



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 02:42 PM UTC

PDB ID : 7L05 / pdb_00007l05
Title : Complex of novel maytansinoid M24 bound to T2R-TTL (two tubulin alpha/beta heterodimers, RB3 stathmin-like domain, and tubulin tyrosine ligase)
Authors : Franklin, M.C.
Deposited on : 2020-12-11
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

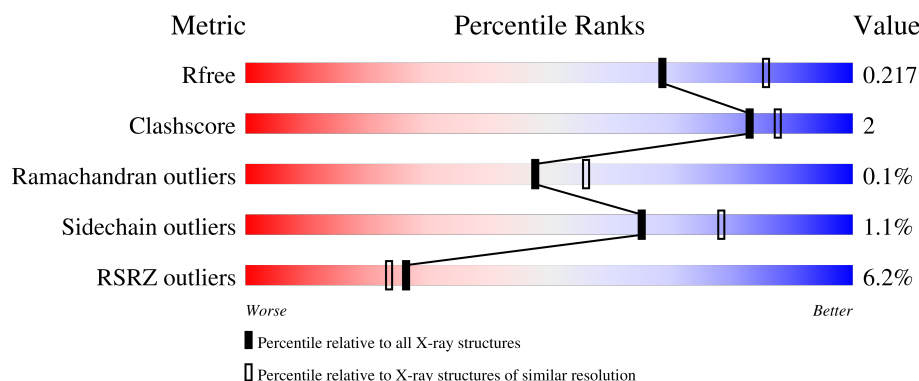
1 Overall quality at a glance

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	 4% 92% 5% •
1	C	451	 2% 88% 10% •
2	B	445	 2% 87% 7% 5%
2	D	445	 7% 86% 8% 6%

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Mol	Chain	Length	Quality of chain
3	E	149	5% 78% 19%
4	F	384	16% 84% 5% 11%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 18587 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	1	0
			3434	2173	583	656	22			
1	C	440	Total	C	N	O	S	0	8	0
			3471	2197	586	664	24			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	5	0
			3325	2095	563	641	26			
2	D	420	Total	C	N	O	S	0	5	0
			3309	2082	558	643	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	3	0
			1017	629	184	198	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	cloning artifact	UNP P63043
E	146	HIS	-	expression tag	UNP P63043
E	147	HIS	-	expression tag	UNP P63043
E	148	HIS	-	expression tag	UNP P63043
E	149	HIS	-	expression tag	UNP P63043
E	150	HIS	-	expression tag	UNP P63043
E	151	HIS	-	expression tag	UNP P63043

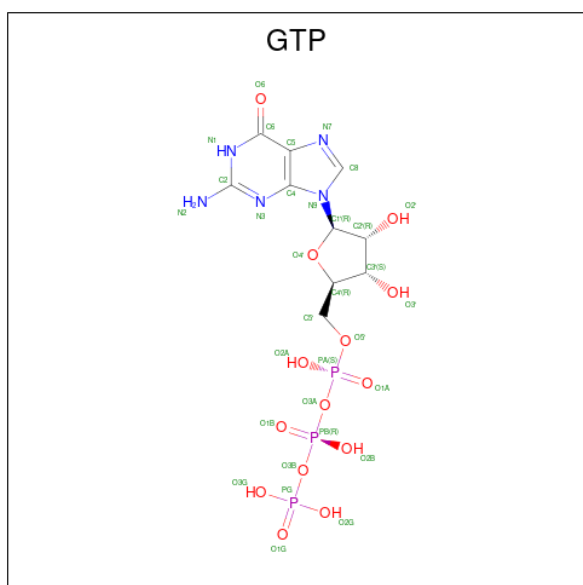
- Molecule 4 is a protein called Tubulin Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	342	Total	C	N	O	S	0	4	0
			2838	1828	486	510	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 (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	C	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		

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

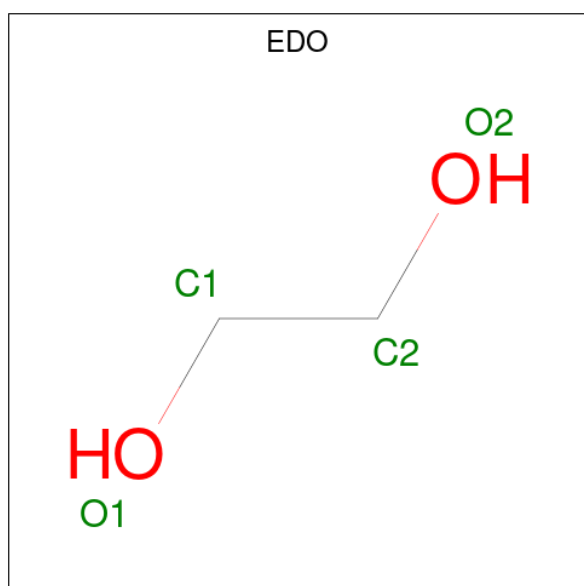
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

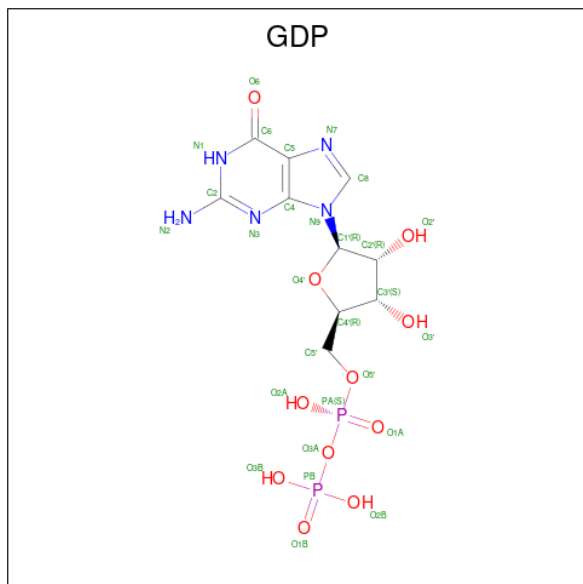
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total 1	Cl 1	0	0

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



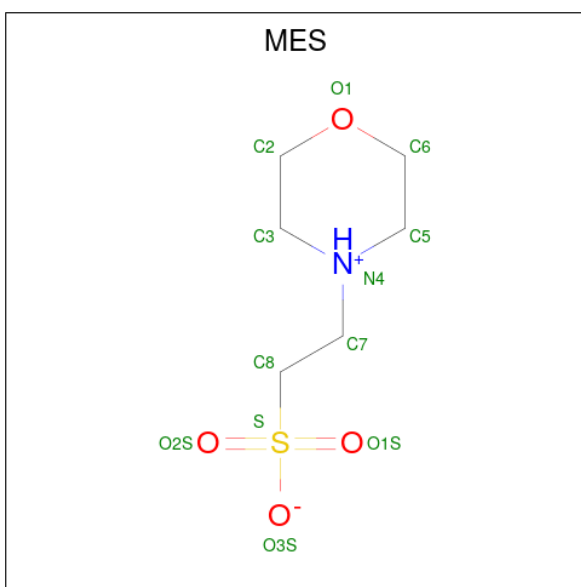
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		

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



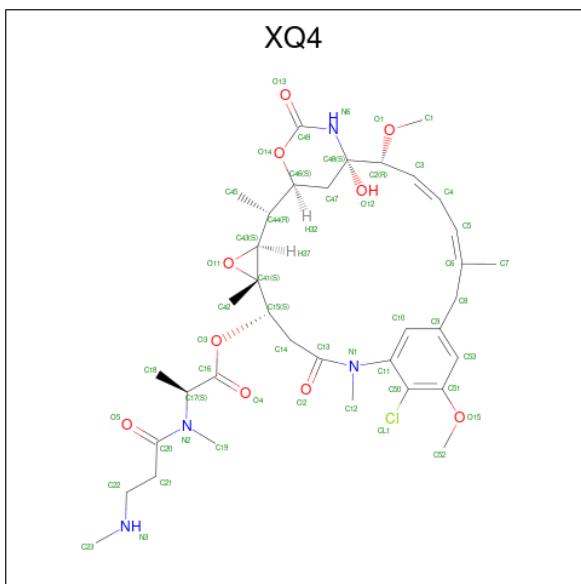
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
10	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



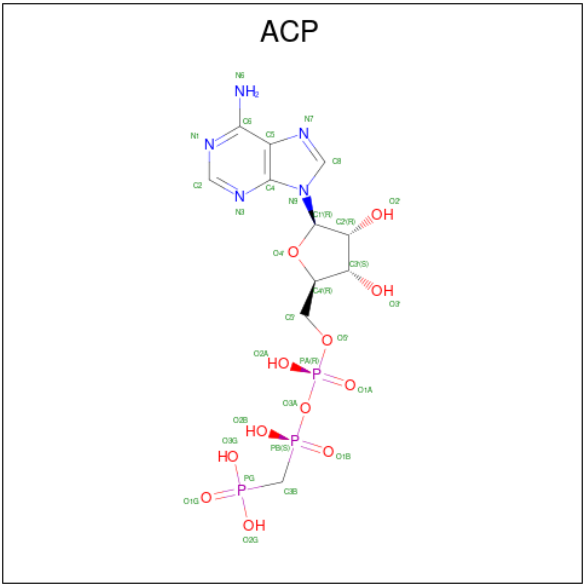
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 12 is (1S,2R,3S,5S,6S,16E,18E,20R,21S)-11-chloro-21-hydroxy-12,20-dimethoxy-2,5,9,16-tetramethyl-8,23-dioxo-4,24-dioxo-9,22-diazatetracyclo[19.3.1.1 10,14 .0 3,5]hexacos-10(26),11,13,16,18-pentaen-6-yl (2S)-2-{methyl[3-(methylamino)propanoyl]amino}propanoate (non-preferred name) (CCD ID: XQ4) (formula: C₃₆H₅₁ClN₄O₁₀).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	Cl	N	O	0	0
			51	36	1	4	10		

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

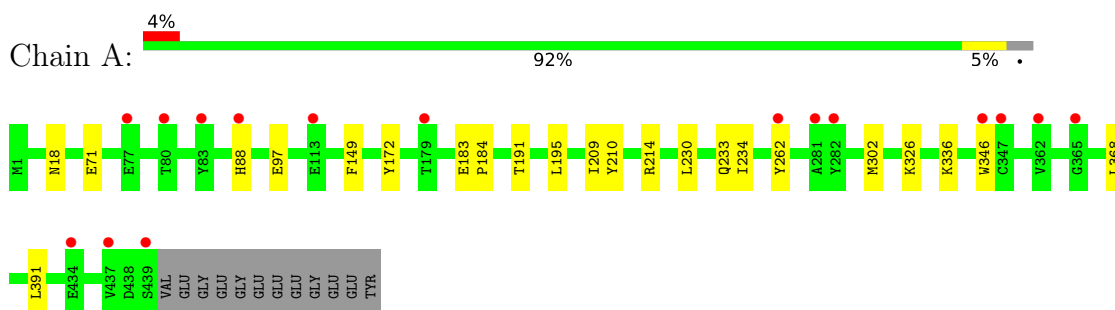
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	200	Total	O	0	0
			200	200		
14	B	176	Total	O	0	0
			176	176		
14	C	354	Total	O	0	0
			354	354		
14	D	100	Total	O	0	0
			100	100		
14	E	52	Total	O	0	0
			52	52		
14	F	75	Total	O	0	0
			75	75		

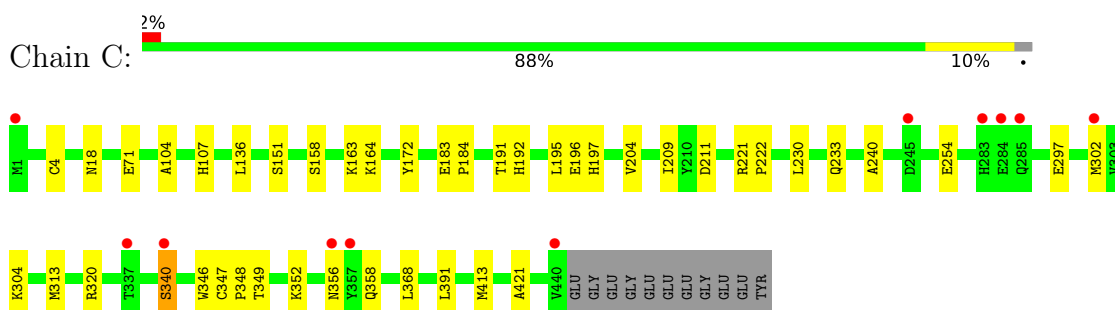
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

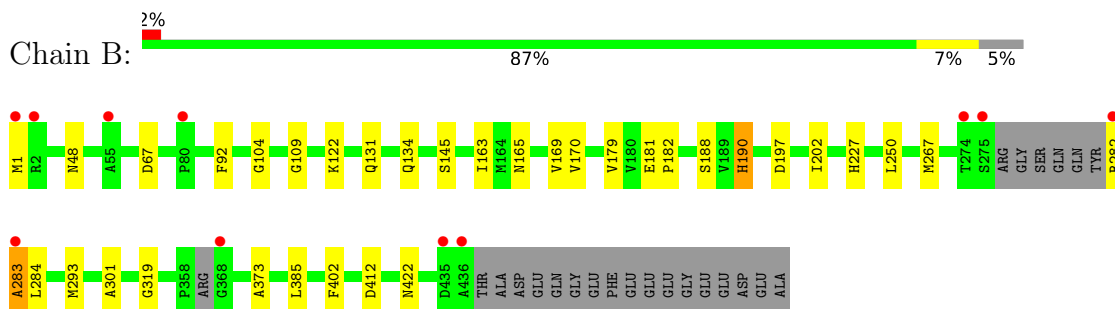
- Molecule 1: Tubulin alpha-1B chain



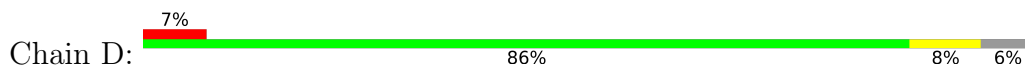
- Molecule 1: Tubulin alpha-1B chain

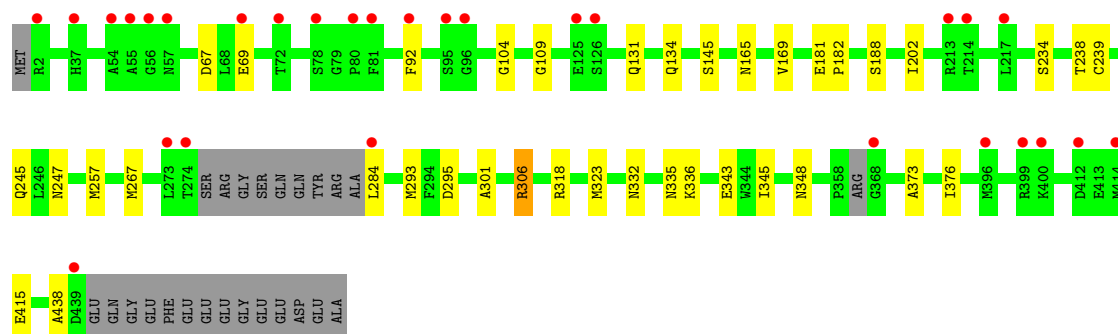


- Molecule 2: Tubulin beta chain

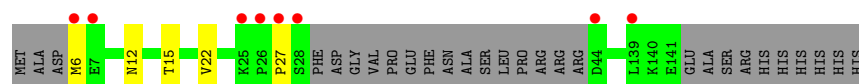
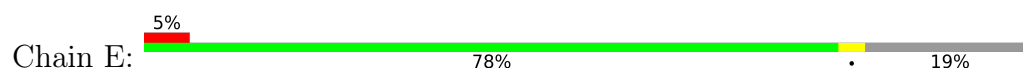


- Molecule 2: Tubulin beta chain

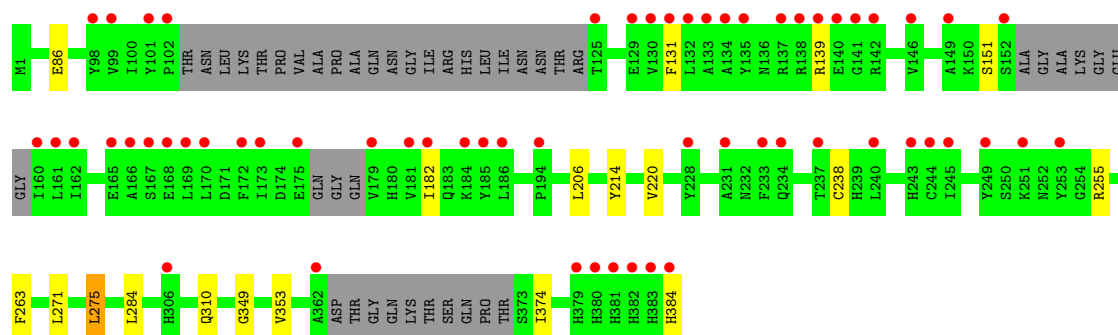
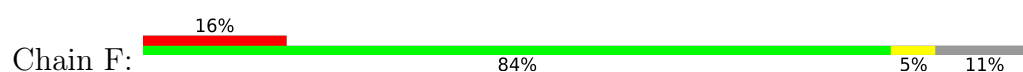




• Molecule 3: Stathmin-4



• Molecule 4: Tubulin Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.09Å 158.04Å 181.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.62 – 2.21 45.62 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.8 (45.62-2.21) 98.0 (45.62-2.21)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.186 , 0.217 0.190 , 0.217	Depositor DCC
R_{free} test set	7466 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18587	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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, XQ4, GTP, MES, EDO, CA, MG, CL, ACP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.00	0/3515	1.31	4/4772 (0.1%)
1	C	1.07	2/3573 (0.1%)	1.31	3/4853 (0.1%)
2	B	1.06	2/3412 (0.1%)	1.34	4/4622 (0.1%)
2	D	1.02	0/3398	1.34	3/4605 (0.1%)
3	E	1.06	0/1035	1.53	0/1373
4	F	1.03	0/2917	1.28	2/3941 (0.1%)
All	All	1.04	4/17850 (0.0%)	1.33	16/24166 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	190	HIS	CE1-NE2	6.90	1.39	1.32
1	C	340	SER	C-O	6.10	1.30	1.23
2	B	227	HIS	CE1-NE2	5.21	1.37	1.32
1	C	222	PRO	C-O	-5.21	1.17	1.23

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	HIS	CB-CA-C	8.25	121.38	109.26
2	B	131	GLN	CB-CA-C	-6.37	99.05	110.70
1	A	88	HIS	CA-CB-CG	6.24	120.04	113.80
2	B	319	GLY	CA-C-O	-6.10	117.92	122.37
1	A	18	ASN	CB-CA-C	-6.09	101.06	110.81

There are no chirality outliers.

There are no planarity outliers.

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	3434	0	3346	10	0
1	C	3471	0	3392	23	0
2	B	3325	0	3222	23	0
2	D	3309	0	3190	22	1
3	E	1017	0	1040	2	0
4	F	2838	0	2818	6	1
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	A	4	0	6	0	0
9	B	8	0	12	0	0
10	B	28	0	12	0	0
10	D	28	0	12	0	0
11	B	12	0	13	3	0
12	D	51	0	0	0	0
13	F	31	0	14	0	0
14	A	200	0	0	0	0
14	B	176	0	0	1	0
14	C	354	0	0	2	0
14	D	100	0	0	4	0
14	E	52	0	0	1	0
14	F	75	0	0	0	0
All	All	18587	0	17101	83	1

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 2.

The worst 5 of 83 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:HIS:CD2	2:B:422[A]:ASN:HD22	1.93	0.85
2:B:190:HIS:HD2	2:B:422[A]:ASN:HD22	1.23	0.81
1:A:209:ILE:HD11	1:A:302:MET:SD	2.26	0.74
2:B:170:VAL:HG11	2:B:385[A]:LEU:HD11	1.69	0.73
1:A:234:ILE:HD13	1:A:302:MET:SD	2.31	0.71

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:335:ASN:OD1	4:F:384:HIS:NE2[3_545]	2.08	0.12

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	438/451 (97%)	431 (98%)	7 (2%)	0	100	100
1	C	446/451 (99%)	435 (98%)	11 (2%)	0	100	100
2	B	420/445 (94%)	411 (98%)	8 (2%)	1 (0%)	43	50
2	D	419/445 (94%)	413 (99%)	6 (1%)	0	100	100
3	E	120/149 (80%)	119 (99%)	0	1 (1%)	16	15
4	F	336/384 (88%)	327 (97%)	9 (3%)	0	100	100
All	All	2179/2325 (94%)	2136 (98%)	41 (2%)	2 (0%)	48	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	283	ALA
3	E	27	PRO

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	371/379 (98%)	368 (99%)	3 (1%)	73	84
1	C	379/379 (100%)	374 (99%)	5 (1%)	61	75
2	B	367/381 (96%)	365 (100%)	2 (0%)	81	89
2	D	366/381 (96%)	362 (99%)	4 (1%)	65	78
3	E	112/133 (84%)	111 (99%)	1 (1%)	70	82
4	F	314/342 (92%)	304 (97%)	10 (3%)	34	45
All	All	1909/1995 (96%)	1884 (99%)	25 (1%)	65	75

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	15	THR
4	F	238	CYS
4	F	310	GLN
4	F	151	SER
4	F	255	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	14	ASN
2	D	165	ASN
2	D	134	GLN
2	D	329	GLN
1	C	107	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	$\# Z > 2$
9	EDO	A	506	-	3,3,3	0.12	0	2,2,2	0.06	0
9	EDO	B	505	-	3,3,3	0.40	0	2,2,2	0.72	0
10	GDP	B	501	6	29,30,30	1.46	5 (17%)	45,47,47	1.73	10 (22%)
12	XQ4	D	503	-	52,54,54	1.66	7 (13%)	59,80,80	2.37	19 (32%)
13	ACP	F	502	6	31,33,33	0.73	1 (3%)	47,52,52	0.70	0
9	EDO	B	504	-	3,3,3	0.14	0	2,2,2	0.22	0
5	GTP	C	501	6	33,34,34	0.67	1 (3%)	50,54,54	0.67	0
11	MES	B	506	-	12,12,12	0.84	0	15,16,16	1.42	3 (20%)
10	GDP	D	501	6	29,30,30	1.12	2 (6%)	45,47,47	1.67	7 (15%)
5	GTP	A	501	6	33,34,34	0.69	1 (3%)	50,54,54	0.66	1 (2%)

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
9	EDO	A	506	-	-	1/1/1/1	-
9	EDO	B	505	-	-	1/1/1/1	-
10	GDP	B	501	6	-	5/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	XQ4	D	503	-	-	14/62/88/88	0/2/4/4
13	ACP	F	502	6	-	7/19/38/38	0/3/3/3
9	EDO	B	504	-	-	1/1/1/1	-
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
11	MES	B	506	-	-	1/6/14/14	0/1/1/1
10	GDP	D	501	6	-	5/16/32/32	0/3/3/3
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	503	XQ4	O14-C49	6.81	1.45	1.35
12	D	503	XQ4	C41-C43	5.25	1.54	1.47
10	B	501	GDP	PA-O3A	4.73	1.64	1.59
12	D	503	XQ4	O3-C16	4.50	1.44	1.34
12	D	503	XQ4	O11-C41	-3.63	1.41	1.46

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	503	XQ4	O11-C43-C44	-9.04	106.57	117.41
12	D	503	XQ4	C41-O11-C43	7.46	65.04	60.81
10	D	501	GDP	C5-C4-N3	-5.33	119.91	128.39
12	D	503	XQ4	O11-C43-C41	-5.02	56.42	59.82
10	D	501	GDP	C2-N3-C4	4.68	120.35	112.30

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

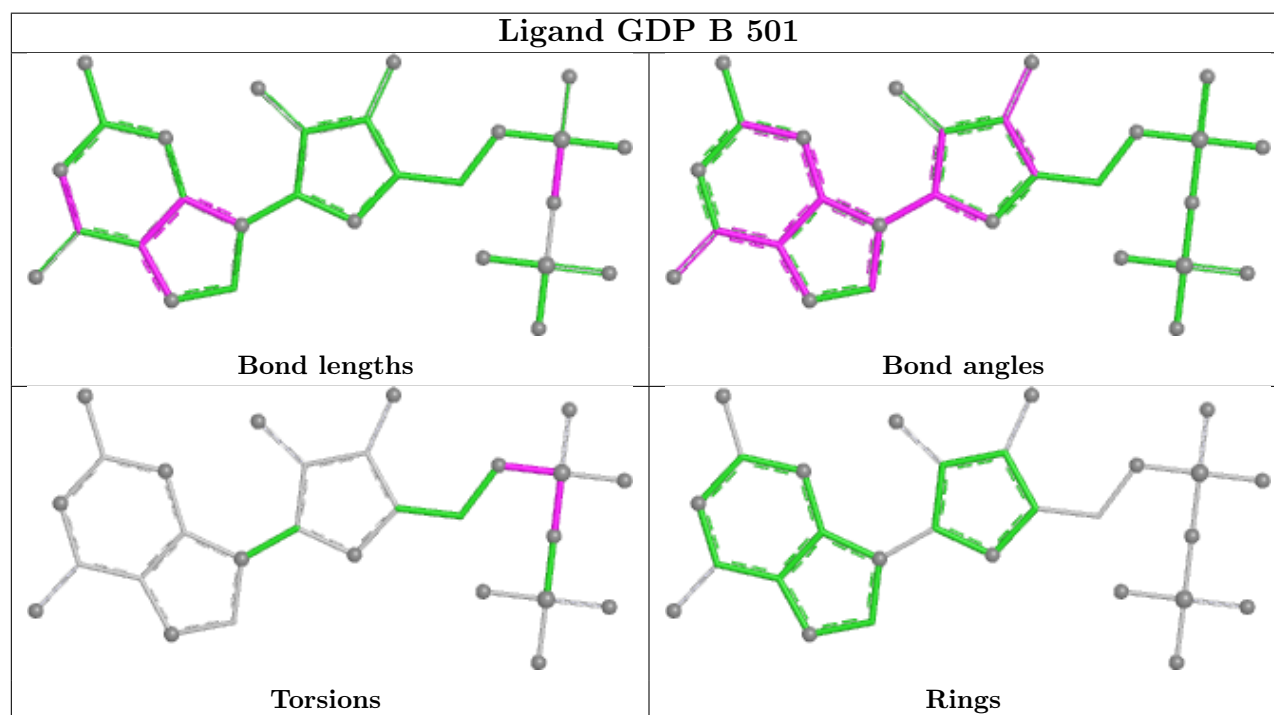
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

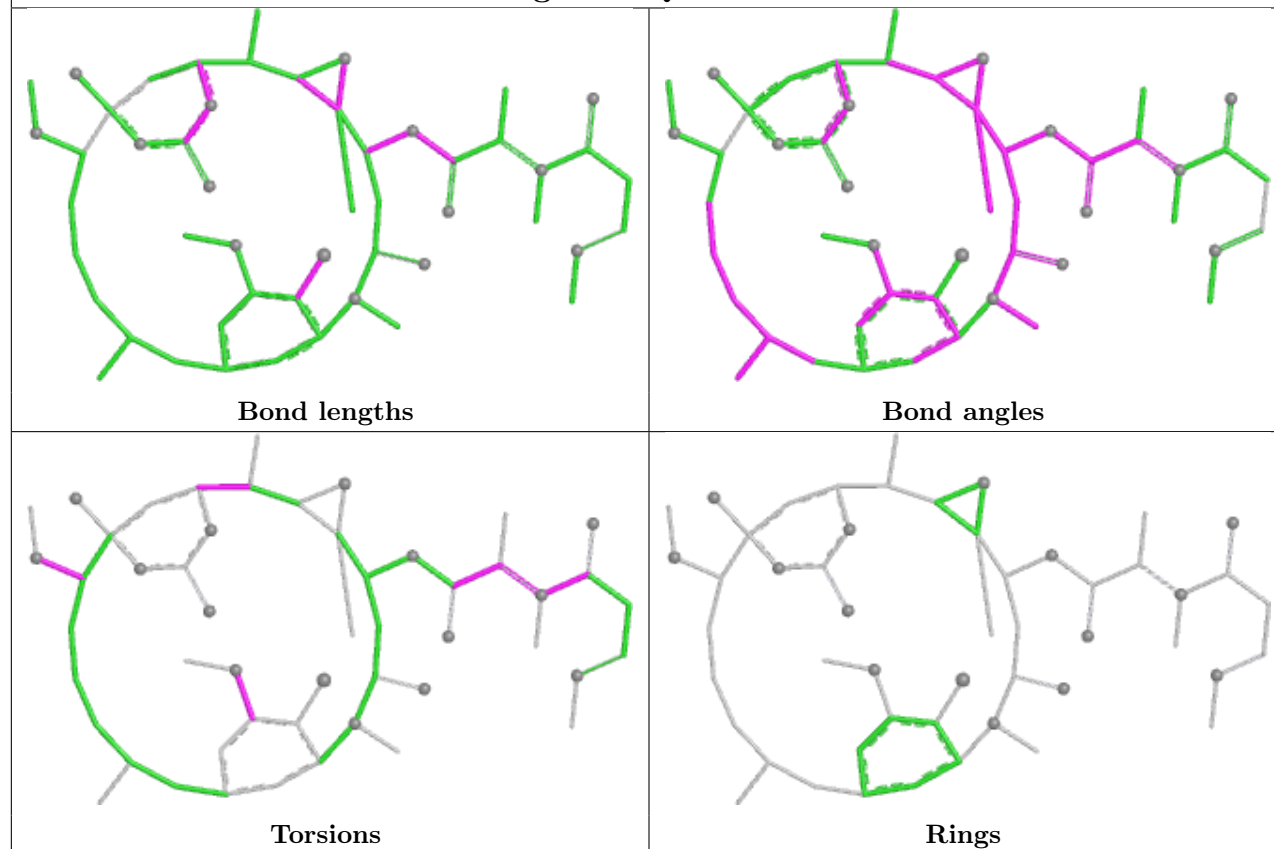
1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	506	MES	3	0

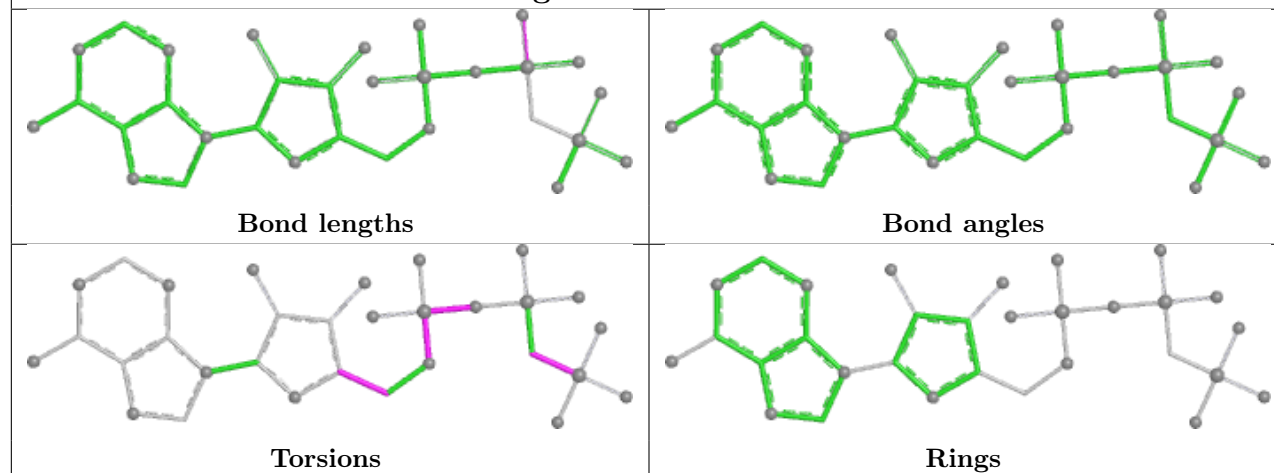
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

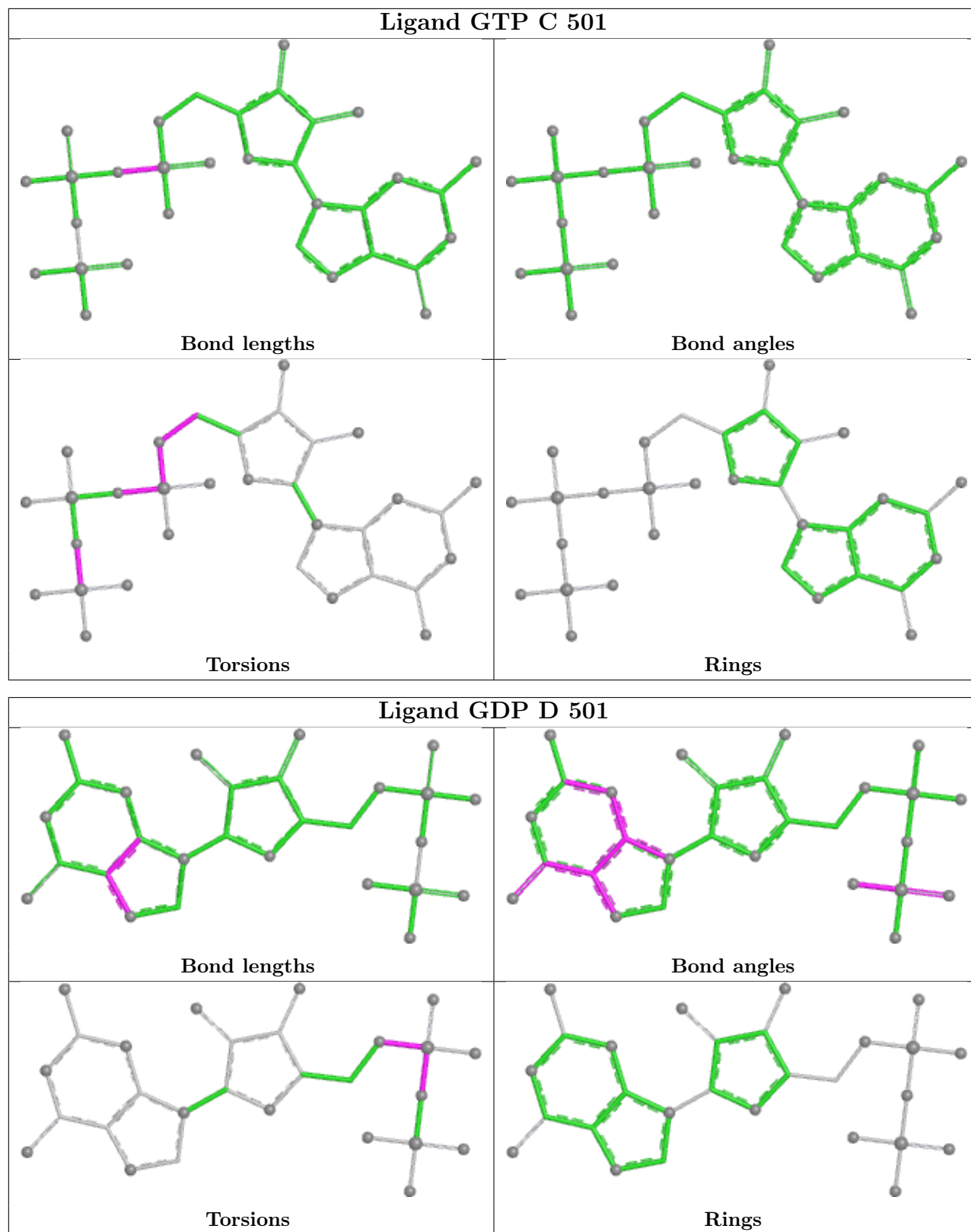


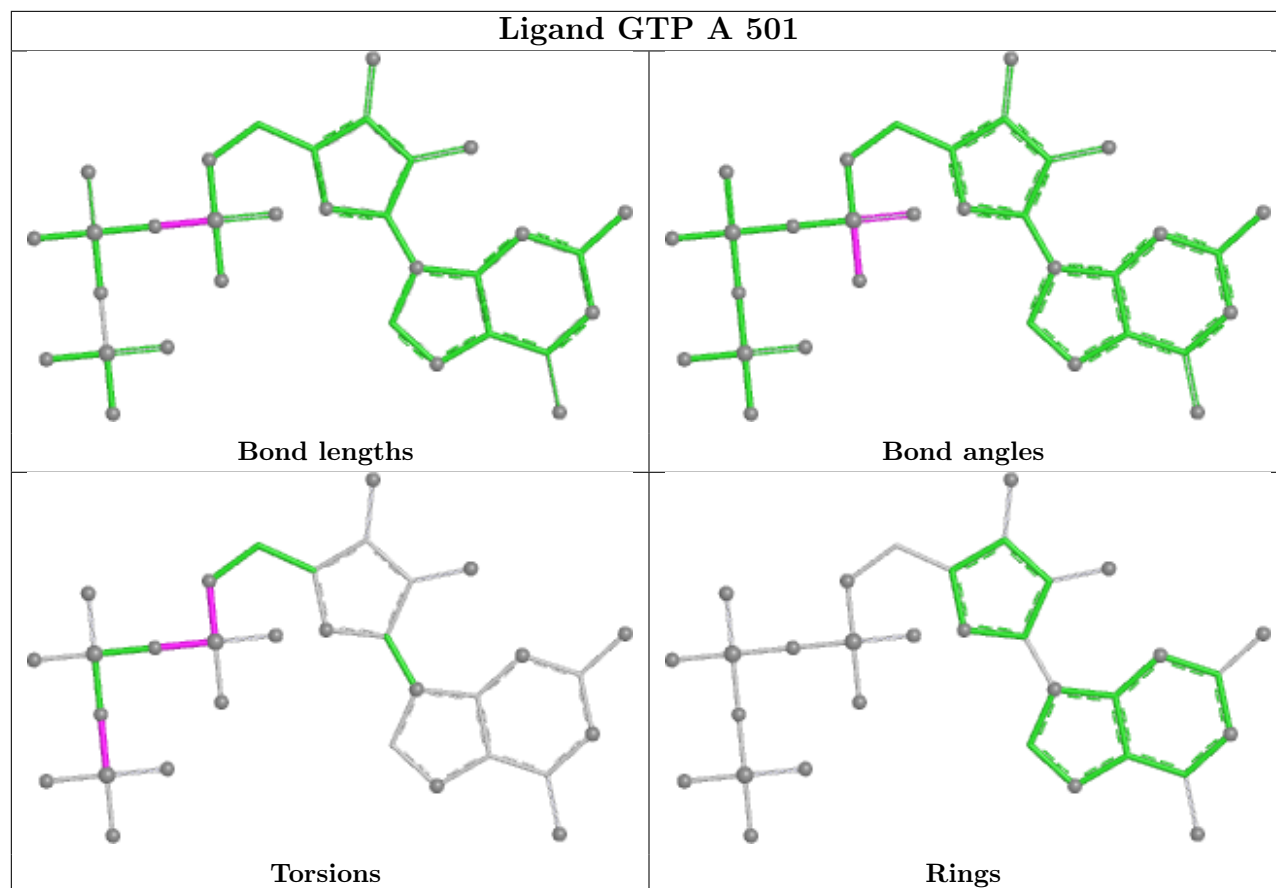
Ligand XQ4 D 503



Ligand ACP F 502







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	439/451 (97%)	0.08	16 (3%)	46	43	20, 35, 66, 95	1 (0%)
1	C	440/451 (97%)	-0.13	11 (2%)	58	56	12, 25, 46, 68	8 (1%)
2	B	421/445 (94%)	0.03	11 (2%)	57	55	15, 32, 59, 84	6 (1%)
2	D	420/445 (94%)	0.39	29 (6%)	23	20	20, 43, 74, 93	8 (1%)
3	E	121/149 (81%)	0.51	8 (6%)	24	21	19, 45, 86, 101	3 (2%)
4	F	342/384 (89%)	0.87	60 (17%)	4	3	26, 55, 122, 135	4 (1%)
All	All	2183/2325 (93%)	0.24	135 (6%)	26	23	12, 37, 81, 135	30 (1%)

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	MET	6.6
4	F	382	HIS	5.9
4	F	179	VAL	5.7
4	F	384	HIS	5.4
4	F	130	VAL	5.2

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 ⓘ

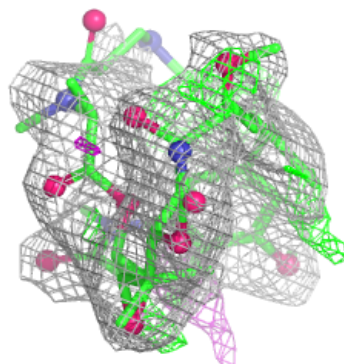
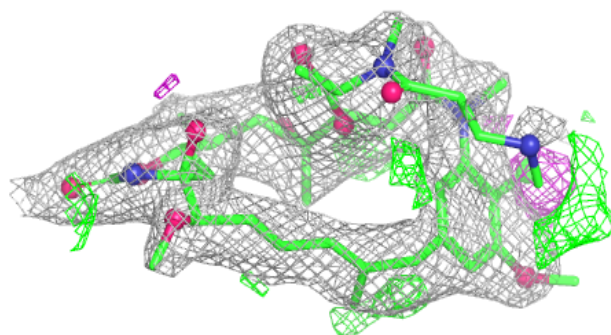
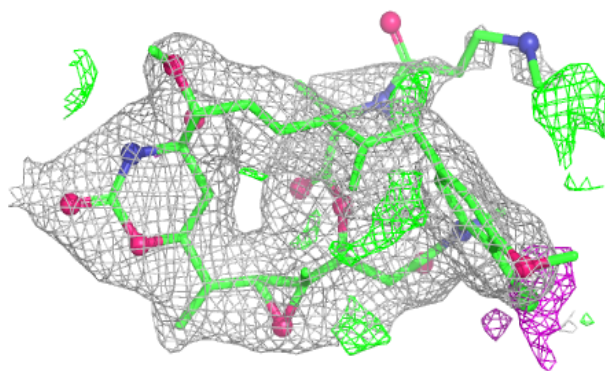
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	EDO	A	506	4/4	0.62	0.28	57,59,59,60	0
12	XQ4	D	503	51/51	0.80	0.19	52,66,102,112	0
13	ACP	F	502	31/31	0.80	0.14	49,69,87,94	0
7	CA	A	505	1/1	0.83	0.12	69,69,69,69	0
9	EDO	B	504	4/4	0.86	0.18	46,47,48,48	0
9	EDO	B	505	4/4	0.87	0.14	39,40,40,40	0
8	CL	A	504	1/1	0.90	0.10	57,57,57,57	0
6	MG	F	501	1/1	0.91	0.13	62,62,62,62	0
7	CA	B	503	1/1	0.91	0.12	61,61,61,61	0
6	MG	D	502	1/1	0.94	0.07	47,47,47,47	0
7	CA	A	503	1/1	0.94	0.07	44,44,44,44	0
10	GDP	D	501	28/28	0.95	0.08	32,37,41,45	0
11	MES	B	506	12/12	0.95	0.09	32,34,37,41	0
7	CA	C	503	1/1	0.98	0.07	28,28,28,28	0
6	MG	C	502	1/1	0.98	0.06	17,17,17,17	0
6	MG	A	502	1/1	0.98	0.04	21,21,21,21	0
6	MG	B	502	1/1	0.99	0.02	13,13,13,13	0
5	GTP	C	501	32/32	0.99	0.04	13,14,16,18	0
5	GTP	A	501	32/32	0.99	0.04	17,19,20,22	0
10	GDP	B	501	28/28	0.99	0.04	13,17,19,21	0

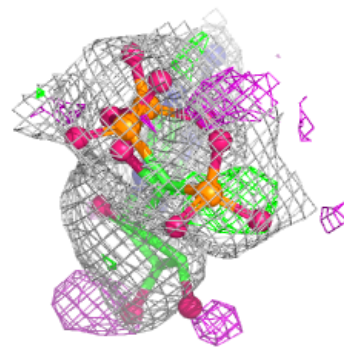
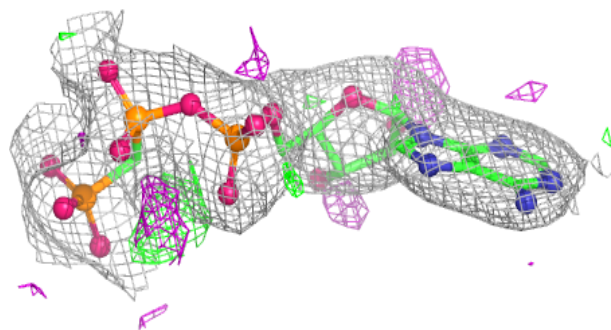
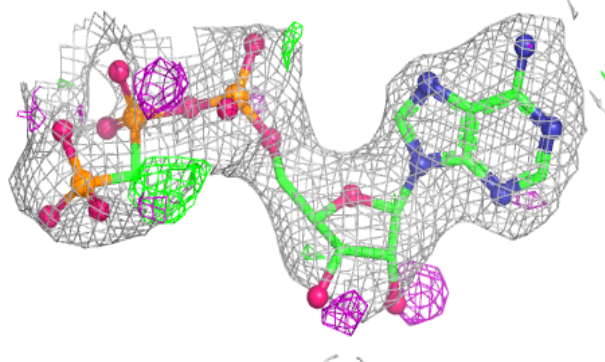
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around XQ4 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)

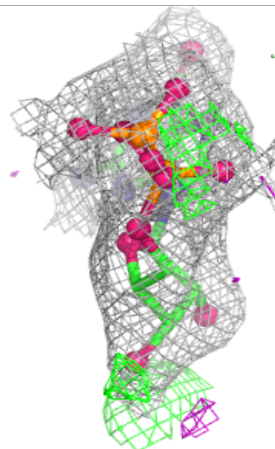
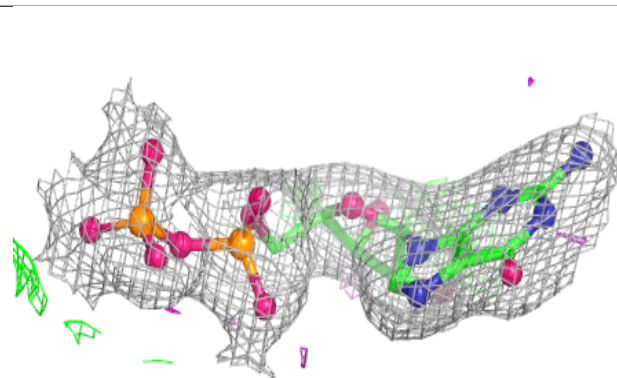
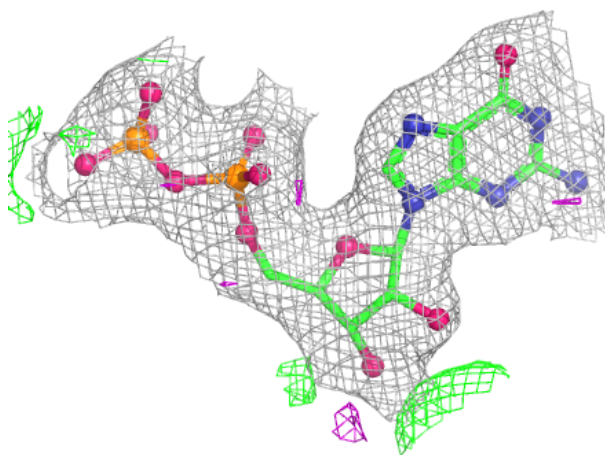
**Electron density around ACP F 502:**

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



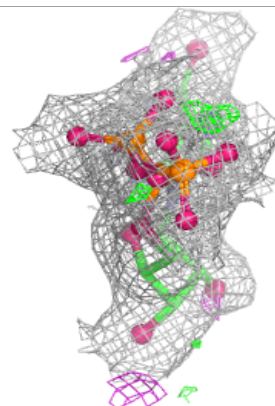
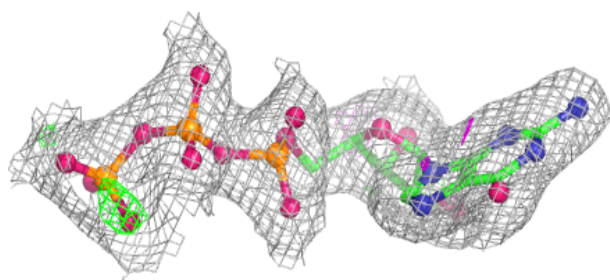
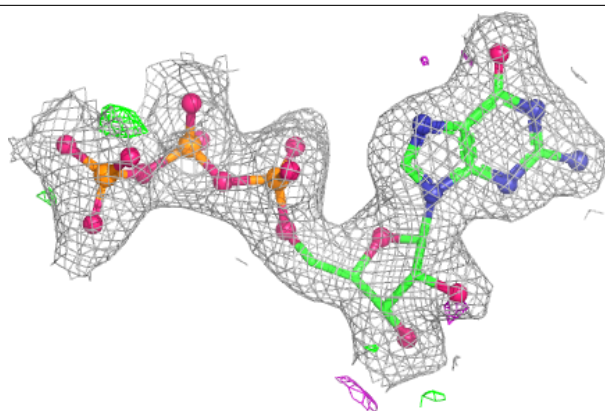
Electron density around GDP D 501:

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

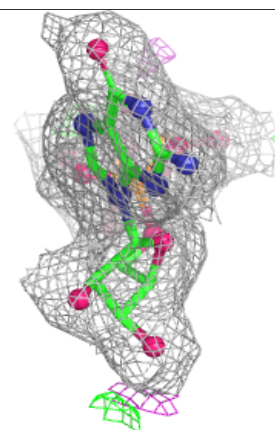
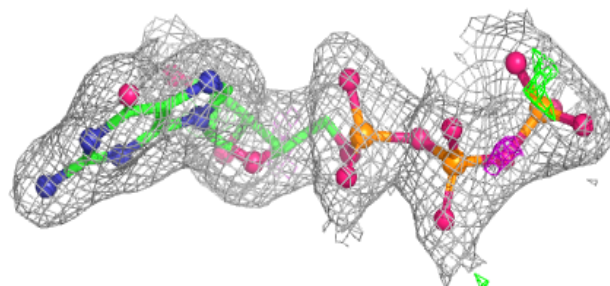
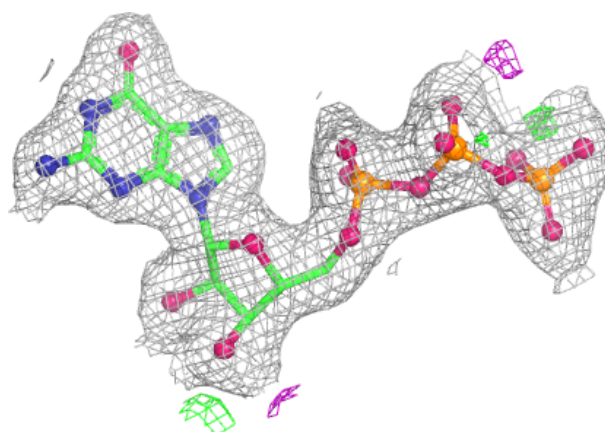


Electron density around GTP C 501:

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

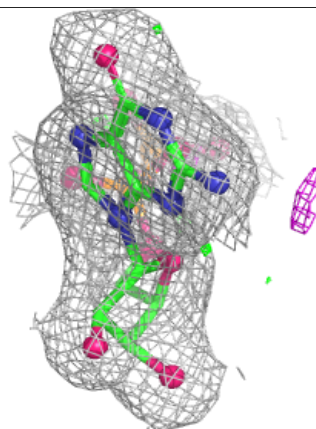
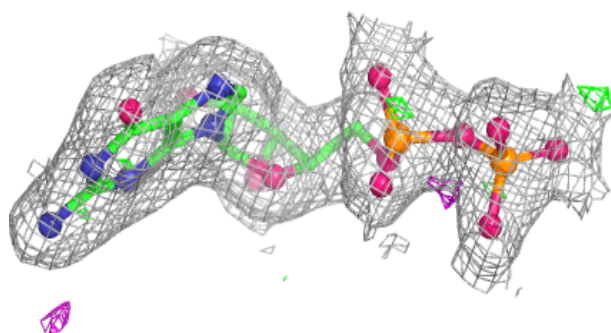
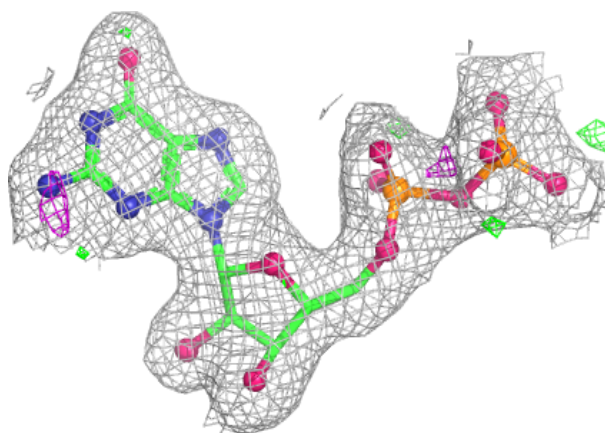
**Electron density around GTP A 501:**

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



Electron density around GDP B 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.