



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 7, 2022 – 08:18 PM JST

PDB ID : 7E4P  
Title : Crystal structure of tubulin in complex with Ansamitocin P3  
Authors : Wang, Y.; Li, W.  
Deposited on : 2021-02-14  
Resolution : 2.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.26  
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) : 2.26

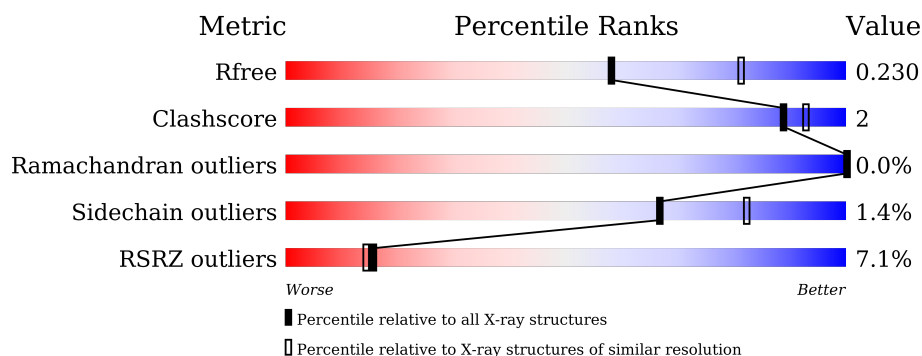
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	440	<div> <div>2%</div> <div>96%</div> <div>..</div> </div>
1	C	440	<div> <div>2%</div> <div>96%</div> <div>.</div> </div>
2	B	431	<div> <div>5%</div> <div>95%</div> <div>..</div> </div>
2	D	431	<div> <div>8%</div> <div>91%</div> <div>6% .</div> </div>
3	E	138	<div> <div>6%</div> <div>86%</div> <div>. 12%</div> </div>
4	F	380	<div> <div>20%</div> <div>79%</div> <div>9% 12%</div> </div>

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 35098 atoms, of which 16873 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	H	N	O	S	0	0	0
			6733	2163	3317	581	650	22			
1	C	440	Total	C	H	N	O	S	0	0	0
			6772	2175	3335	584	656	22			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	427	Total	C	H	N	O	S	0	0	0
			6589	2110	3228	576	649	26			
2	D	421	Total	C	H	N	O	S	0	0	0
			6488	2080	3179	562	640	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	121	Total	C	H	N	O	S	0	0	0
			2013	617	1013	181	197	5			

- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

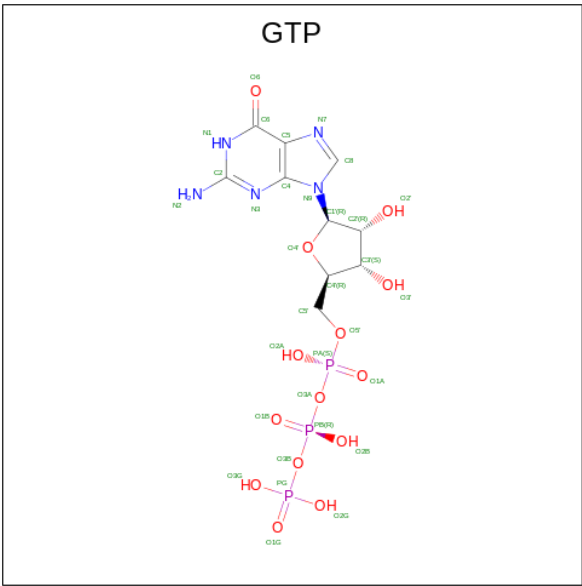
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	336	Total	C	H	N	O	S	0	0	0
			5446	1773	2685	473	501	14			

There are 2 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

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:

C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	C	1	Total	C	H	N	O	P	0	0
			42	10	10	5	14	3		
5	D	1	Total	C	H	N	O	P	0	0
			41	10	9	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	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

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

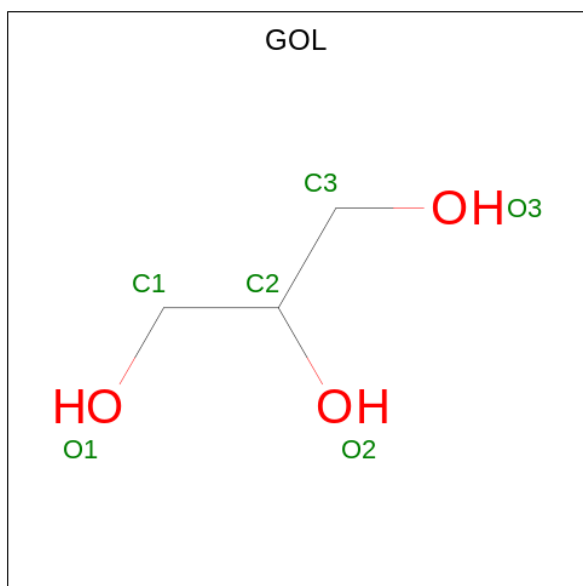
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		

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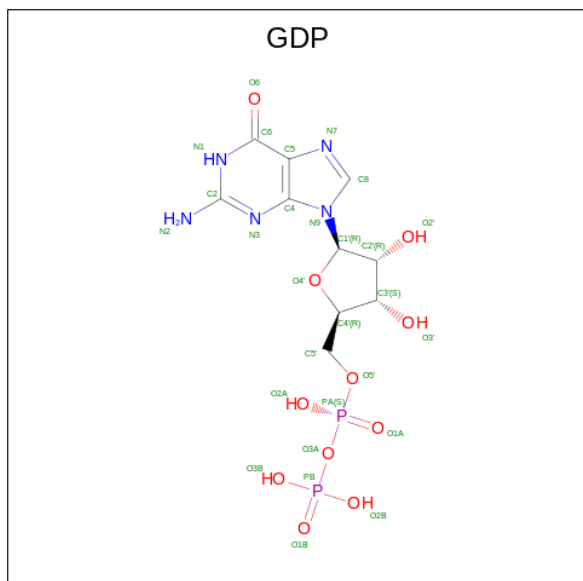
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



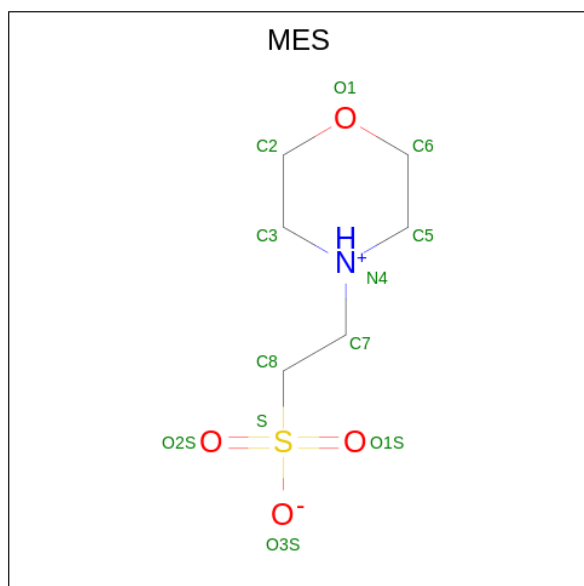
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



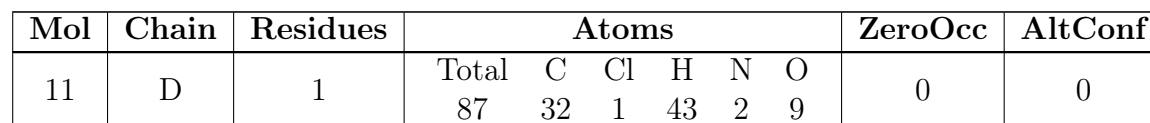
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		

- Molecule 11 is (1S,2S,3S,5S,6S,16Z,18Z,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 ]hexacosa-10(26),11,13,16,18-pentaen-6-yl 2-methylpropanoate (three-letter code: BKF) (formula:  $C_{32}H_{43}ClN_2O_9$ ) (labeled as "Ligand of Interest" by depositor).



- # ACP
- 
- The chemical structure of Adenosine 3'-phosphate (ACP) is shown. It consists of an adenosine moiety (adenine base and ribose sugar) linked to a triphosphate chain. The adenosine moiety is represented by a blue and red structure, with the adenine base and ribose sugar. The triphosphate chain is shown in purple and red, with the three phosphate groups labeled P1, P2, and P3. The structure is labeled with atom names and numbers, such as N1, N2, N3, N4, N5, N6, N7, N8, N9, O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779, O780, O781, O782, O783, O784, O785, O786, O787, O788, O789, O790, O791, O792, O793, O794, O795, O796, O797, O798, O799, O800, O801, O802, O803, O804, O805

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
12	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	162	Total 162	O 162	0	0
13	B	135	Total 135	O 135	0	0
13	C	260	Total 260	O 260	0	0
13	D	70	Total 70	O 70	0	0
13	E	21	Total 21	O 21	0	0
13	F	69	Total 69	O 69	0	0

### 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.

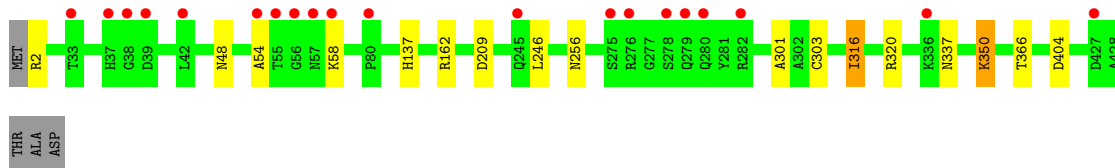
- Molecule 1: Tubulin alpha-1B chain



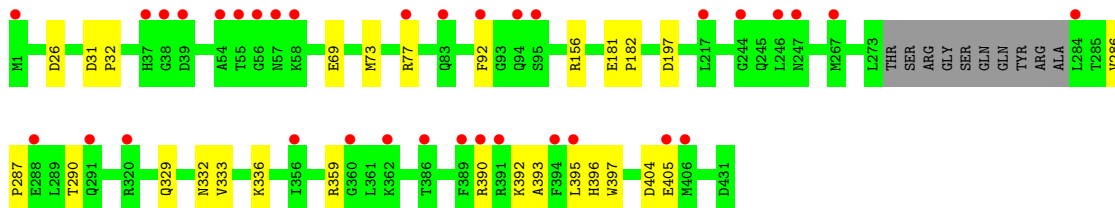
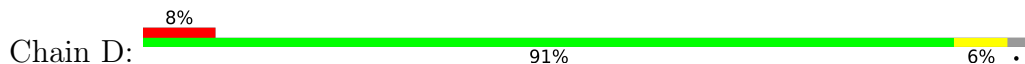
- Molecule 1: Tubulin alpha-1B chain



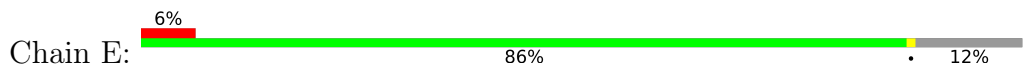
- Molecule 2: Tubulin beta-2B chain

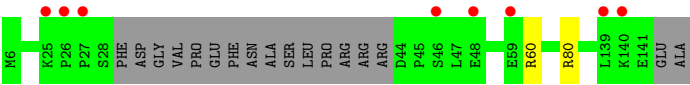


- Molecule 2: Tubulin beta-2B chain

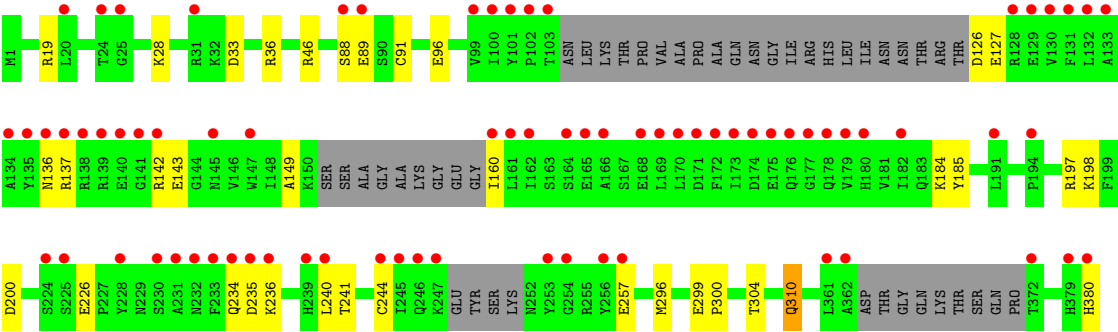
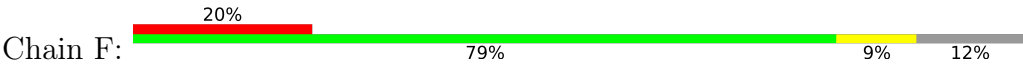


- Molecule 3: Stathmin-4





● 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, $\alpha$ , $\beta$ , $\gamma$	105.40Å 158.57Å 181.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.25 – 2.40 47.25 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.25-2.40) 97.0 (47.25-2.40)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.213 , 0.229 0.217 , 0.230	Depositor DCC
$R_{free}$ test set	1155 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	35098	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GOL, MES, GDP, GTP, ACP, MG, BKF

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	0.24	0/3494	0.42	0/4743
1	C	0.24	0/3515	0.42	0/4772
2	B	0.23	0/3436	0.40	0/4654
2	D	0.24	0/3382	0.41	0/4581
3	E	0.22	0/1008	0.35	0/1337
4	F	0.25	0/2823	0.42	0/3813
All	All	0.24	0/17658	0.41	0/23900

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	88	SER	Mainchain

### 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	3416	3317	3330	11	0
1	C	3437	3335	3348	9	1
2	B	3361	3228	3238	11	0
2	D	3309	3179	3189	17	0
3	E	1000	1013	1018	1	1
4	F	2761	2685	2733	15	0
5	A	32	10	12	1	0
5	C	32	10	12	0	0
5	D	32	9	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	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	8	8	0	0
9	B	28	10	12	0	0
10	B	12	12	12	0	0
11	D	44	43	0	1	0
12	F	31	14	14	0	0
13	A	162	0	0	4	0
13	B	135	0	0	7	0
13	C	260	0	0	5	0
13	D	70	0	0	5	0
13	E	21	0	0	0	0
13	F	69	0	0	2	0
All	All	18225	16873	16938	64	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 64 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:ASP:OD1	2:D:359:ARG:NH2	2.22	0.72
1:C:358:GLN:NE2	13:C:603:HOH:O	2.22	0.72
2:D:392:LYS:C	13:D:614:HOH:O	2.29	0.70
4:F:36:ARG:NH2	13:F:502:HOH:O	2.27	0.66
1:A:2:ARG:NH2	13:A:606:HOH:O	2.28	0.66

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)
1:C:366:GLY:O	3:E:80:ARG:NH2[4_545]	2.17	0.03

## 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	435/440 (99%)	424 (98%)	11 (2%)	0	100	100
1	C	438/440 (100%)	428 (98%)	10 (2%)	0	100	100
2	B	425/431 (99%)	414 (97%)	11 (3%)	0	100	100
2	D	417/431 (97%)	409 (98%)	8 (2%)	0	100	100
3	E	117/138 (85%)	115 (98%)	2 (2%)	0	100	100
4	F	326/380 (86%)	313 (96%)	12 (4%)	1 (0%)	41	55
All	All	2158/2260 (96%)	2103 (98%)	54 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	89	GLU

### 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	368/371 (99%)	363 (99%)	5 (1%)	67	82
1	C	371/371 (100%)	367 (99%)	4 (1%)	73	87
2	B	369/372 (99%)	365 (99%)	4 (1%)	73	87
2	D	364/372 (98%)	363 (100%)	1 (0%)	92	97
3	E	109/123 (89%)	109 (100%)	0	100	100
4	F	303/338 (90%)	291 (96%)	12 (4%)	31	49
All	All	1884/1947 (97%)	1858 (99%)	26 (1%)	67	82

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	19	ARG
4	F	136	ASN
4	F	244	CYS
4	F	91	CYS
4	F	137	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	190	HIS
4	F	246	GLN
4	F	310	GLN

### 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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GTP	D	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.89	6 (18%)
8	GOL	A	504	-	5,5,5	0.38	0	5,5,5	0.20	0
12	ACP	F	401	6	27,33,33	4.48	6 (22%)	32,52,52	1.63	6 (18%)
5	GTP	A	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.80	7 (21%)
10	MES	B	503	-	12,12,12	2.26	1 (8%)	14,16,16	2.50	5 (35%)
9	GDP	B	501	6	24,30,30	1.13	2 (8%)	31,47,47	1.91	8 (25%)
11	BKF	D	502	-	45,47,47	2.91	15 (33%)	53,71,71	3.64	26 (49%)
5	GTP	C	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.77	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	D	501	6	-	9/18/38/38	0/3/3/3
8	GOL	A	504	-	-	2/4/4/4	-
12	ACP	F	401	6	-	8/15/38/38	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
11	BKF	D	502	-	-	21/49/76/76	0/2/4/4
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	PB-O3A	20.62	1.81	1.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	502	BKF	C08-N07	7.95	1.51	1.35
12	F	401	ACP	PA-O5'	7.68	1.90	1.59
10	B	503	MES	C8-S	-7.60	1.66	1.77
11	D	502	BKF	C12-C14	7.31	1.56	1.47

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	502	BKF	C10-C08-N07	11.60	131.98	118.89
11	D	502	BKF	C01-C06-N07	8.75	129.69	120.71
11	D	502	BKF	C05-C06-C01	-8.27	111.99	122.53
11	D	502	BKF	C28-C26-C25	-7.62	102.94	122.59
11	D	502	BKF	C12-O34-C14	6.71	64.83	60.79

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A

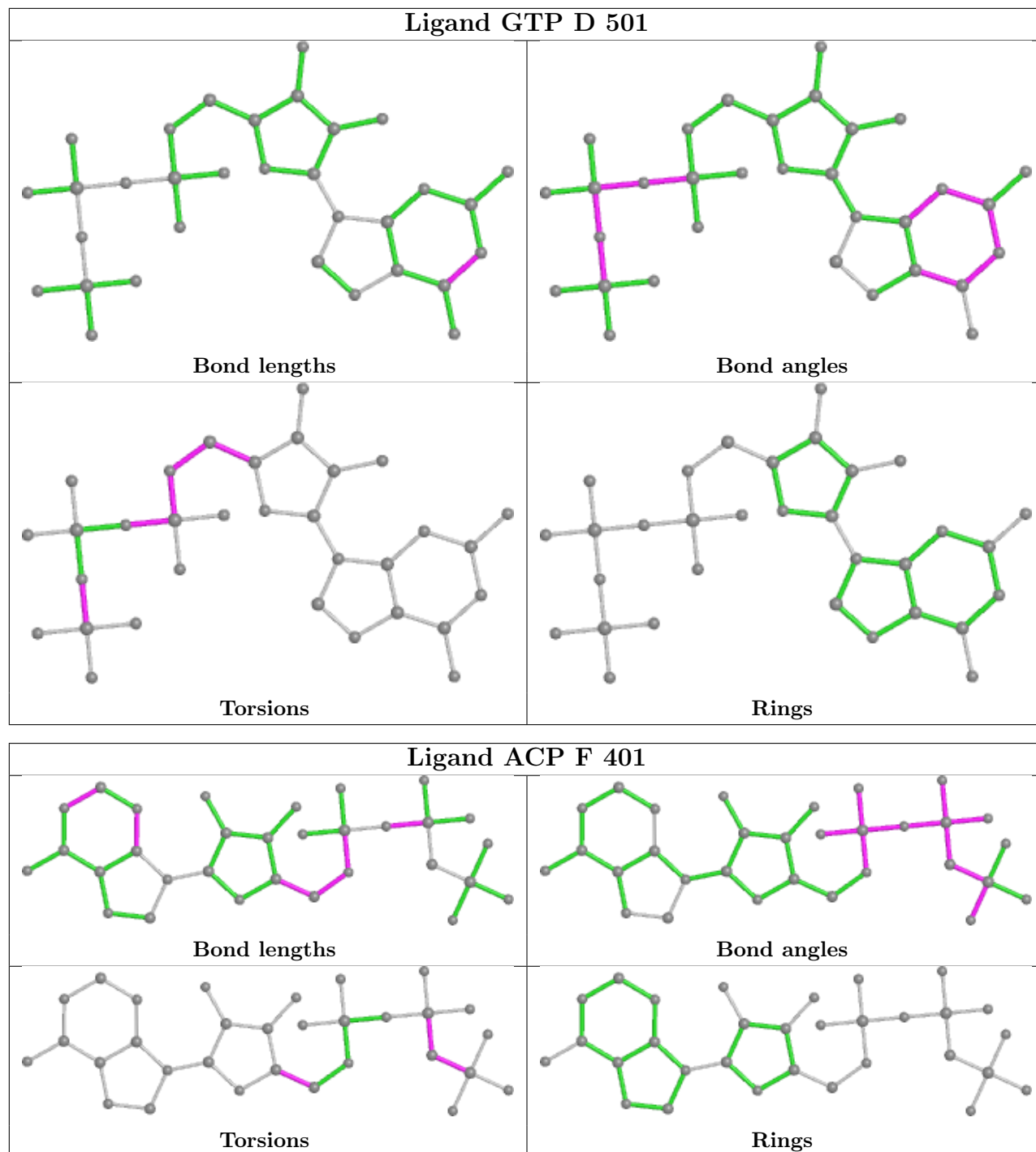
There are no ring outliers.

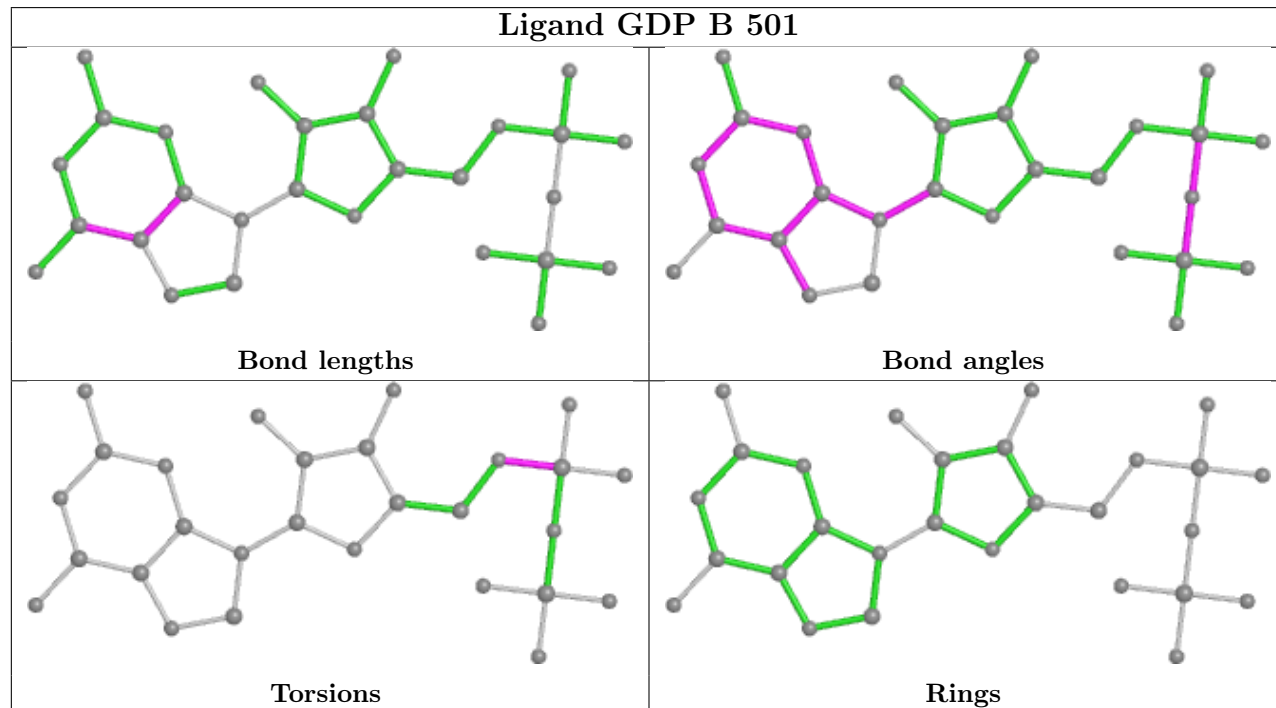
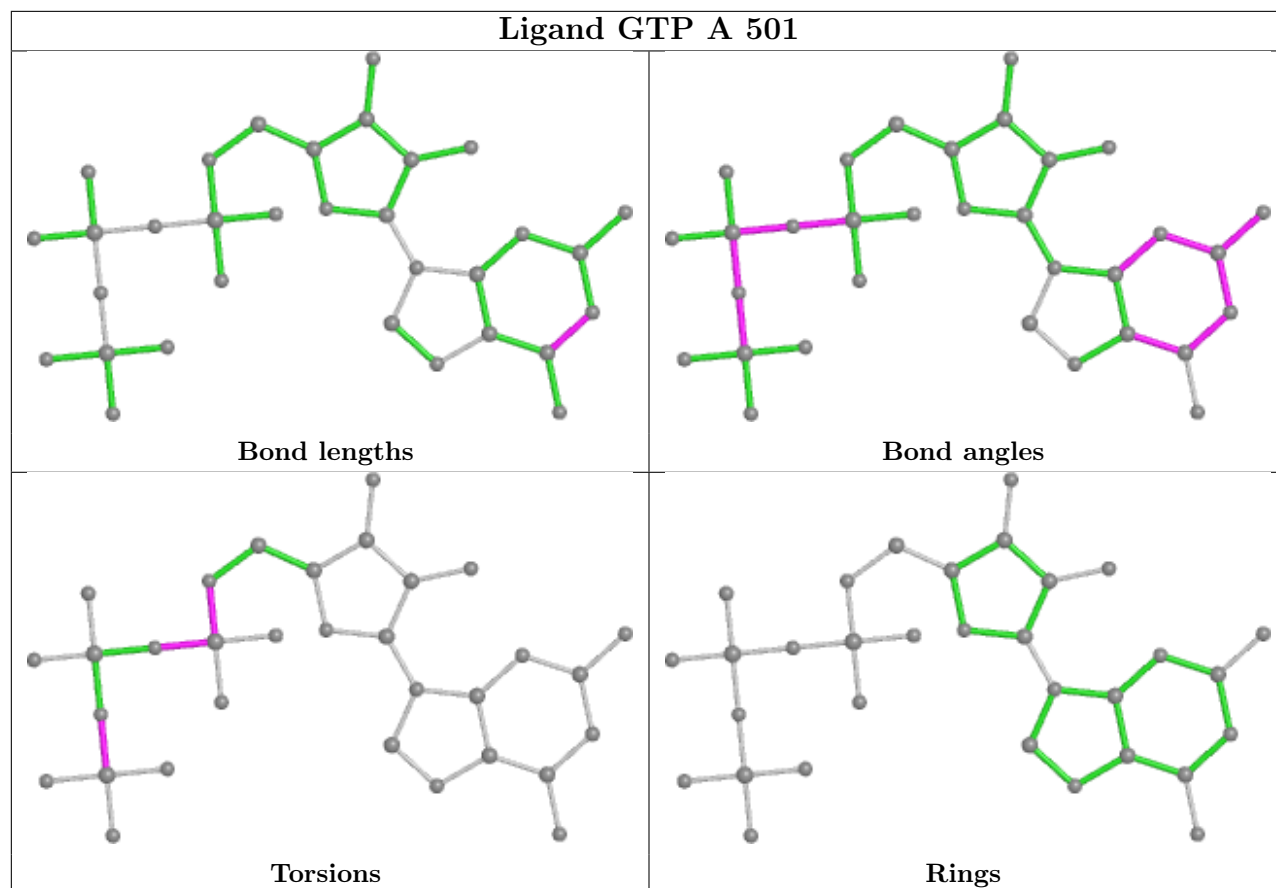
2 monomers are involved in 2 short contacts:

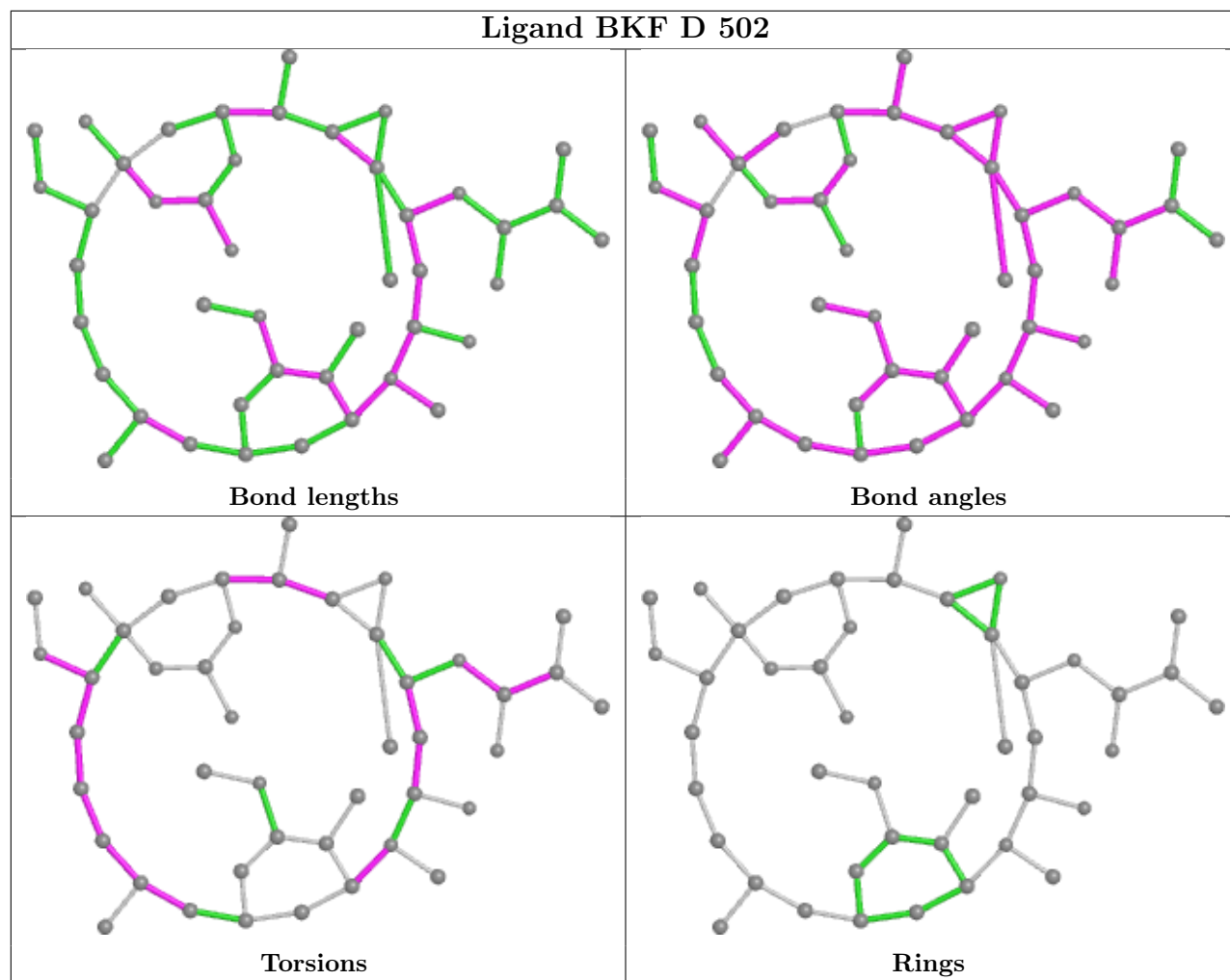
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
11	D	502	BKF	1	0

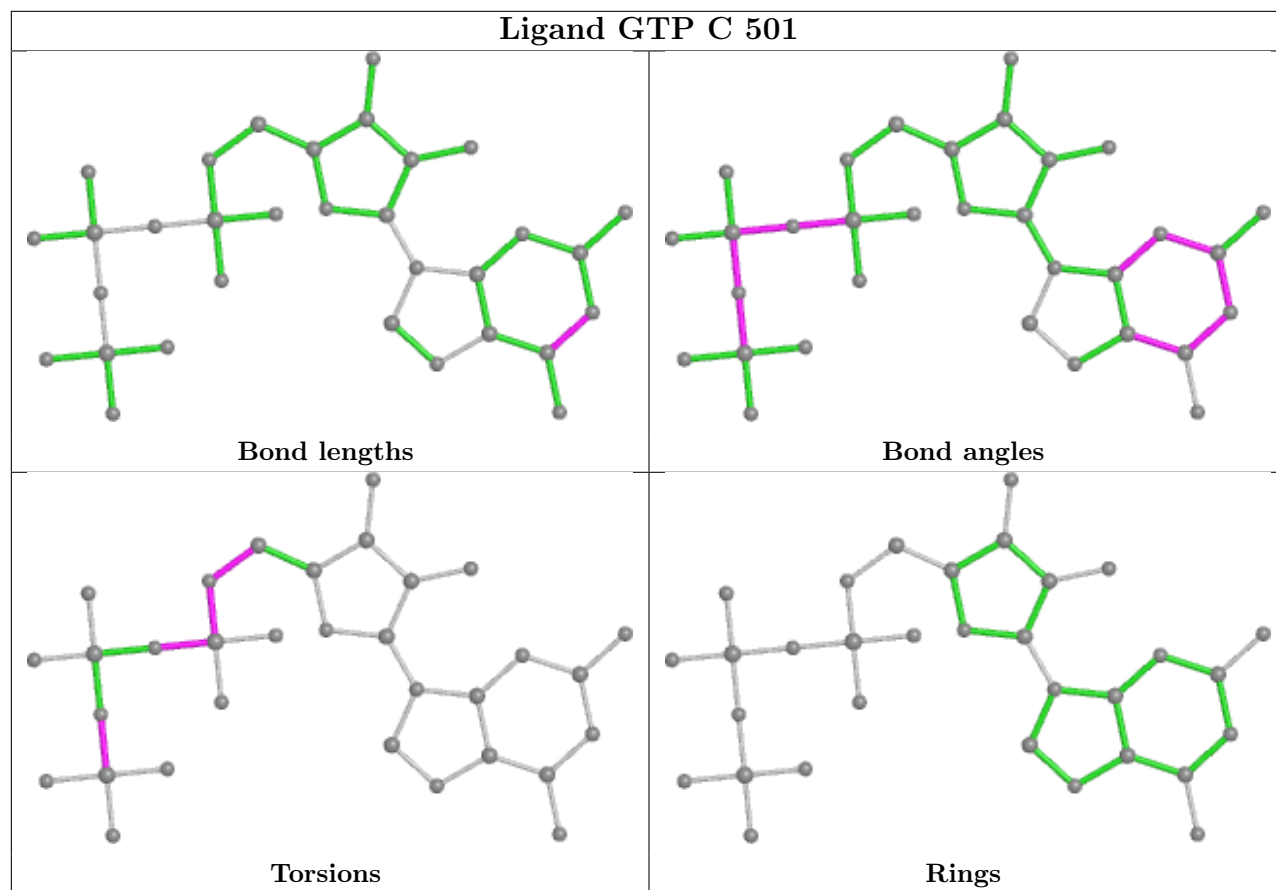
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	437/440 (99%)	0.19	10 (2%) 60 58	22, 37, 62, 90	0
1	C	440/440 (100%)	-0.07	7 (1%) 72 70	16, 28, 49, 64	0
2	B	427/431 (99%)	0.25	20 (4%) 31 30	17, 37, 68, 115	0
2	D	421/431 (97%)	0.54	34 (8%) 12 11	26, 49, 82, 103	0
3	E	121/138 (87%)	0.50	8 (6%) 18 17	25, 50, 79, 98	0
4	F	336/380 (88%)	0.96	75 (22%) 0 0	28, 56, 120, 141	0
All	All	2182/2260 (96%)	0.35	154 (7%) 16 14	16, 41, 84, 141	0

The worst 5 of 154 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	231	ALA	8.1
4	F	176	GLN	7.0
4	F	173	ILE	6.8
4	F	380	HIS	6.6
4	F	177	GLY	6.4

### 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

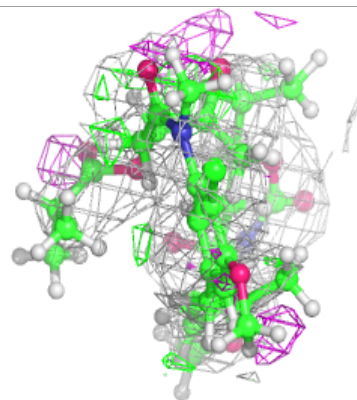
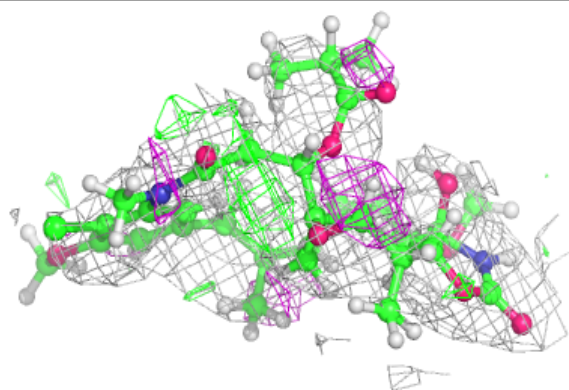
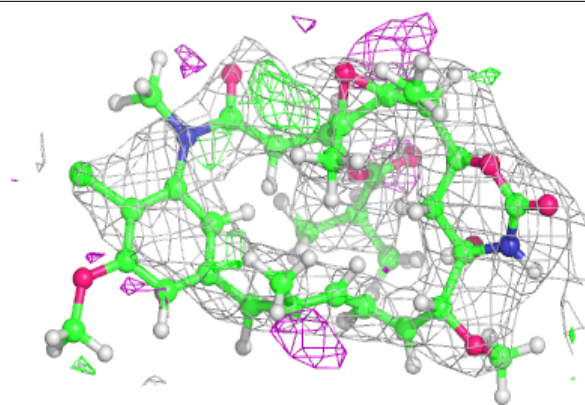
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
11	BKF	D	502	44/44	0.80	0.33	51,73,97,149	0
7	CA	A	503	1/1	0.84	0.07	56,56,56,56	0
8	GOL	A	504	6/6	0.86	0.13	36,49,58,59	0
6	MG	D	503	1/1	0.90	0.08	69,69,69,69	0
6	MG	B	502	1/1	0.91	0.26	24,24,24,24	0
6	MG	C	502	1/1	0.91	0.31	27,27,27,27	0
12	ACP	F	401	31/31	0.91	0.15	61,79,100,116	0
5	GTP	D	501	32/32	0.93	0.15	44,53,69,79	0
6	MG	F	402	1/1	0.94	0.17	69,69,69,69	0
10	MES	B	503	12/12	0.95	0.11	33,41,50,57	0
6	MG	A	502	1/1	0.97	0.17	25,25,25,25	0
9	GDP	B	501	28/28	0.97	0.20	18,26,32,38	0
5	GTP	C	501	32/32	0.97	0.18	18,23,30,31	0
5	GTP	A	501	32/32	0.97	0.23	22,27,34,38	0
7	CA	C	503	1/1	0.97	0.09	37,37,37,37	0

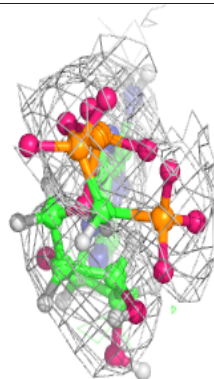
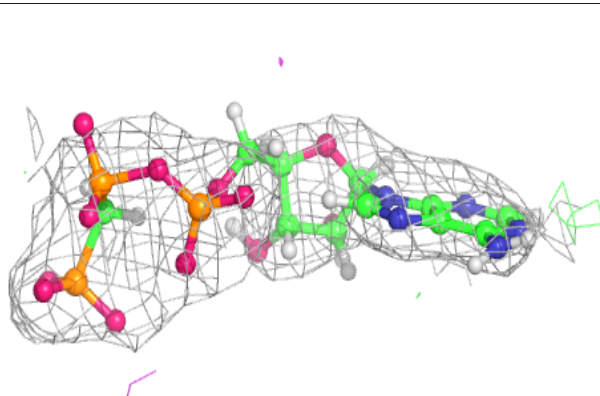
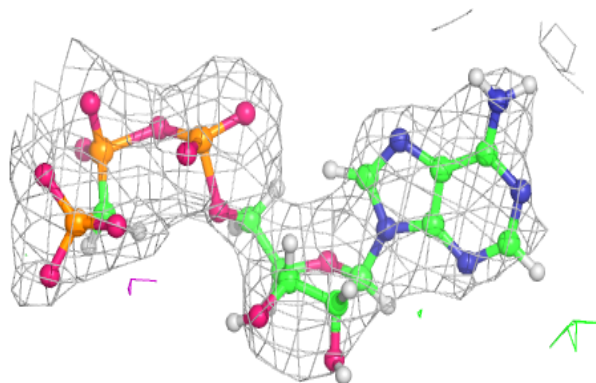
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around BKF 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)

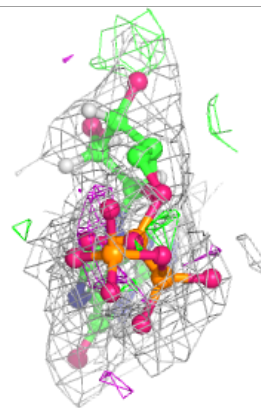
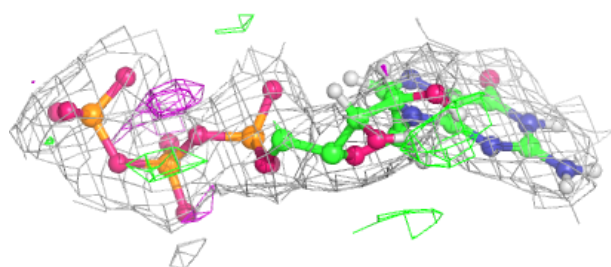
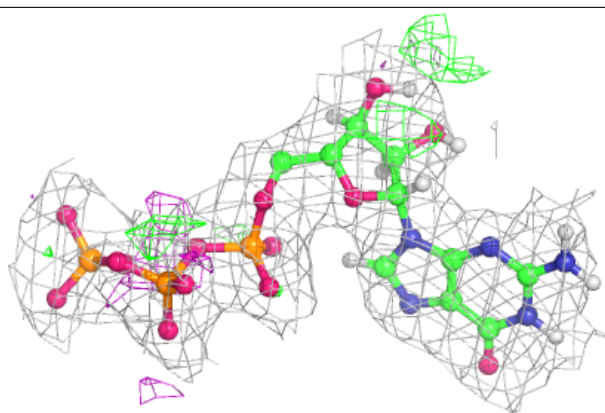
**Electron density around ACP F 401:**

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



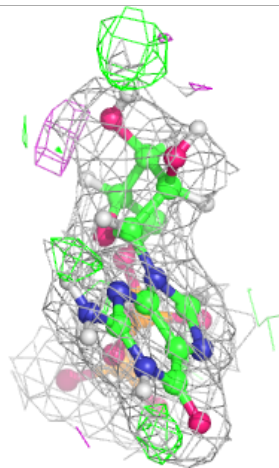
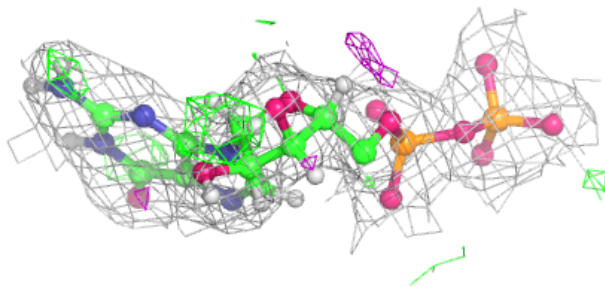
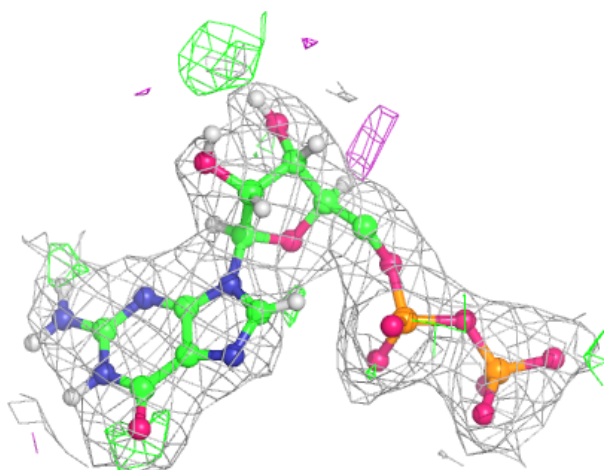
**Electron density around GTP D 501:**

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



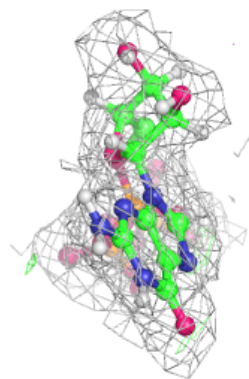
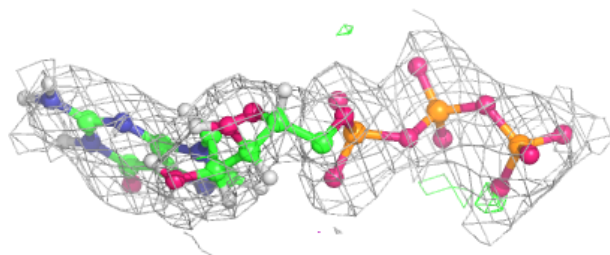
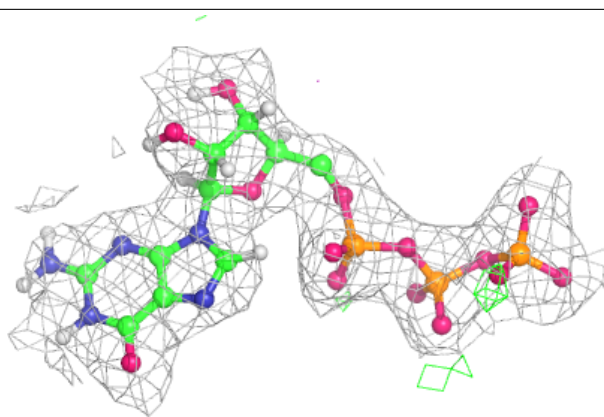
**Electron density around GDP B 501:**

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

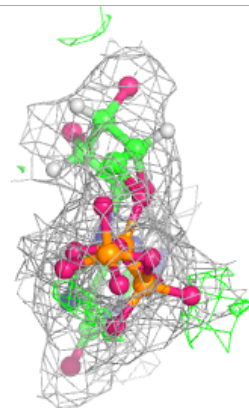
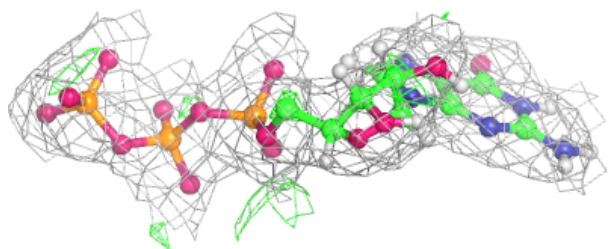
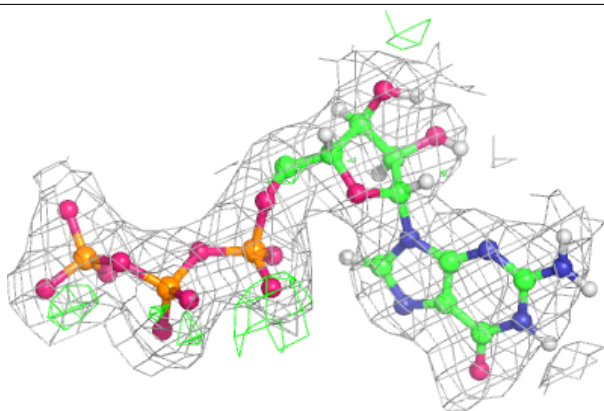


**Electron density around GTP C 501:**

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

**Electron density around GTP A 501:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.