



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2022 – 12:12 PM JST

PDB ID : 7CNO
Title : Phomopsin A in complex with tubulin
Authors : Wu, C.Y.; Wang, Y.X.
Deposited on : 2020-08-02
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
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) : 2.27

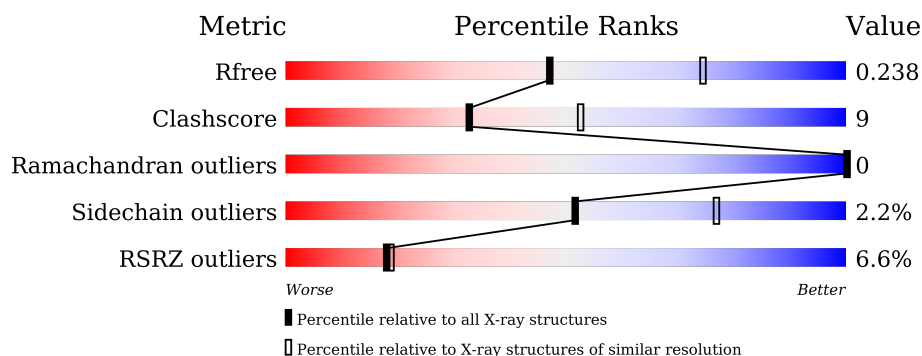
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 13%; height: 10px; background-color: yellow;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div>
1	C	451	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 84%; height: 10px; background-color: green;"></div> <div style="width: 13%; height: 10px; background-color: yellow;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div>
2	B	445	<div> <div style="width: 2%; height: 10px; background-color: red;"></div> <div style="width: 83%; height: 10px; background-color: green;"></div> <div style="width: 13%; height: 10px; background-color: yellow;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div>
2	D	445	<div> <div style="width: 10%; height: 10px; background-color: red;"></div> <div style="width: 66%; height: 10px; background-color: green;"></div> <div style="width: 28%; height: 10px; background-color: yellow;"></div> <div style="width: 5%; height: 10px; background-color: grey;"></div> </div>
3	E	143	<div> <div style="width: 10%; height: 10px; background-color: red;"></div> <div style="width: 69%; height: 10px; background-color: green;"></div> <div style="width: 14%; height: 10px; background-color: yellow;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div>
4	G	384	<div> <div style="width: 18%; height: 10px; background-color: red;"></div> <div style="width: 66%; height: 10px; background-color: green;"></div> <div style="width: 21%; height: 10px; background-color: yellow;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MES	B	504	-	-	X	-
9	GDP	D	501	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18166 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	437	Total	C	N	O	S	0	5	0
			3439	2178	584	653	24			
1	C	440	Total	C	N	O	S	0	8	0
			3463	2193	584	662	24			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	4	0
			3383	2127	577	652	27			
2	D	422	Total	C	N	O	S	0	5	0
			3325	2090	563	645	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	4	0
			1027	634	185	202	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

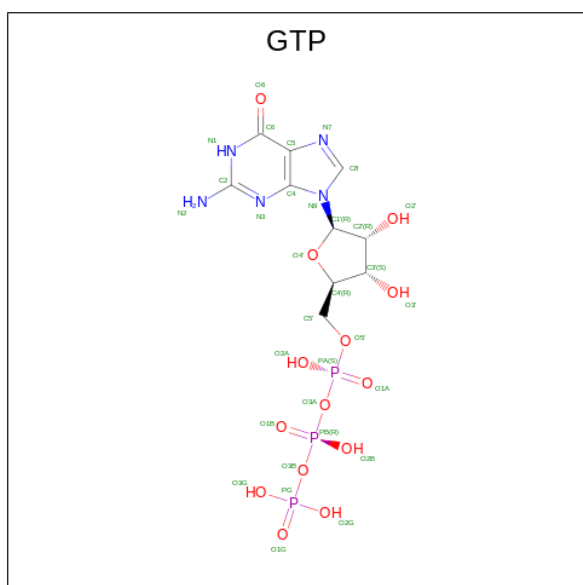
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	338	Total	C	N	O	S	0	0	0
			2757	1770	469	504	14			

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	2	Total	Mg	0	0
			2	2		
6	C	1	Total	Mg	0	0
			1	1		

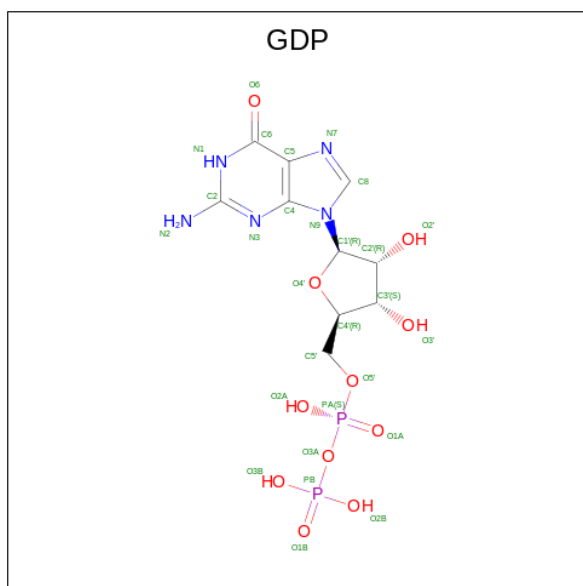
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

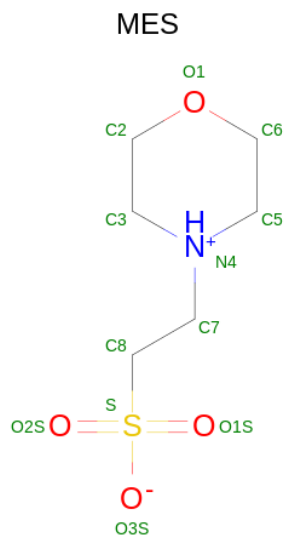
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



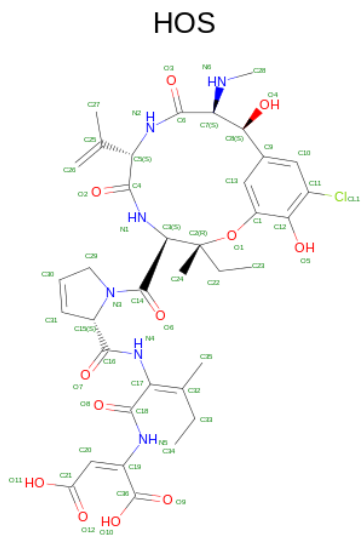
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C N O P 28 10 5 11 2	0	0
9	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



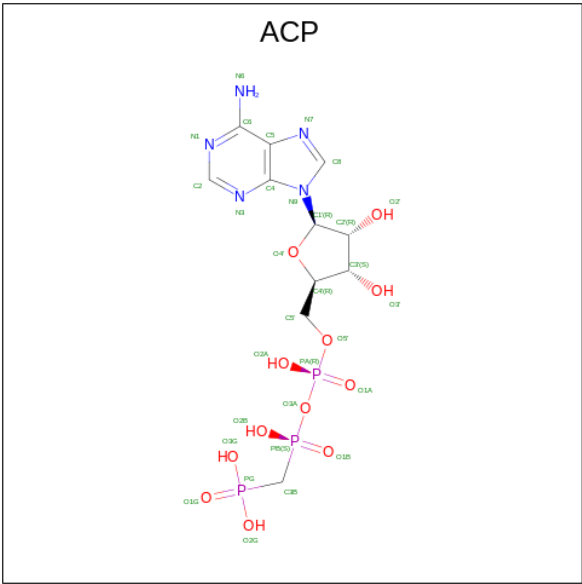
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total 12	C 6	N 1	O 4	S 1	0	0
10	B	1	Total 12	C 6	N 1	O 4	S 1	0	0

- Molecule 11 is Phomopsin A (three-letter code: HOS) (formula: $\text{C}_{36}\text{H}_{45}\text{ClN}_6\text{O}_{12}$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total 55	C 36	Cl 1	N 6	O 12	0	0
11	D	1	Total 55	C 36	Cl 1	N 6	O 12	0	0

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

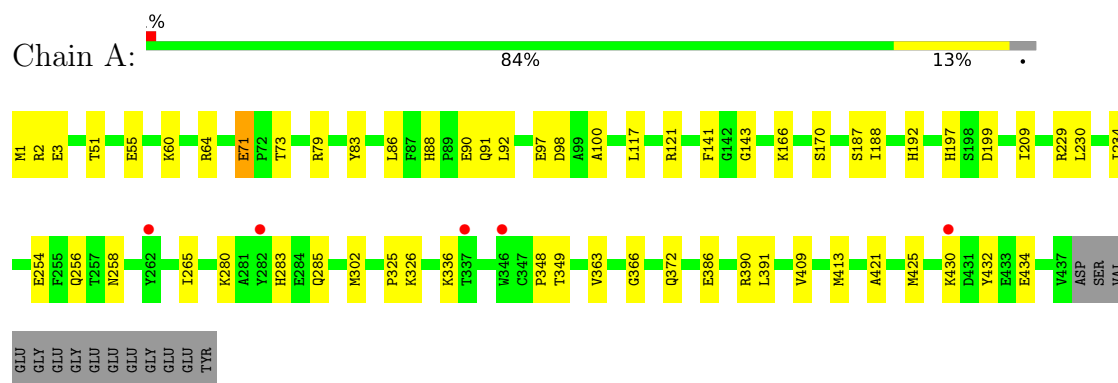
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	110	Total	O	0	0
			110	110		
13	B	132	Total	O	0	0
			132	132		
13	C	144	Total	O	0	0
			144	144		
13	D	32	Total	O	0	0
			32	32		
13	E	19	Total	O	0	0
			19	19		
13	G	41	Total	O	0	0
			41	41		

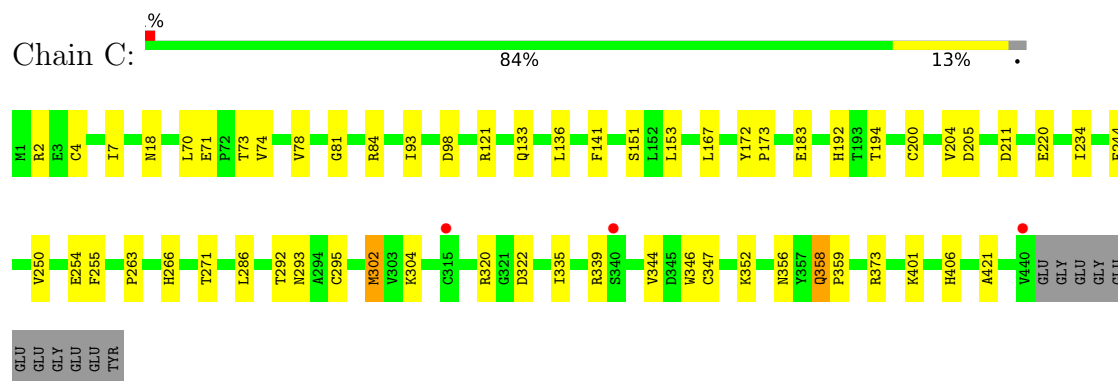
3 Residue-property plots [i](#)

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.

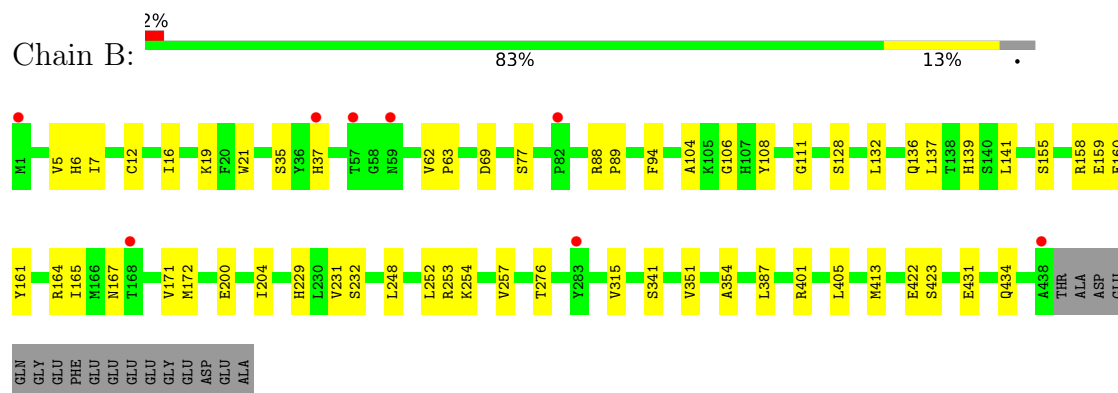
- Molecule 1: Tubulin alpha-1B chain



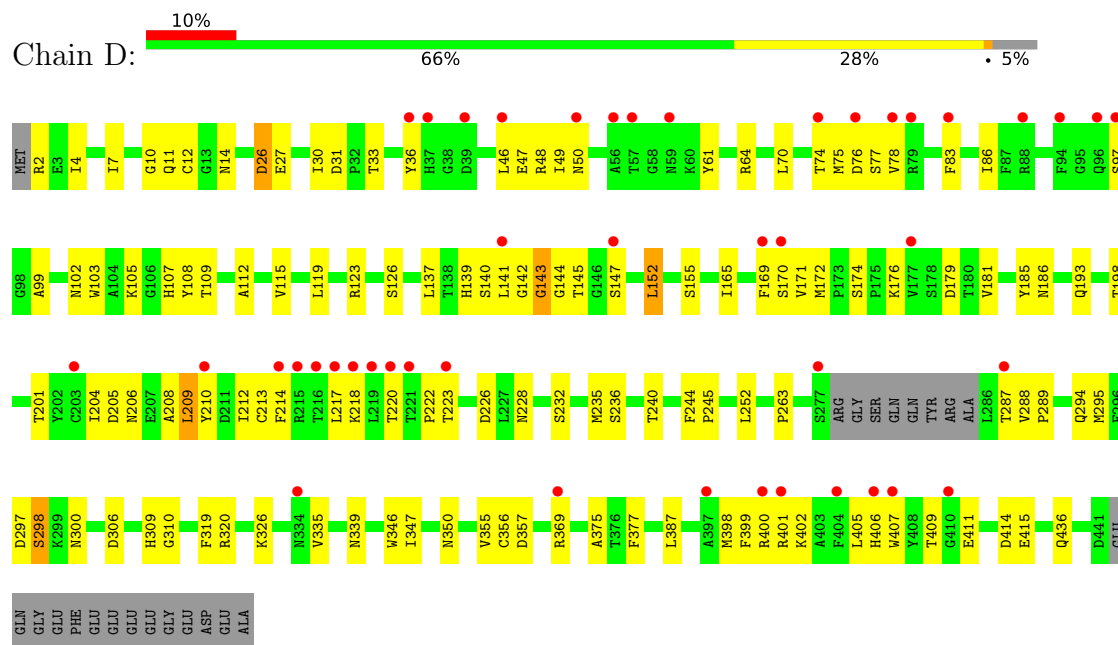
- Molecule 1: Tubulin alpha-1B chain



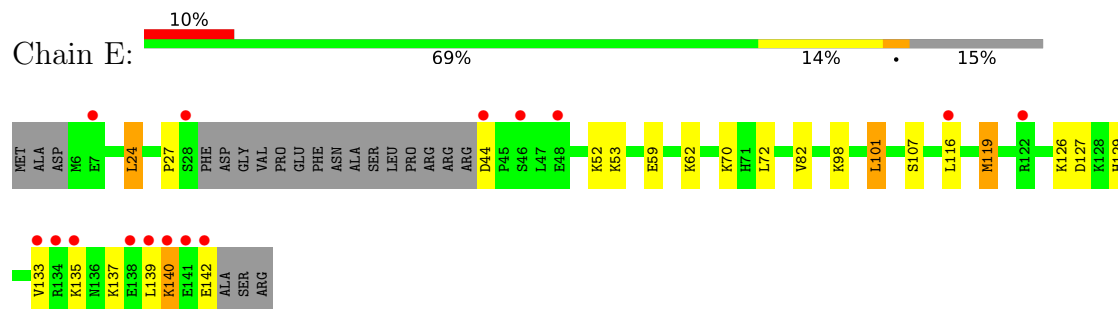
- Molecule 2: Tubulin beta chain



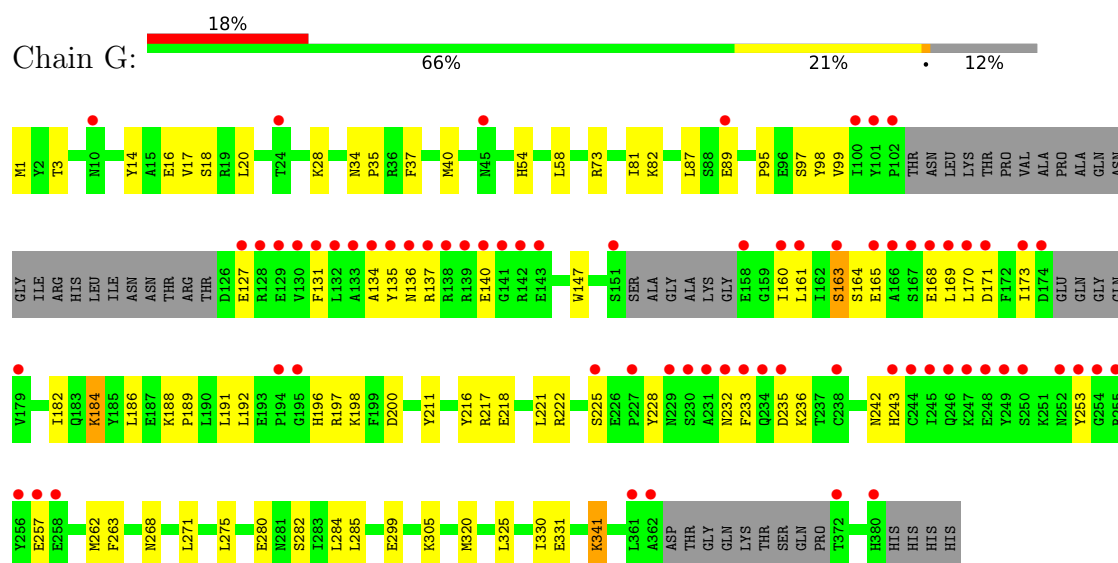
- Molecule 2: Tubulin beta chain



- 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	105.28Å 155.22Å 184.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.70 – 2.50 30.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.7 (30.70-2.50) 95.7 (30.70-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.187 , 0.239 0.188 , 0.238	Depositor DCC
R_{free} test set	5039 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.3	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	0.94	EDS
Total number of atoms	18166	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: HOS, CA, MG, GDP, GTP, MES, 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	0.44	0/3532	0.58	0/4794
1	C	0.47	0/3562	0.63	0/4835
2	B	0.44	0/3467	0.58	0/4696
2	D	0.40	0/3412	0.62	2/4623 (0.0%)
3	E	0.42	0/1048	0.55	0/1392
4	G	0.40	0/2819	0.56	0/3810
All	All	0.43	0/17840	0.59	2/24150 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	209	LEU	CA-CB-CG	8.56	135.00	115.30
2	D	143	GLY	C-N-CA	-5.42	110.92	122.30

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	3439	0	3365	43	0
1	C	3463	0	3381	43	0
2	B	3383	0	3264	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3325	0	3200	105	0
3	E	1027	0	1041	19	0
4	G	2757	0	2708	59	0
5	A	32	0	12	1	0
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	0	12	1	0
9	D	28	0	12	9	0
10	B	24	0	25	7	0
11	B	55	0	43	0	0
11	D	55	0	42	12	0
12	G	31	0	14	6	0
13	A	110	0	0	4	0
13	B	132	0	0	0	0
13	C	144	0	0	3	0
13	D	32	0	0	1	0
13	E	19	0	0	2	0
13	G	41	0	0	2	0
All	All	18166	0	17131	303	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 9.

The worst 5 of 303 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:158:ARG:NE	10:B:504:MES:H62	1.69	1.07
2:D:11:GLN:HB3	9:D:501:GDP:O2A	1.62	0.99
11:D:502:HOS:H28B	11:D:502:HOS:HN2	1.26	0.98
2:B:158:ARG:HE	10:B:504:MES:H62	1.35	0.89
4:G:40:MET:SD	13:G:538:HOH:O	2.31	0.88

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	440/451 (98%)	428 (97%)	12 (3%)	0	100	100
1	C	445/451 (99%)	434 (98%)	11 (2%)	0	100	100
2	B	430/445 (97%)	412 (96%)	18 (4%)	0	100	100
2	D	422/445 (95%)	403 (96%)	19 (4%)	0	100	100
3	E	122/143 (85%)	121 (99%)	1 (1%)	0	100	100
4	G	328/384 (85%)	314 (96%)	14 (4%)	0	100	100
All	All	2187/2319 (94%)	2112 (97%)	75 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	373/379 (98%)	372 (100%)	1 (0%)	92	97
1	C	377/379 (100%)	372 (99%)	5 (1%)	69	87
2	B	371/383 (97%)	364 (98%)	7 (2%)	57	80
2	D	367/383 (96%)	358 (98%)	9 (2%)	47	73
3	E	113/127 (89%)	103 (91%)	10 (9%)	10	19
4	G	301/342 (88%)	290 (96%)	11 (4%)	34	60
All	All	1902/1993 (95%)	1859 (98%)	43 (2%)	52	76

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	127	ASP
4	G	163	SER
3	E	135	LYS
4	G	18	SER
4	G	217	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	15	GLN
2	D	193	GLN
4	G	380	HIS
2	D	309	HIS
4	G	234	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	HOS	B	507	-	45,57,57	3.11	21 (46%)	43,83,83	1.66	9 (20%)
9	GDP	B	501	6	24,30,30	1.11	1 (4%)	31,47,47	1.88	6 (19%)
9	GDP	D	501	-	24,30,30	2.02	8 (33%)	31,47,47	2.24	12 (38%)
5	GTP	A	501	6	26,34,34	1.07	1 (3%)	33,54,54	1.71	6 (18%)
5	GTP	C	501	6	26,34,34	1.06	1 (3%)	33,54,54	1.85	8 (24%)
12	ACP	G	401	-	27,33,33	1.37	4 (14%)	32,52,52	1.68	5 (15%)
10	MES	B	504	-	12,12,12	0.55	0	14,16,16	1.85	2 (14%)
10	MES	B	505	-	12,12,12	2.11	1 (8%)	14,16,16	2.53	5 (35%)
11	HOS	D	502	-	45,57,57	1.76	11 (24%)	43,83,83	3.06	10 (23%)

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
11	HOS	B	507	-	-	9/76/92/92	0/2/3/3
9	GDP	B	501	6	-	4/12/32/32	0/3/3/3
9	GDP	D	501	-	-	4/12/32/32	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
12	ACP	G	401	-	-	5/15/38/38	0/3/3/3
10	MES	B	504	-	-	3/6/14/14	0/1/1/1
10	MES	B	505	-	-	1/6/14/14	0/1/1/1
11	HOS	D	502	-	-	20/76/92/92	0/2/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	507	HOS	C16-N4	8.23	1.51	1.36
10	B	505	MES	C8-S	-6.94	1.67	1.77
11	B	507	HOS	C17-C18	6.43	1.58	1.47
11	B	507	HOS	C14-N3	5.78	1.47	1.34
11	B	507	HOS	C18-N5	5.70	1.48	1.37

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	502	HOS	C17-C18-N5	11.07	132.97	115.81
11	D	502	HOS	C31-C15-C16	-9.38	95.35	110.11
11	D	502	HOS	O8-C18-C17	-9.15	108.66	120.91
11	B	507	HOS	C14-C3-N1	-5.97	100.83	107.34
5	C	501	GTP	N3-C2-N1	-5.66	119.67	127.22

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A

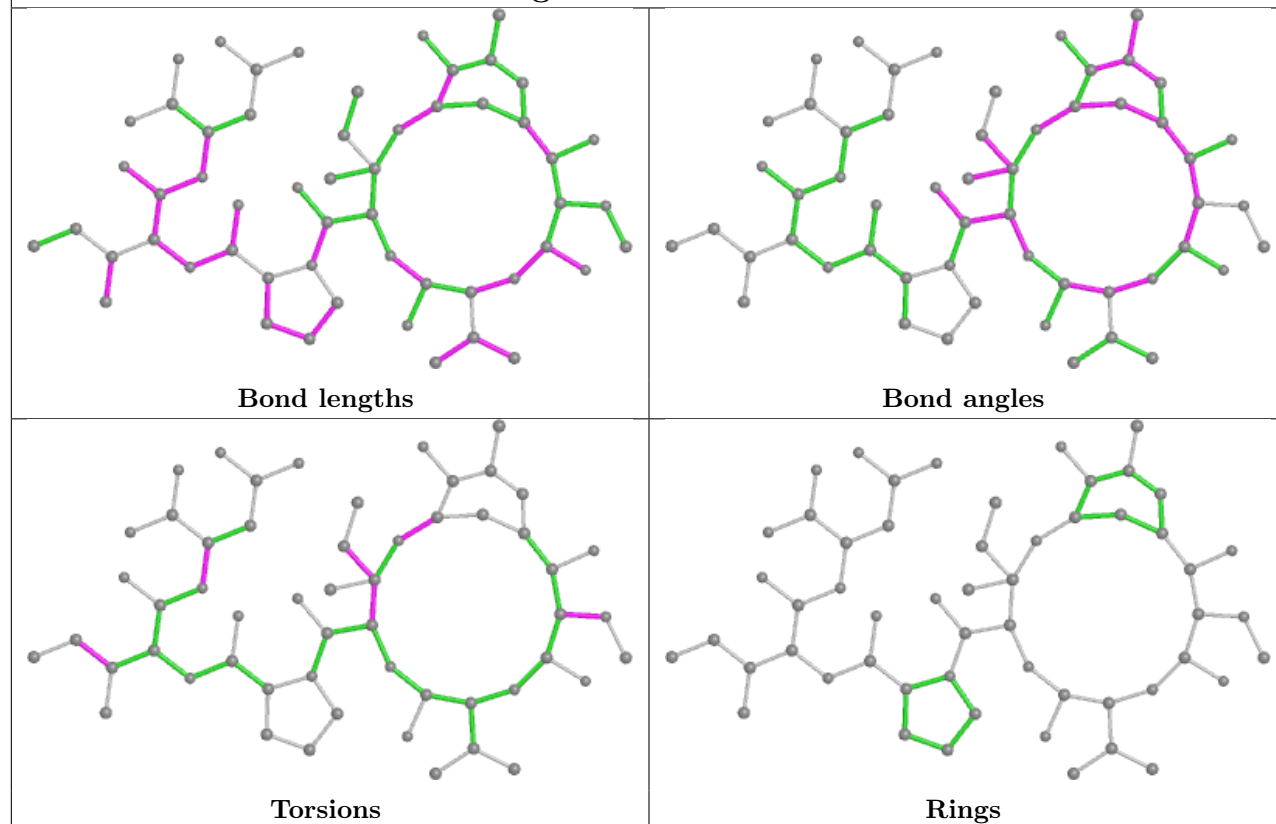
There are no ring outliers.

7 monomers are involved in 37 short contacts:

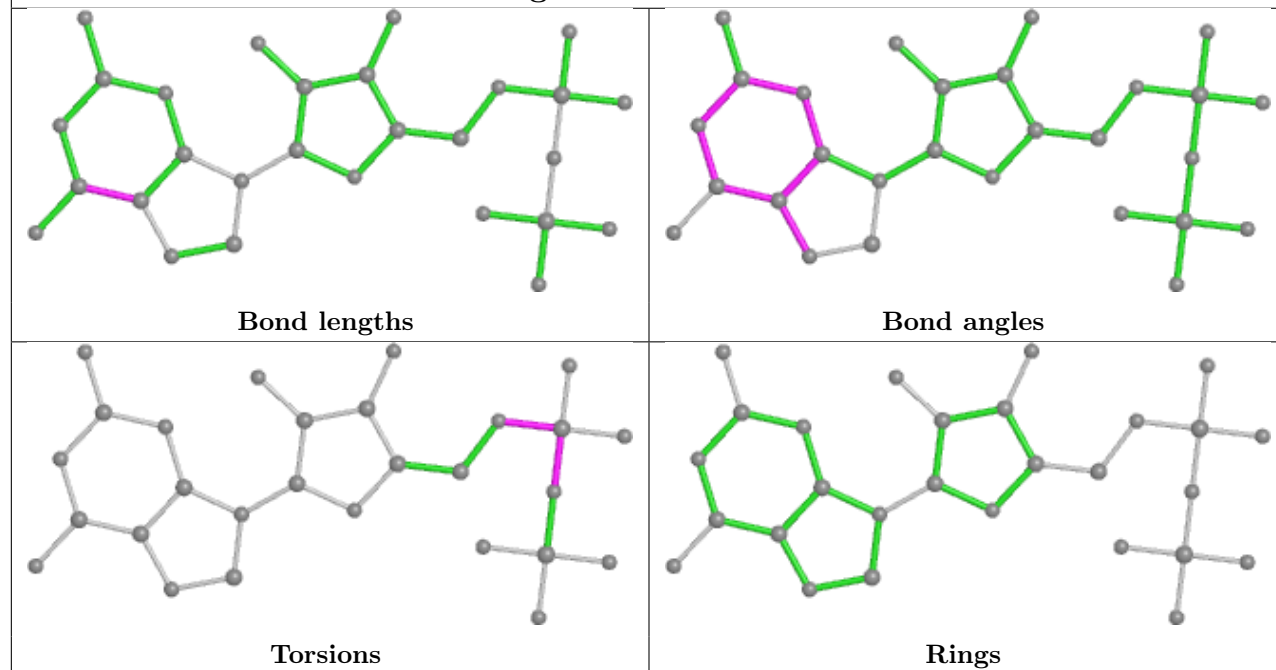
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	501	GDP	1	0
9	D	501	GDP	9	0
5	A	501	GTP	1	0
5	C	501	GTP	1	0
12	G	401	ACP	6	0
10	B	504	MES	7	0
11	D	502	HOS	12	0

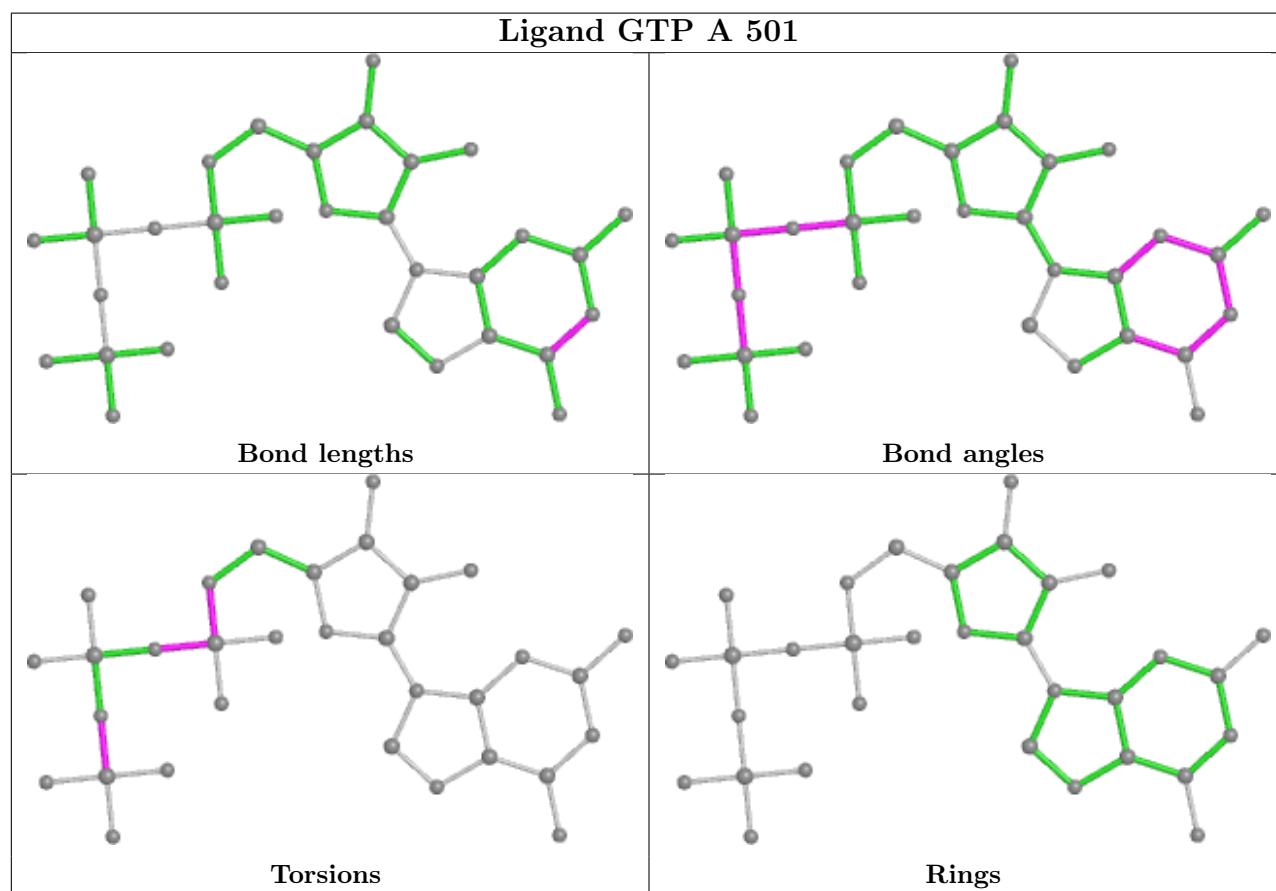
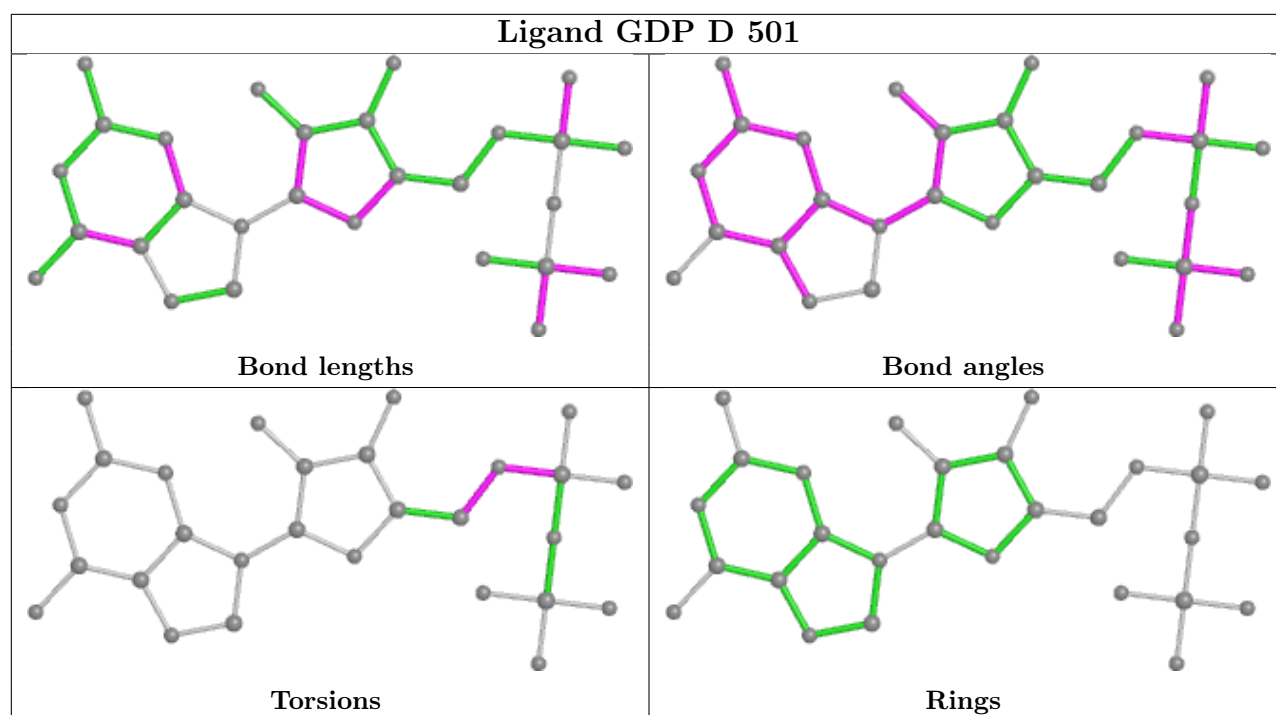
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

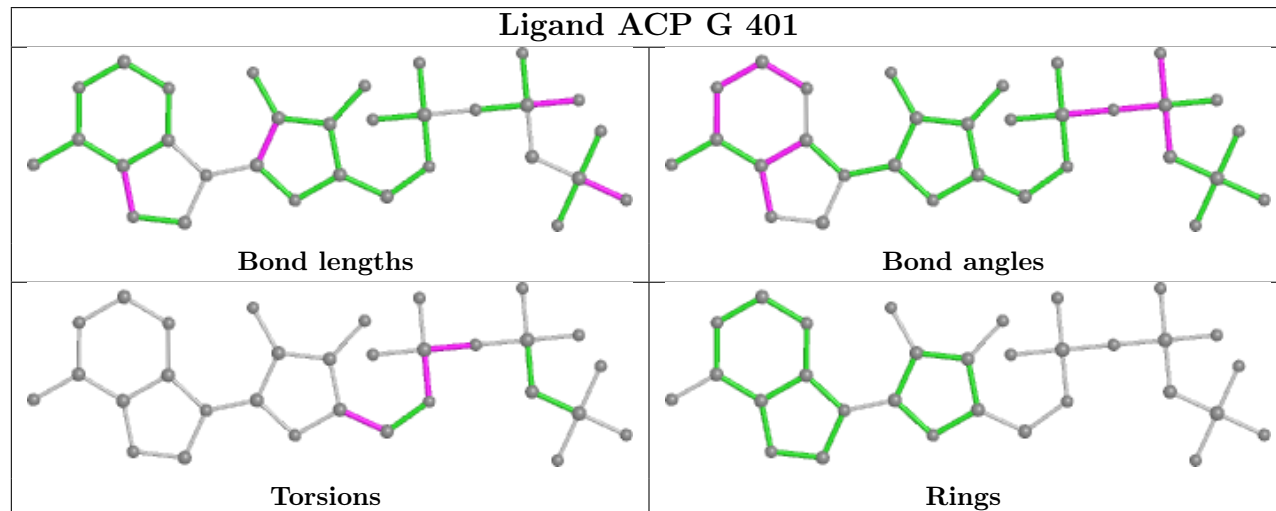
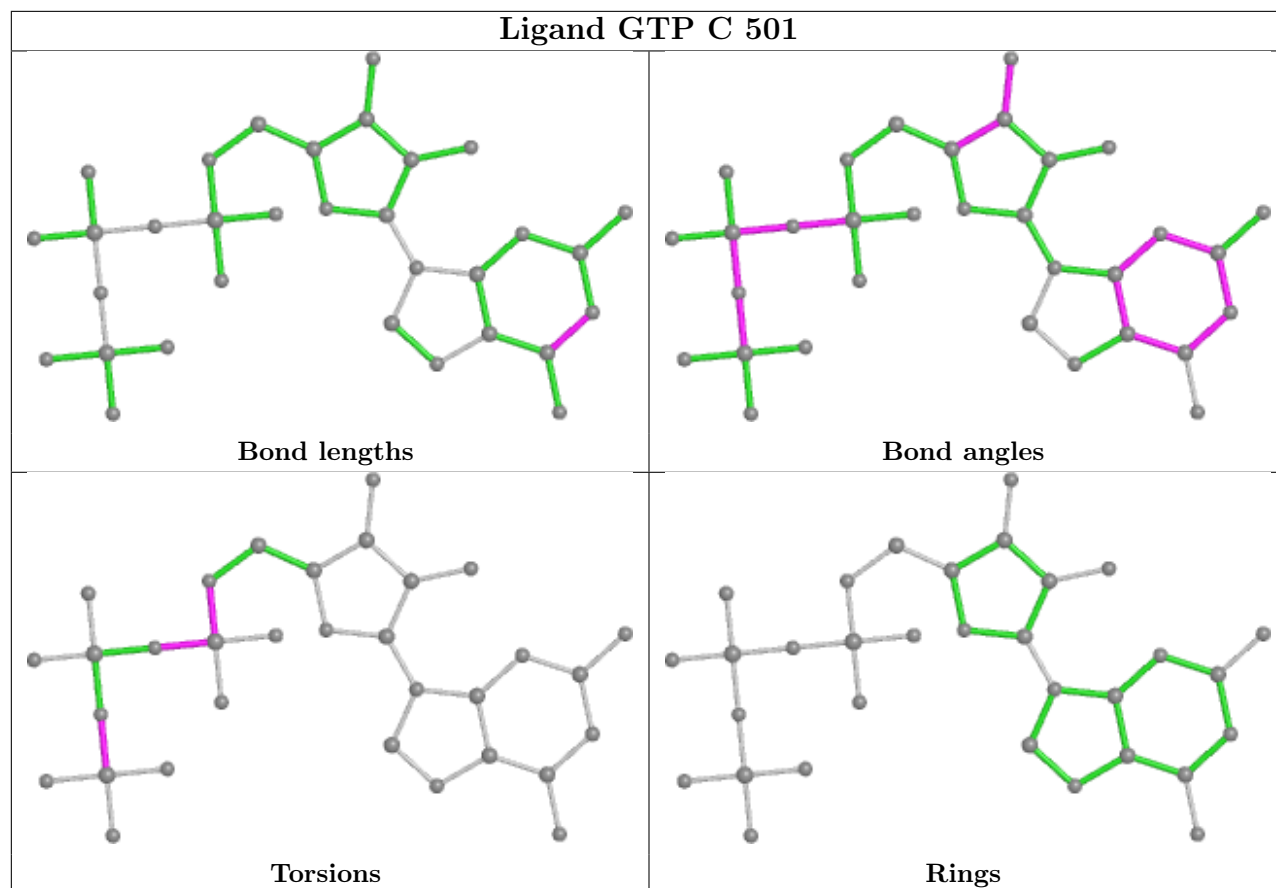
Ligand HOS B 507

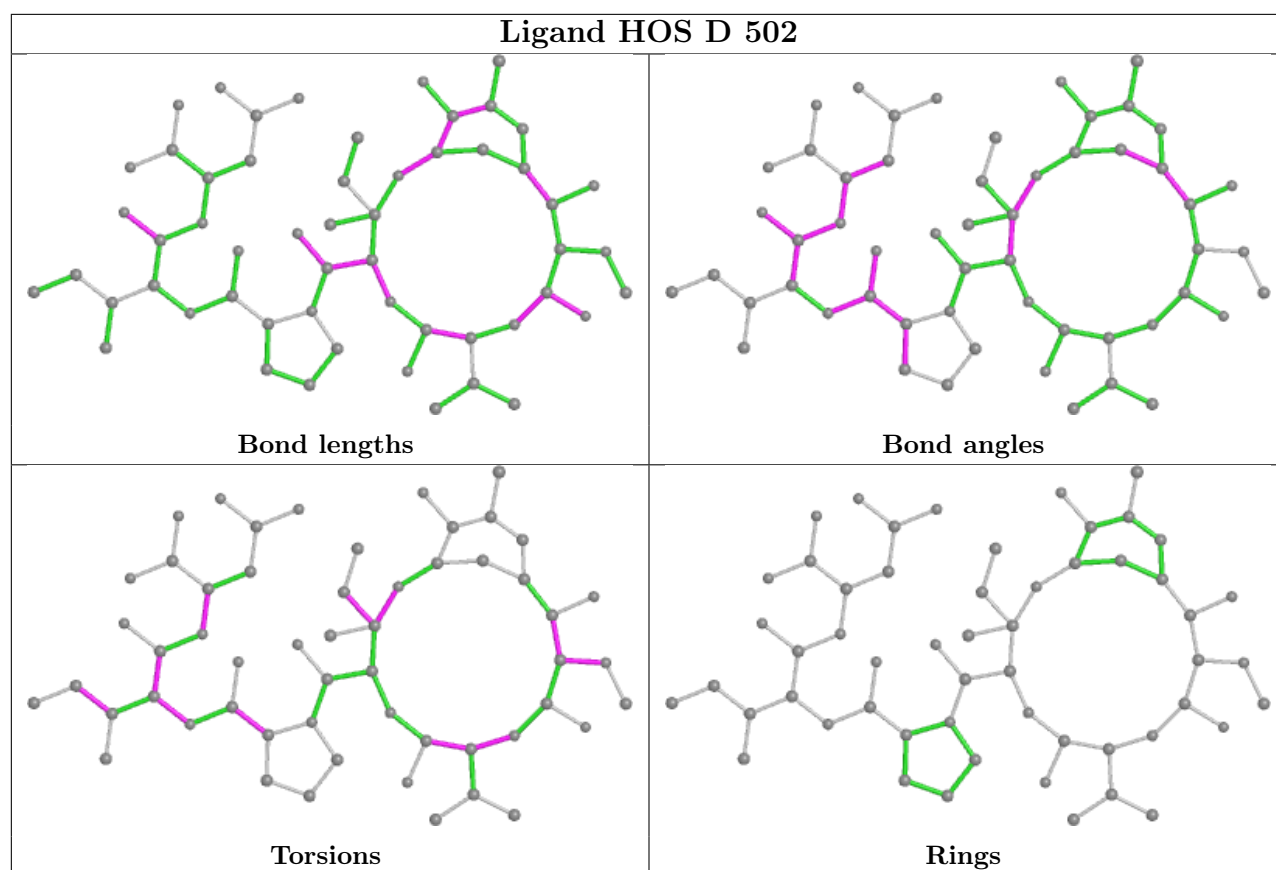


Ligand GDP B 501









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	437/451 (96%)	-0.15	5 (1%) 80 82	20, 39, 69, 92	0
1	C	440/451 (97%)	-0.29	3 (0%) 87 89	18, 33, 60, 172	0
2	B	428/445 (96%)	-0.17	8 (1%) 66 69	17, 34, 67, 111	1 (0%)
2	D	422/445 (94%)	0.46	44 (10%) 6 6	28, 63, 99, 136	4 (0%)
3	E	122/143 (85%)	0.60	15 (12%) 4 3	30, 56, 97, 129	0
4	G	338/384 (88%)	0.75	70 (20%) 1 0	27, 63, 130, 158	0
All	All	2187/2319 (94%)	0.12	145 (6%) 18 19	17, 45, 99, 172	5 (0%)

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	315	CYS	11.9
2	D	404	PHE	6.6
4	G	134	ALA	5.9
4	G	132	LEU	5.8
4	G	137	ARG	5.8

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 monosaccharides in this entry.

6.4 Ligands ⓘ

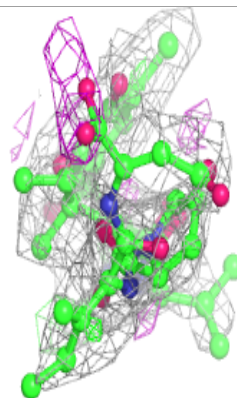
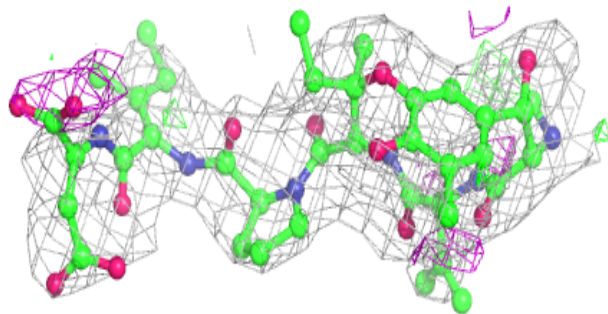
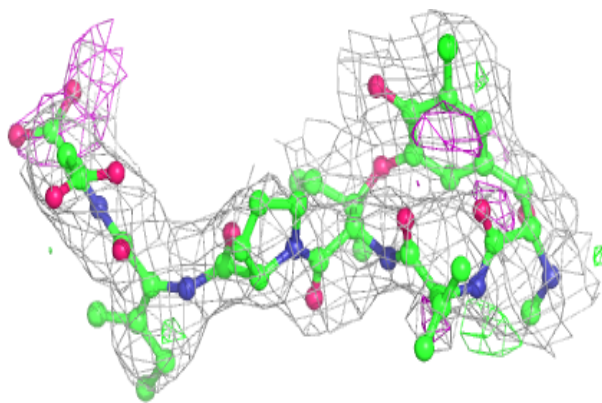
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	B	503	1/1	0.76	0.18	74,74,74,74	0
6	MG	A	502	1/1	0.81	0.09	32,32,32,32	0
11	HOS	D	502	55/55	0.82	0.32	53,73,99,125	0
9	GDP	D	501	28/28	0.86	0.20	44,57,72,88	0
12	ACP	G	401	31/31	0.87	0.17	68,95,122,124	0
6	MG	B	502	1/1	0.92	0.14	42,42,42,42	0
10	MES	B	504	12/12	0.92	0.20	32,57,71,81	0
7	CA	E	201	1/1	0.92	0.07	75,75,75,75	0
8	CL	A	504	1/1	0.92	0.14	60,60,60,60	0
6	MG	C	502	1/1	0.94	0.12	33,33,33,33	0
10	MES	B	505	12/12	0.94	0.17	45,52,62,72	0
6	MG	B	506	1/1	0.95	0.21	58,58,58,58	0
11	HOS	B	507	55/55	0.96	0.15	20,32,71,82	0
7	CA	A	503	1/1	0.97	0.04	64,64,64,64	0
7	CA	C	503	1/1	0.97	0.04	45,45,45,45	0
5	GTP	A	501	32/32	0.98	0.11	21,27,34,35	0
5	GTP	C	501	32/32	0.99	0.11	18,24,29,31	0
9	GDP	B	501	28/28	0.99	0.12	14,22,28,36	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.

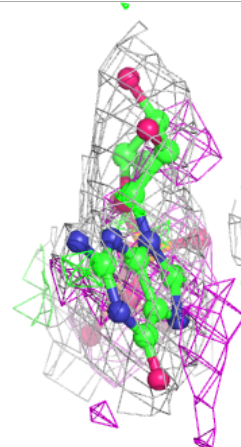
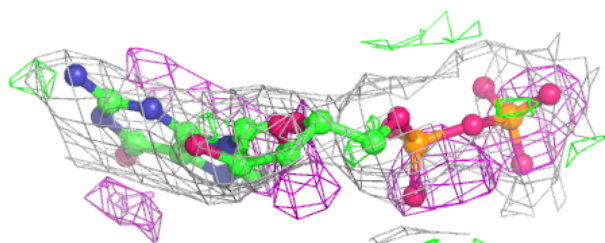
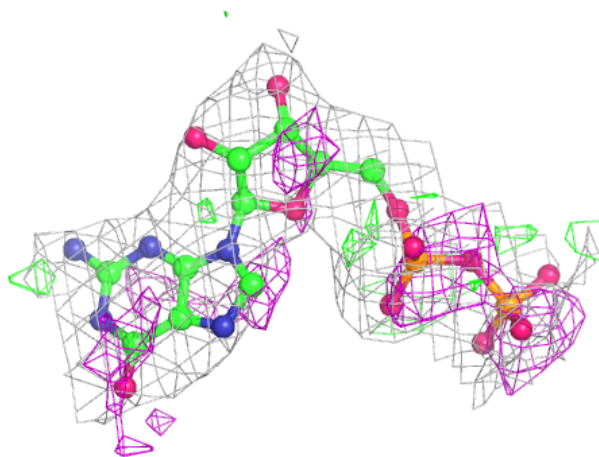
Electron density around HOS D 502:

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



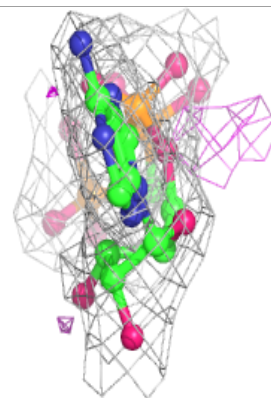
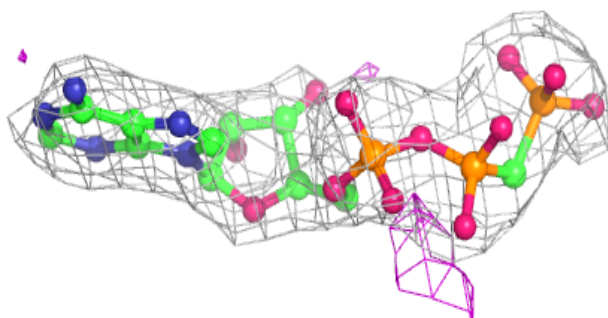
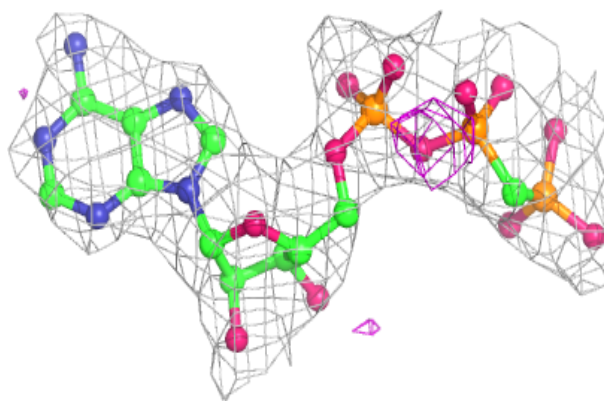
Electron density around GDP D 501:

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

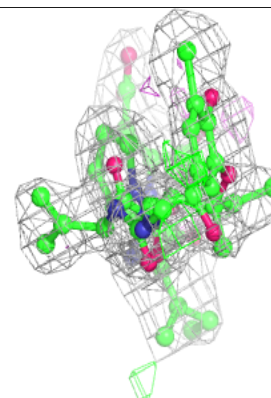
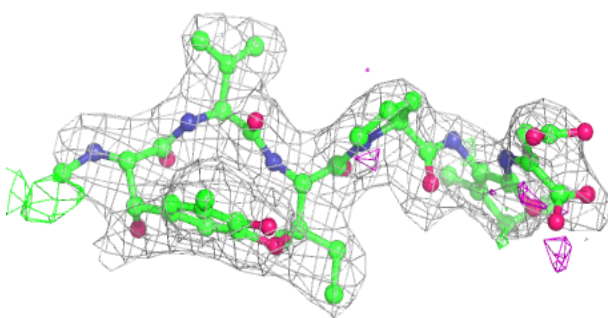
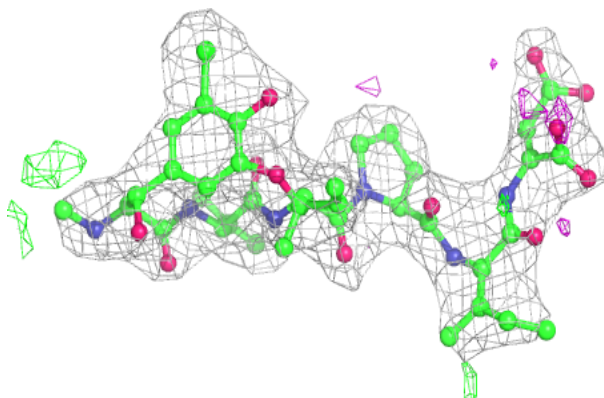


Electron density around ACP G 401:

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

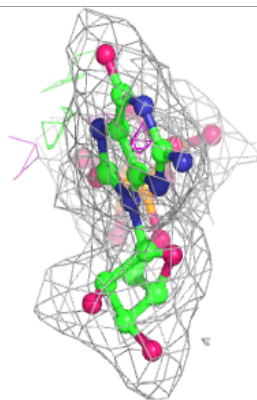
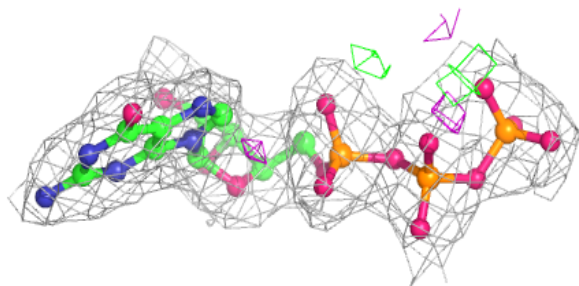
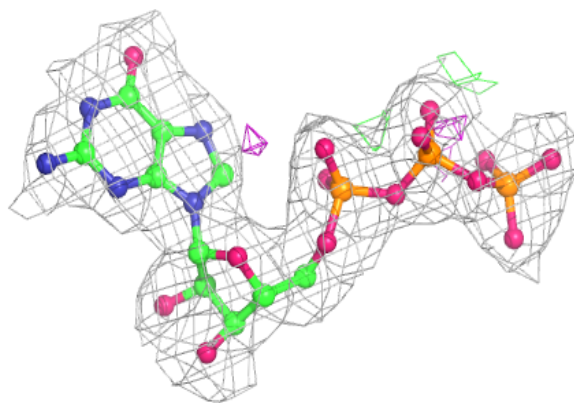
**Electron density around HOS B 507:**

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

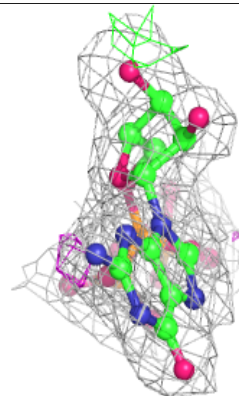
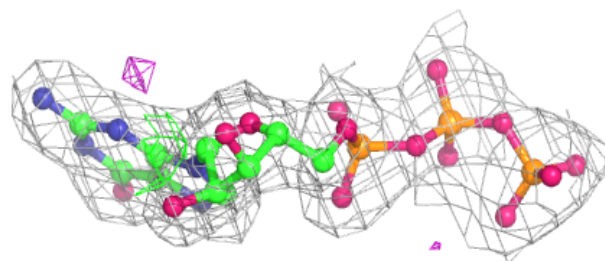
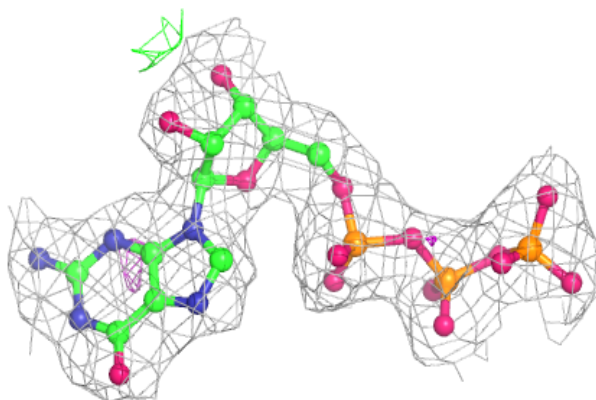


Electron density around GTP A 501:

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

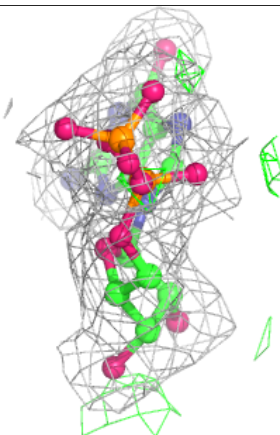
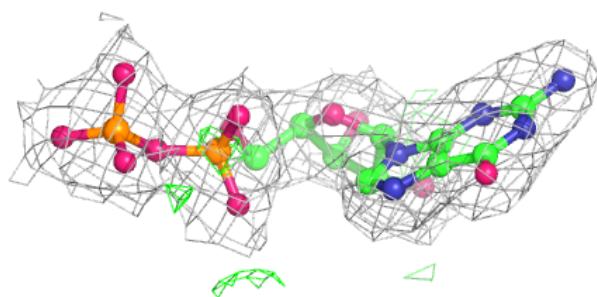
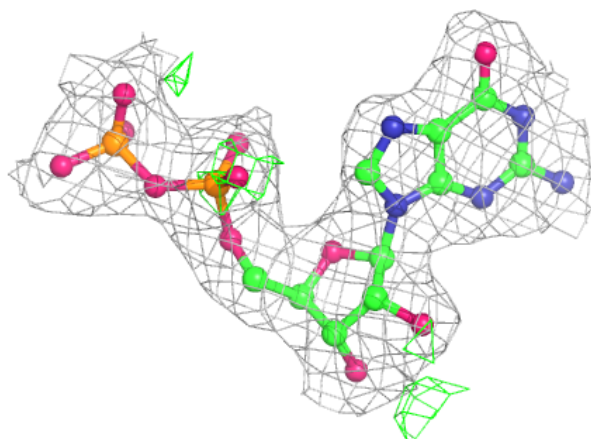
**Electron density around GTP C 501:**

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



Electron density around 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 [i](#)

There are no such residues in this entry.