	-	9,9,9	0.21	0	8,8,8	0.06	0
8	GOL	F	504	-	5,5,5	0.04	0	5,5,5	0.19	0
9	PEG	B	506	-	6,6,6	0.19	0	5,5,5	0.24	0
5	GTP	A	501	6	33,34,34	0.55	0	50,54,54	0.56	0
8	GOL	B	504	-	5,5,5	0.07	0	5,5,5	0.22	0
12	PGE	D	401	-	9,9,9	0.26	0	8,8,8	0.25	0
12	PGE	F	506	-	9,9,9	0.12	0	8,8,8	0.22	0
8	GOL	B	502	-	5,5,5	0.09	0	5,5,5	0.36	0
9	PEG	F	507	-	6,6,6	0.19	0	5,5,5	0.13	0
8	GOL	B	503	-	5,5,5	0.09	0	5,5,5	0.29	0
8	GOL	F	502	-	5,5,5	0.14	0	5,5,5	0.32	0
7	GDP	B	501	-	29,30,30	0.41	0	45,47,47	0.54	0
7	GDP	F	501	-	29,30,30	0.41	0	45,47,47	0.50	0
12	PGE	H	401	-	9,9,9	0.25	0	8,8,8	0.24	0
11	P6G	B	508	-	18,18,18	0.22	0	17,17,17	0.14	0
5	GTP	E	501	6	33,34,34	0.54	0	50,54,54	0.55	0
8	GOL	B	505	-	5,5,5	0.15	0	5,5,5	0.35	0
12	PGE	B	509	-	9,9,9	0.24	0	8,8,8	0.12	0
8	GOL	F	503	-	5,5,5	0.12	0	5,5,5	0.35	0

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	1PE	B	507	-	-	5/13/13/13	-
12	PGE	F	505	-	-	4/7/7/7	-
8	GOL	F	504	-	-	2/4/4/4	-
9	PEG	B	506	-	-	4/4/4/4	-
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
8	GOL	B	504	-	-	0/4/4/4	-
12	PGE	D	401	-	-	4/7/7/7	-
12	PGE	F	506	-	-	6/7/7/7	-
8	GOL	B	502	-	-	2/4/4/4	-
9	PEG	F	507	-	-	2/4/4/4	-
8	GOL	B	503	-	-	0/4/4/4	-
8	GOL	F	502	-	-	0/4/4/4	-
7	GDP	B	501	-	-	5/16/32/32	0/3/3/3
7	GDP	F	501	-	-	5/16/32/32	0/3/3/3
12	PGE	H	401	-	-	6/7/7/7	-
11	P6G	B	508	-	-	2/16/16/16	-
5	GTP	E	501	6	-	6/22/38/38	0/3/3/3
8	GOL	B	505	-	-	0/4/4/4	-
12	PGE	B	509	-	-	4/7/7/7	-
8	GOL	F	503	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	E	501	GTP	C5'-O5'-PA-O3A
5	E	501	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

12 monomers are involved in 26 short contacts:

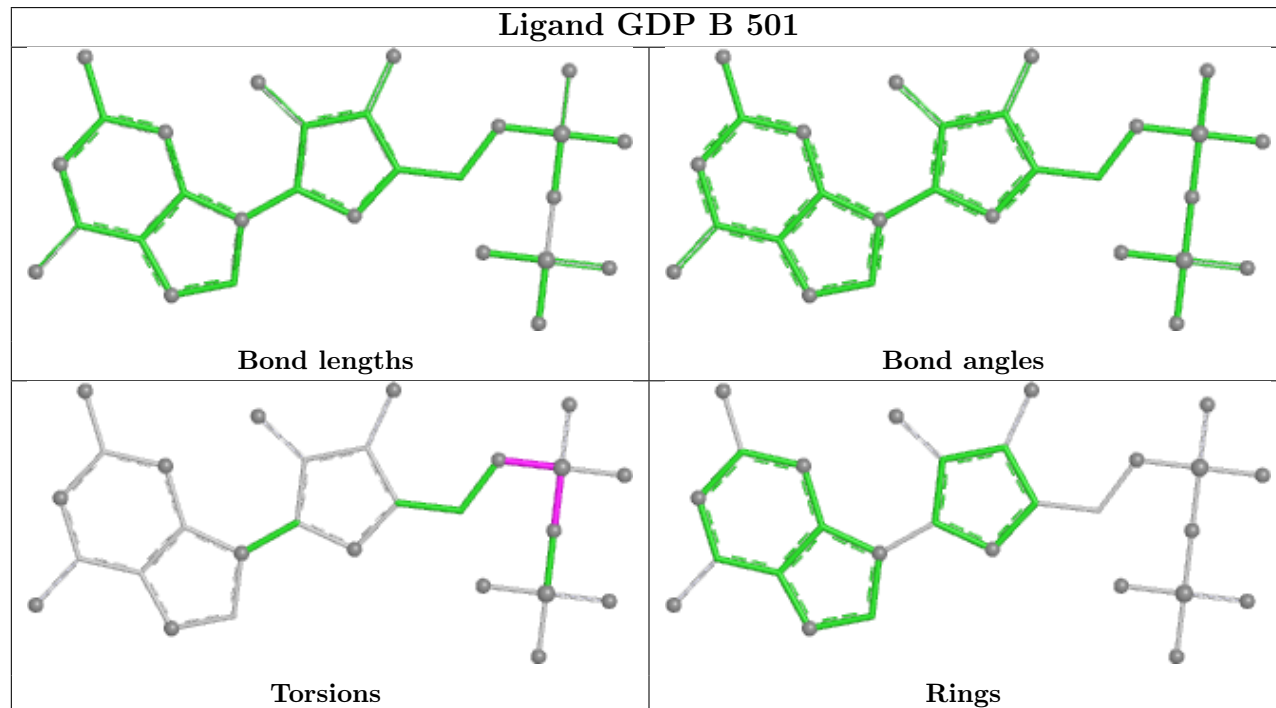
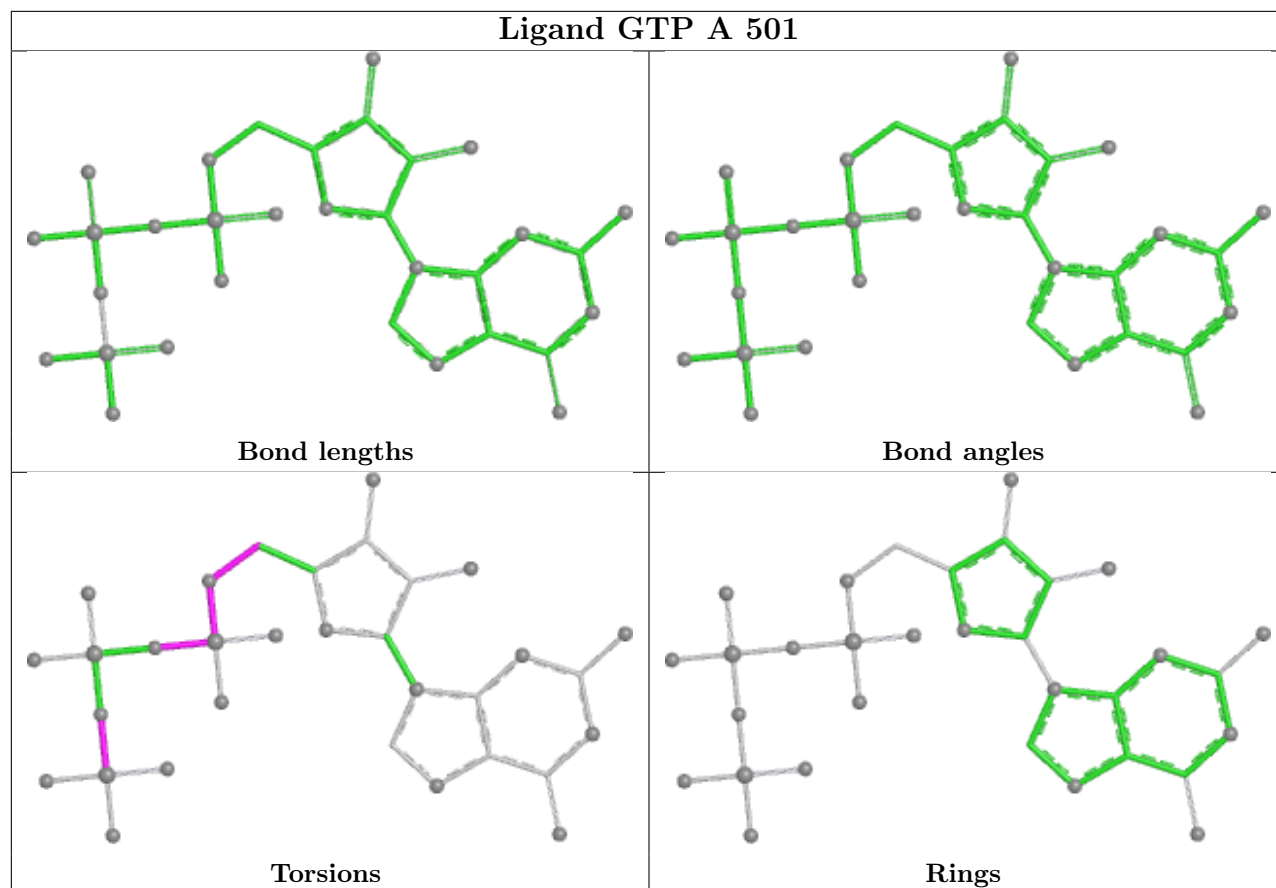
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	507	1PE	5	0

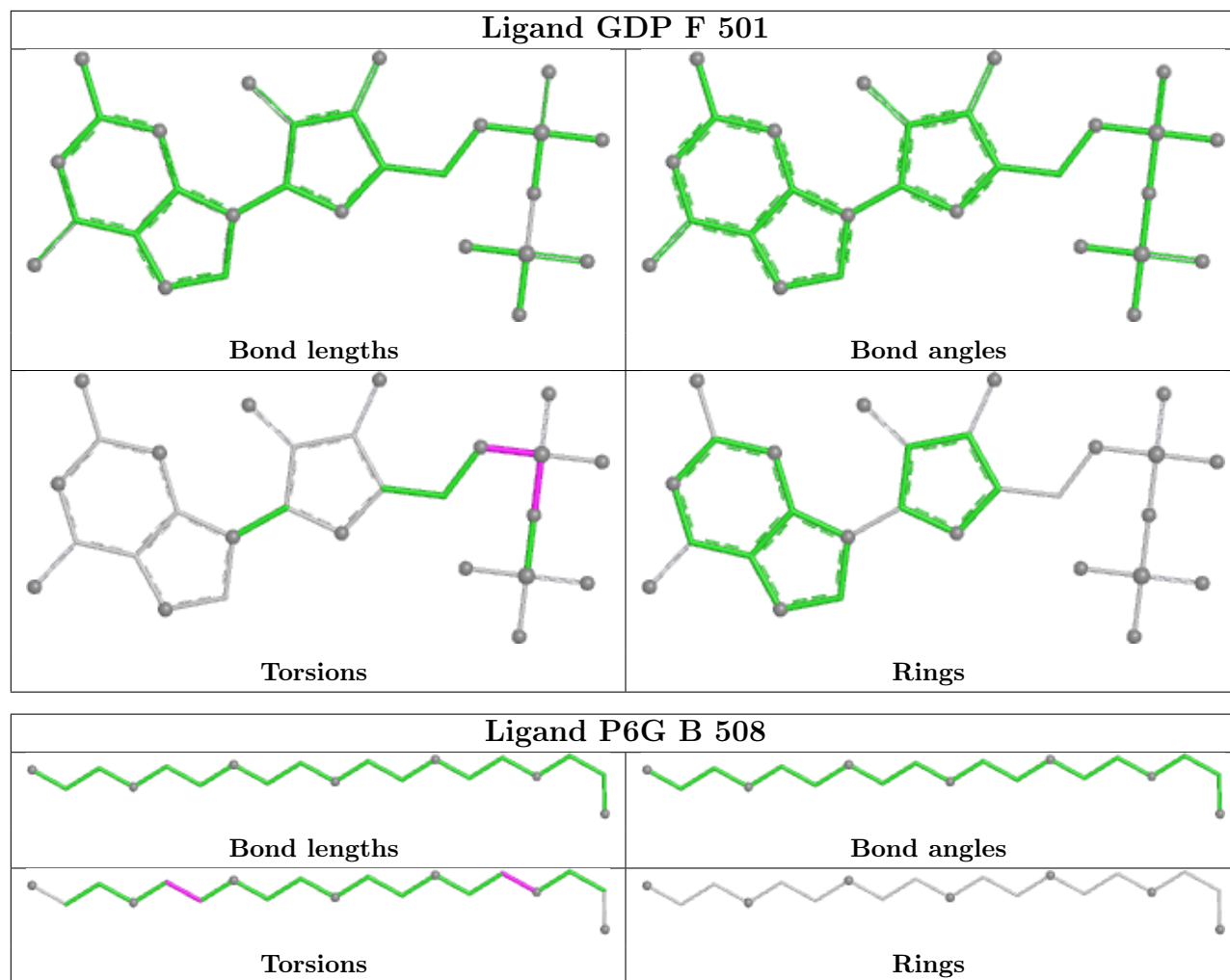
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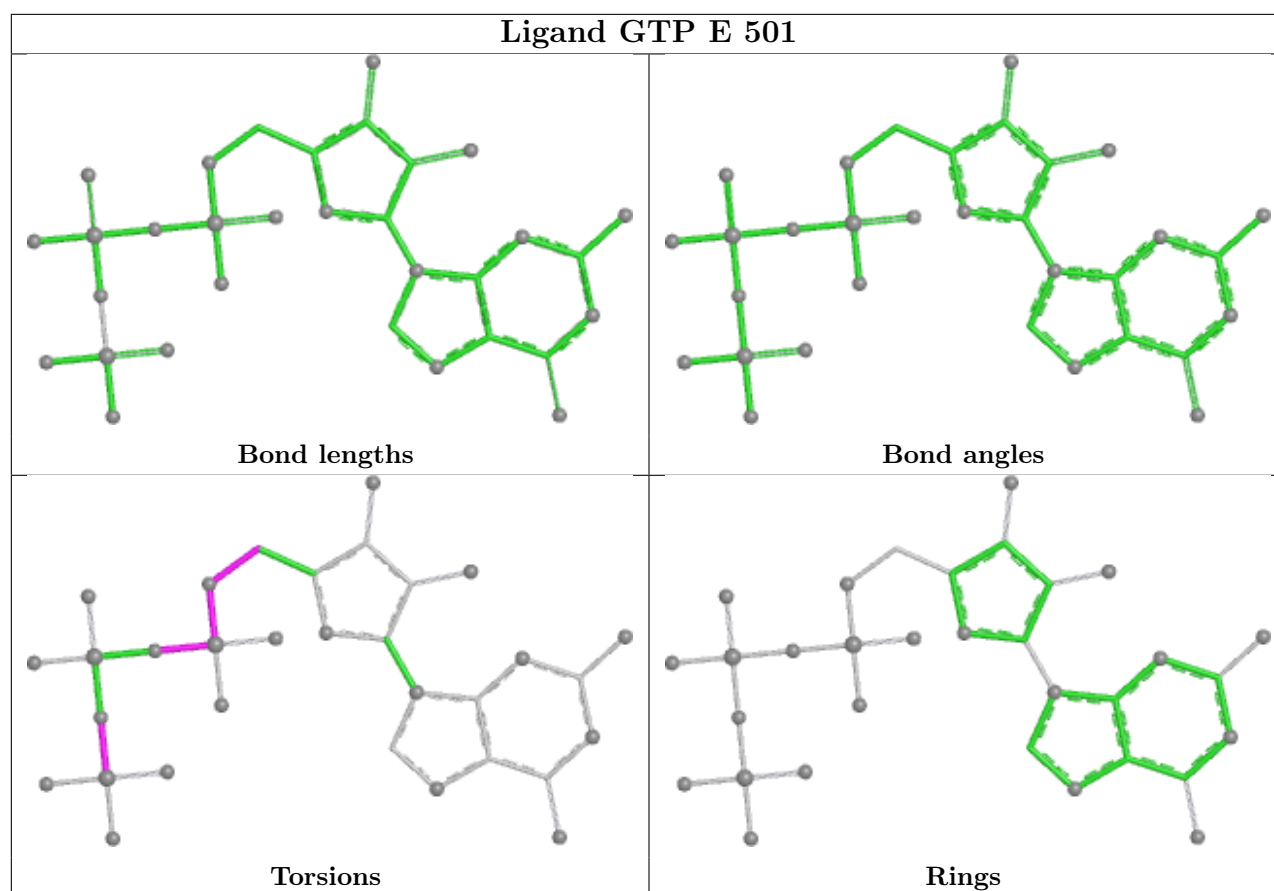
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	504	GOL	1	0
8	B	504	GOL	1	0
12	D	401	PGE	7	0
12	F	506	PGE	3	0
9	F	507	PEG	1	0
8	F	502	GOL	1	0
7	B	501	GDP	1	0
7	F	501	GDP	1	0
12	H	401	PGE	3	0
11	B	508	P6G	1	0
12	B	509	PGE	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	425/451 (94%)	0.83	59 (13%) 6 5	21, 58, 91, 124	3 (0%)
1	E	426/451 (94%)	0.57	34 (7%) 18 16	22, 48, 73, 92	3 (0%)
2	B	431/445 (96%)	-0.27	4 (0%) 81 79	13, 27, 49, 68	3 (0%)
2	F	431/445 (96%)	-0.22	9 (2%) 63 61	11, 28, 50, 73	6 (1%)
3	C	83/121 (68%)	1.63	23 (27%) 1 1	34, 73, 103, 108	0
3	G	81/121 (66%)	1.50	22 (27%) 1 1	38, 64, 87, 93	0
4	D	155/190 (81%)	0.35	8 (5%) 33 30	21, 47, 81, 92	0
4	H	146/190 (76%)	0.46	4 (2%) 56 53	26, 53, 82, 87	0
All	All	2178/2414 (90%)	0.35	163 (7%) 20 17	11, 41, 84, 124	15 (0%)

The worst 5 of 163 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	GLU	5.9
1	A	38	SER	5.6
3	G	313	VAL	5.6
1	A	283	HIS	5.6
3	C	246	PRO	5.6

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

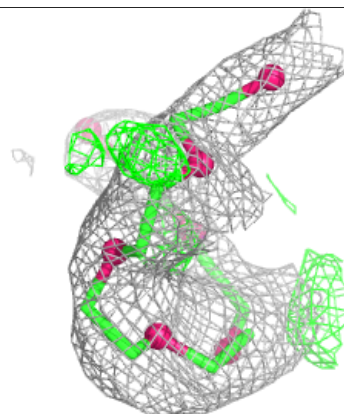
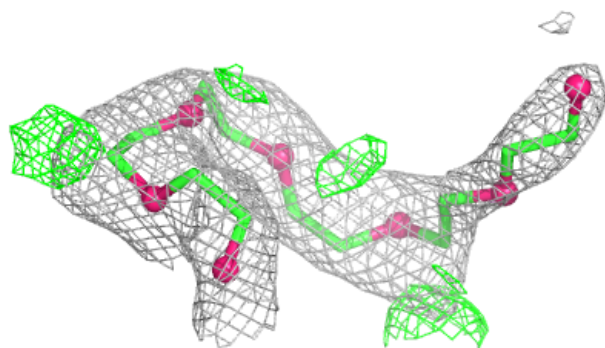
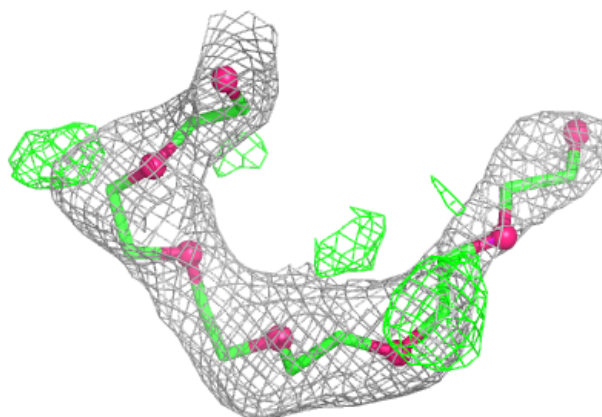
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	B	505	6/6	0.65	0.23	52,53,54,54	0
10	1PE	B	507	16/16	0.77	0.25	83,83,83,83	0
8	GOL	F	502	6/6	0.80	0.19	55,56,56,56	0
12	PGE	H	401	10/10	0.80	0.22	60,62,63,63	0
12	PGE	B	509	10/10	0.81	0.21	68,69,69,69	0
9	PEG	B	506	7/7	0.82	0.15	33,35,36,37	0
8	GOL	F	503	6/6	0.83	0.15	55,55,56,56	0
8	GOL	B	502	6/6	0.84	0.18	73,73,73,73	0
9	PEG	F	507	7/7	0.86	0.18	49,50,51,51	0
12	PGE	F	505	10/10	0.86	0.15	47,47,48,48	0
12	PGE	F	506	10/10	0.86	0.18	59,60,61,61	0
11	P6G	B	508	19/19	0.86	0.18	55,56,58,58	0
12	PGE	D	401	10/10	0.87	0.15	49,50,50,50	0
8	GOL	F	504	6/6	0.89	0.14	62,62,62,62	0
8	GOL	B	504	6/6	0.89	0.11	53,54,54,54	0
8	GOL	B	503	6/6	0.90	0.12	43,44,44,45	0
6	MG	A	502	1/1	0.98	0.06	27,27,27,27	0
7	GDP	B	501	28/28	0.98	0.05	16,19,22,22	0
5	GTP	A	501	32/32	0.98	0.05	24,28,32,33	0
5	GTP	E	501	32/32	0.99	0.04	26,27,28,28	0
7	GDP	F	501	28/28	0.99	0.04	21,22,24,24	0
6	MG	E	502	1/1	0.99	0.06	23,23,23,23	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.

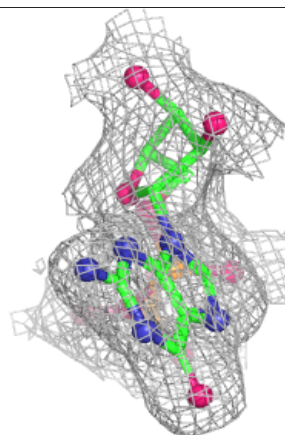
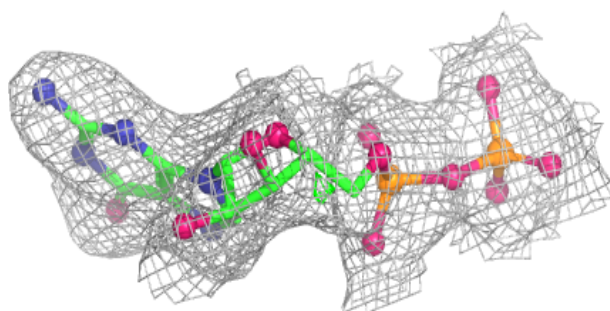
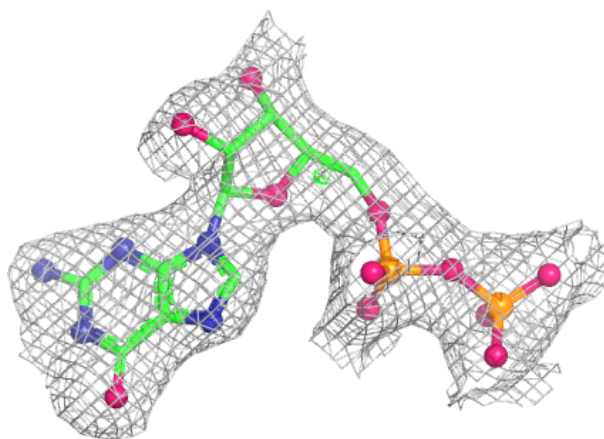
Electron density around P6G B 508:

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

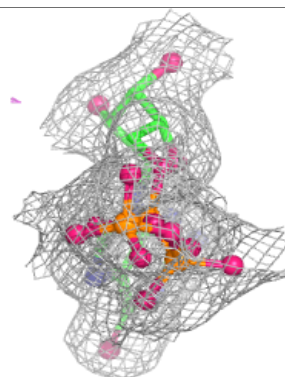
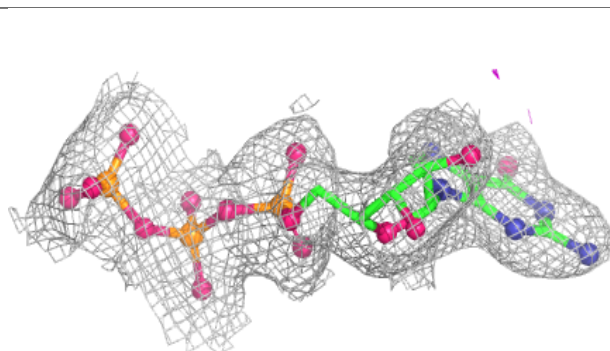
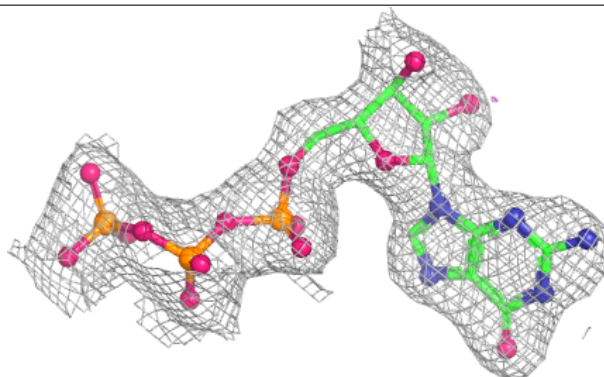


Electron density around GDP B 501:

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

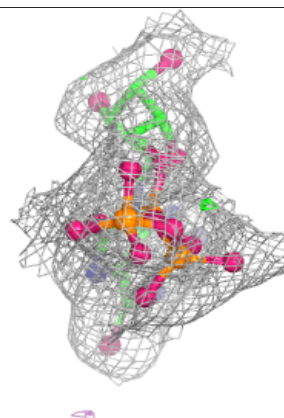
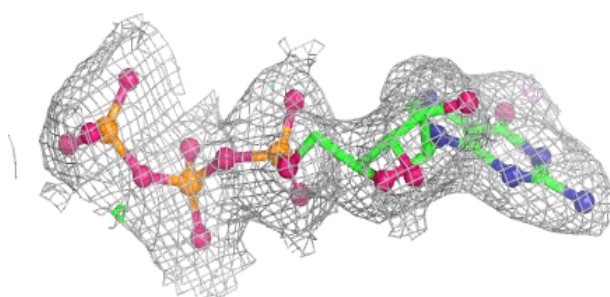
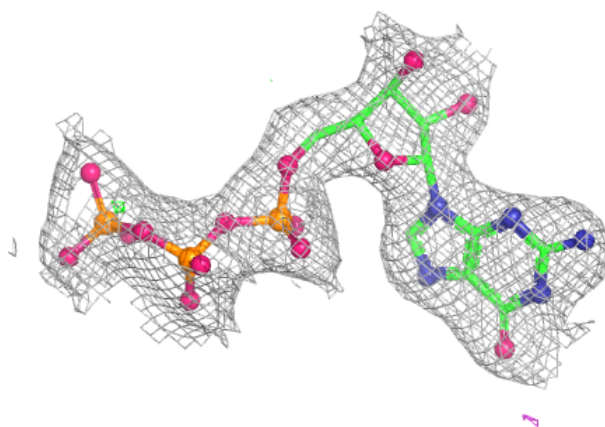
**Electron density around GTP A 501:**

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and green (positive)

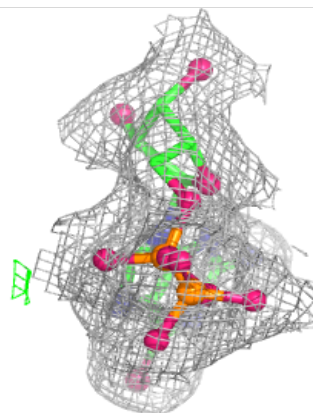
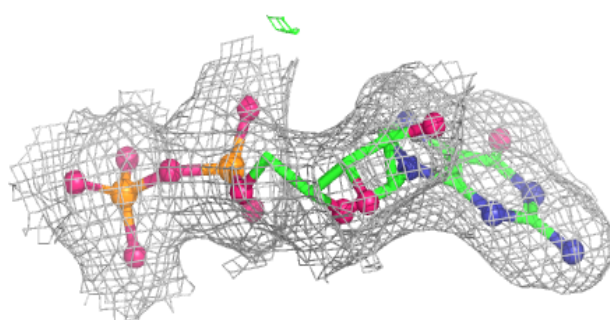
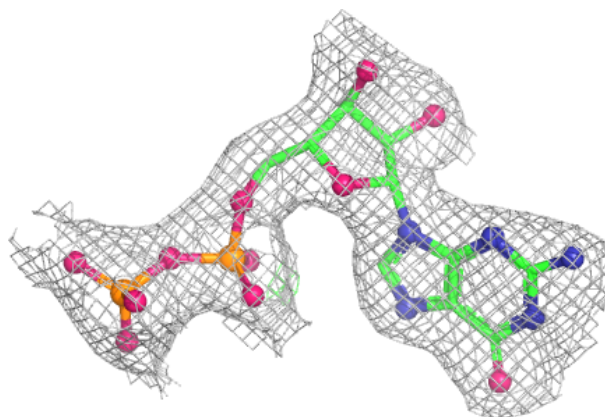


Electron density around GTP E 501:

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

**Electron density around GDP F 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.