



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:10 PM UTC

PDB ID : 8AHM / pdb_00008ahm
Title : Crystal structure of tubulin in complex with C(13)/C(13')-Bis-Desmethyl-Disorazole Z
Authors : Oliva, M.A.; Diaz, J.F.; Altmann, K.H.
Deposited on : 2022-07-22
Resolution : 2.42 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

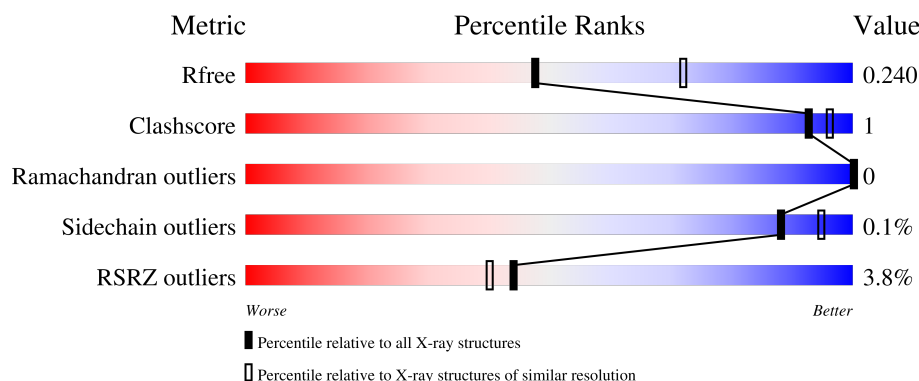
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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 ≥ 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	2% 93% 5% •
1	C	451	2% 93% 5% •
2	B	445	2% 91% 5% •
2	D	445	4% 90% 5% 6%
3	E	189	5% 63% 36%

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Mol	Chain	Length	Quality of chain
4	F	384	8% 79% • 18%

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 34568 atoms, of which 16942 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	5	0
			6793	2175	3358	583	653	24			
1	C	440	Total	C	H	N	O	S	0	14	0
			6914	2212	3413	594	670	25			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	425	Total	C	H	N	O	S	0	8	0
			6633	2120	3257	575	654	27			
2	D	420	Total	C	H	N	O	S	0	0	0
			6481	2075	3181	561	638	26			

- 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	2	0
			2036	623	1026	184	198	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	315	Total	C	H	N	O	S	0	2	0
			5152	1669	2567	436	465	15			

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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

-
- The image displays the chemical structure of Guanosine Triphosphate (GTP). It consists of a guanine base (a purine ring system with an amino group at position 6) linked to a ribose sugar (a five-membered ring with hydroxyl groups at positions 2' and 3'). The ribose is further linked to a chain of three phosphate groups (labeled 1A, 2A, and 3A). The structure is color-coded: the guanine base is blue, the ribose sugar is green, and the phosphate groups are red. The labels N1, N3, N7, N9, C2, C4, C6, C8, C1, C2', C3', C4', C5', C6', C7', C8', C9', 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

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

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

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

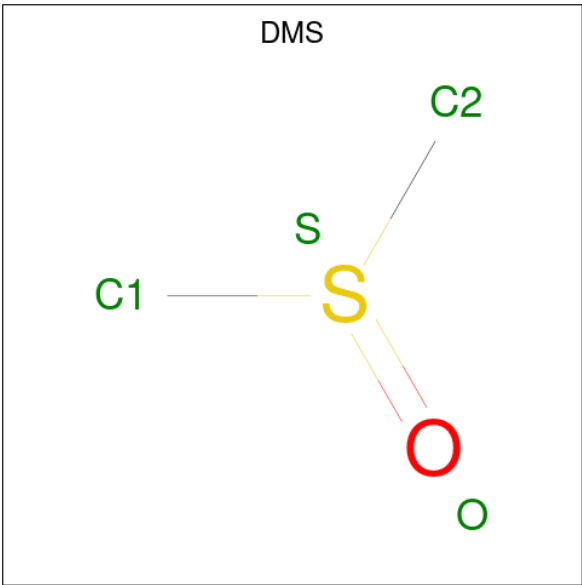


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 8 is CALCIUM ION (CCD ID: CA) (formula: Ca).

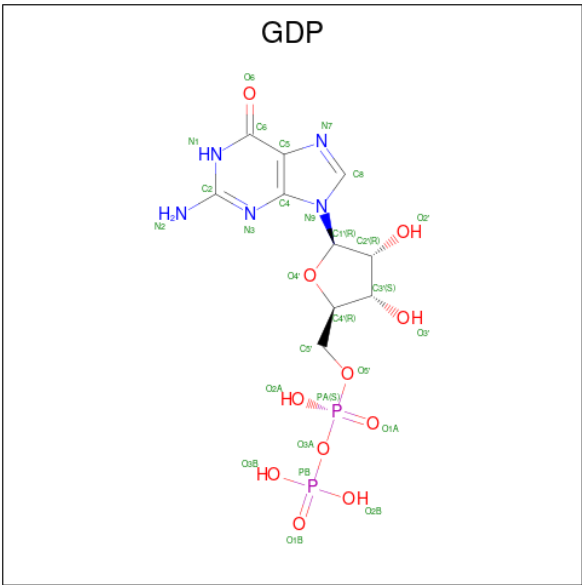
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ca	0	0
			1	1		
8	B	2	Total	Ca	0	0
			2	2		
8	C	1	Total	Ca	0	0
			1	1		

- Molecule 9 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



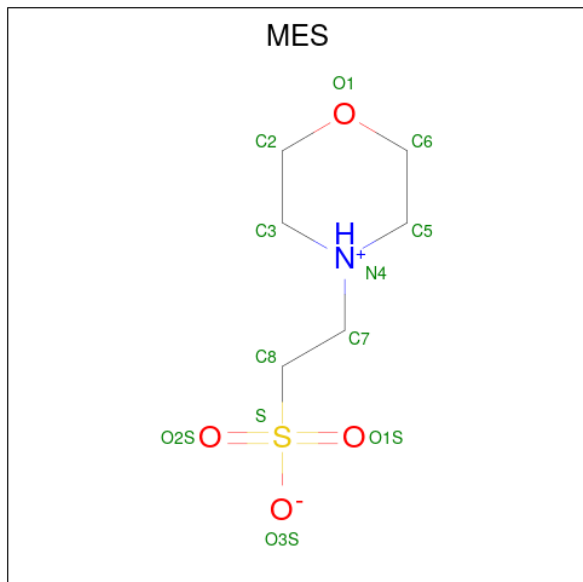
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
9	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

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



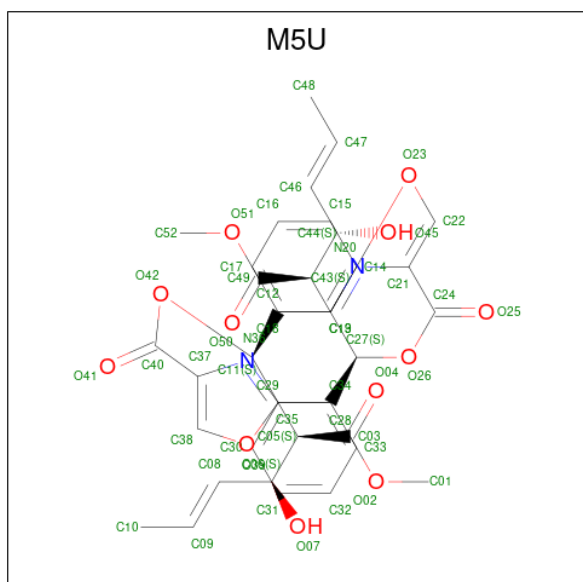
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
10	B	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0
10	D	1	Total 38	C 10	H 10	N 5	O 11	P 2	0	0

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



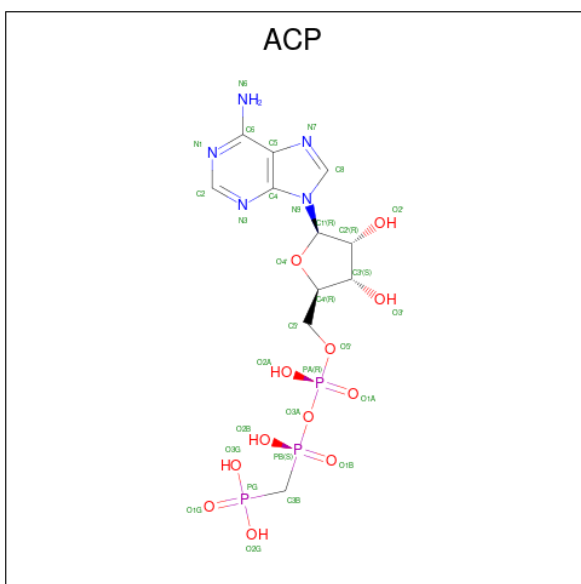
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
11	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 12 is dimethyl 2,2'-((12Z,12Z,4S,6Z,8E,10E,15S,17Z,19E,21E)-2,13-dioxo-3,14-dioxo-1(4,2),12(2,4)-dioxazolacyclodocosaphane-6,8,10,17,19,21-hexaene-4,15-diyl)(2S,2'S,3S,3'S,4E,4'E)-bis(3-hydroxyhex-4-enoate) (CCD ID: M5U) (formula: $C_{38}H_{42}N_2O_{12}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	D	1	Total	C	H	N	O	0	0
			94	38	42	2	12		

- 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	H	N	O	P	0	0
			45	11	14	5	12	3		

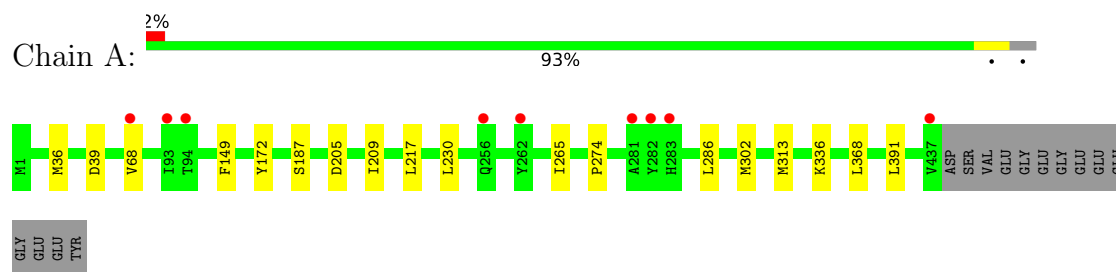
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	33	Total O 33 33	0	0
14	B	32	Total O 32 32	0	0
14	C	80	Total O 80 80	0	0
14	D	13	Total O 13 13	0	0
14	E	2	Total O 2 2	0	0
14	F	9	Total O 9 9	0	0

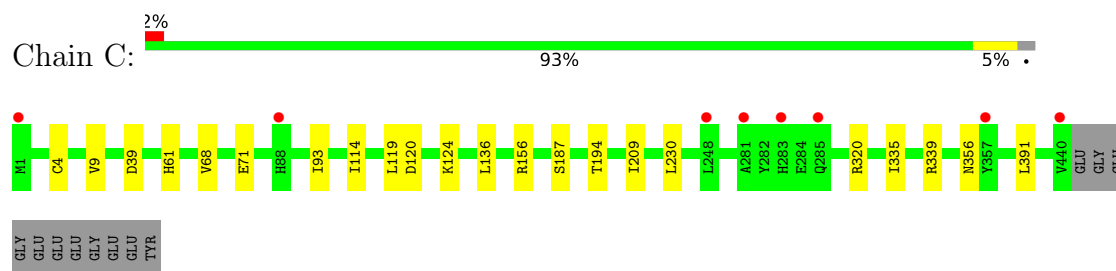
3 Residue-property plots [i](#)

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.

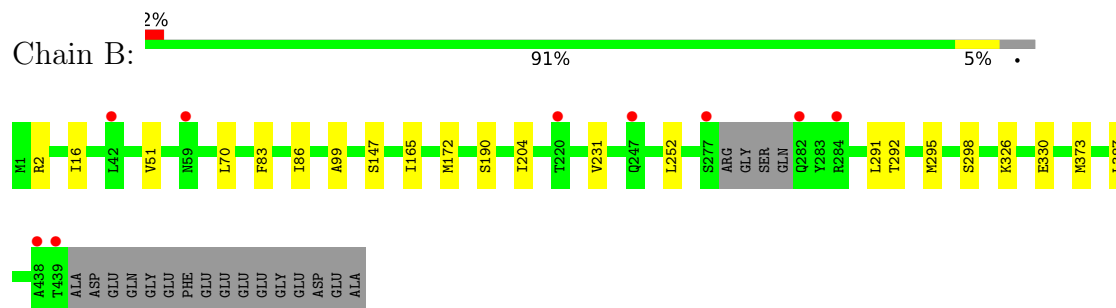
- Molecule 1: Tubulin alpha-1B chain



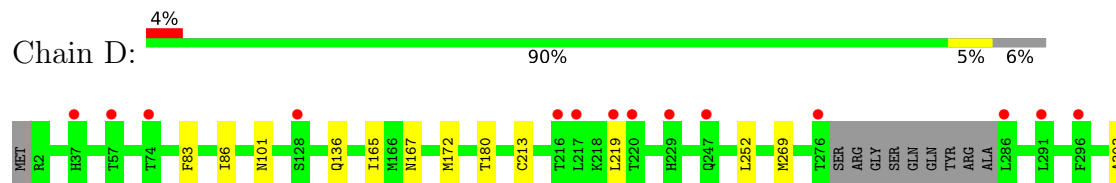
- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta-2B chain

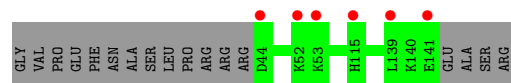
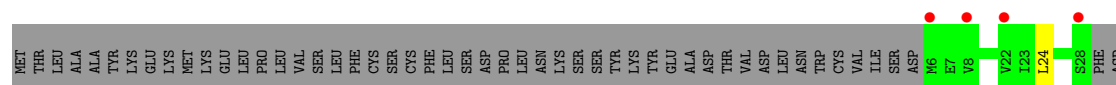


- Molecule 2: Tubulin beta-2B chain

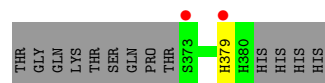
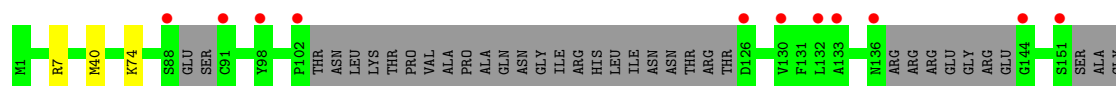
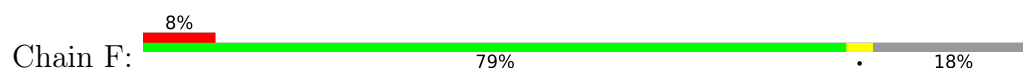




• Molecule 3: Stathmin-4



• 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, α , β , γ	105.05Å 157.80Å 181.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 2.42 49.84 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.84-2.42) 99.8 (49.84-2.42)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.19.1	Depositor
R, R_{free}	0.200 , 0.241 0.199 , 0.240	Depositor DCC
R_{free} test set	5708 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34568	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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, ACP, CA, DMS, MG, GOL, GTP, MES, M5U

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	0.09	0/3529	0.24	0/4791
1	C	0.10	0/3616	0.26	0/4913
2	B	0.09	0/3476	0.24	0/4708
2	D	0.08	0/3373	0.22	0/4570
3	E	0.08	0/1027	0.17	0/1363
4	F	0.08	0/2647	0.22	0/3572
All	All	0.09	0/17668	0.23	0/23917

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3435	3358	3348	10	0
1	C	3501	3413	3382	11	0
2	B	3376	3257	3225	13	0
2	D	3300	3181	3180	11	0
3	E	1010	1026	1014	1	0
4	F	2585	2567	2561	5	0
5	A	32	9	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	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	6	8	8	0	0
8	A	1	0	0	0	0
8	B	2	0	0	0	0
8	C	1	0	0	0	0
9	A	4	6	6	0	0
9	C	4	6	6	0	0
10	B	28	10	12	0	0
10	D	28	10	12	0	0
11	B	24	26	25	1	0
12	D	52	42	0	0	0
13	F	31	14	13	0	0
14	A	33	0	0	0	0
14	B	32	0	0	0	0
14	C	80	0	0	0	0
14	D	13	0	0	1	0
14	E	2	0	0	0	0
14	F	9	0	0	0	0
All	All	17626	16942	16816	50	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 1.

The worst 5 of 50 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)
1:C:120[B]:ASP:OD1	1:C:124:LYS:NZ	2.30	0.64
1:A:336:LYS:HD2	3:E:24:LEU:HD13	1.81	0.62
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.13	0.61
2:B:298:SER:OG	11:B:504:MES:O2S	2.22	0.58
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.87	0.57

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%)	429 (98%)	11 (2%)	0	100	100
1	C	452/451 (100%)	445 (98%)	7 (2%)	0	100	100
2	B	429/445 (96%)	422 (98%)	7 (2%)	0	100	100
2	D	416/445 (94%)	409 (98%)	7 (2%)	0	100	100
3	E	119/189 (63%)	118 (99%)	1 (1%)	0	100	100
4	F	299/384 (78%)	292 (98%)	7 (2%)	0	100	100
All	All	2155/2365 (91%)	2115 (98%)	40 (2%)	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%)	373 (100%)	0	100	100
1	C	384/379 (101%)	383 (100%)	1 (0%)	86	93
2	B	375/383 (98%)	375 (100%)	0	100	100
2	D	363/383 (95%)	363 (100%)	0	100	100
3	E	111/171 (65%)	111 (100%)	0	100	100
4	F	286/342 (84%)	286 (100%)	0	100	100
All	All	1892/2037 (93%)	1891 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	71	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	12	ASN
3	E	136	ASN
4	F	379	HIS
1	C	393	HIS
2	D	101	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 9 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GTP	C	501	6	33,34,34	0.89	0	50,54,54	1.48	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	MES	B	503	-	12,12,12	2.23	1 (8%)	15,16,16	1.50	2 (13%)
11	MES	B	504	-	12,12,12	2.37	1 (8%)	15,16,16	1.42	2 (13%)
10	GDP	D	501	6	29,30,30	1.17	3 (10%)	45,47,47	1.66	5 (11%)
5	GTP	A	501	6	33,34,34	0.94	2 (6%)	50,54,54	1.49	8 (16%)
10	GDP	B	501	6	29,30,30	1.24	5 (17%)	45,47,47	1.62	5 (11%)
13	ACP	F	401	6	31,33,33	3.48	13 (41%)	47,52,52	1.86	14 (29%)
12	M5U	D	503	-	54,54,54	3.06	26 (48%)	62,70,70	4.02	26 (41%)
9	DMS	C	504	-	3,3,3	0.66	0	3,3,3	0.45	0
9	DMS	A	505	-	3,3,3	0.68	0	3,3,3	0.47	0
7	GOL	A	503	-	5,5,5	0.89	0	5,5,5	1.11	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3
11	MES	B	503	-	-	1/6/14/14	0/1/1/1
11	MES	B	504	-	-	3/6/14/14	0/1/1/1
10	GDP	D	501	6	-	5/16/32/32	0/3/3/3
10	GDP	B	501	6	-	4/16/32/32	0/3/3/3
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
13	ACP	F	401	6	-	7/19/38/38	0/3/3/3
12	M5U	D	503	-	-	24/70/70/70	0/2/3/3
7	GOL	A	503	-	-	0/4/4/4	-

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	401	ACP	PA-O3A	9.79	1.70	1.59
12	D	503	M5U	C35-N36	9.13	1.39	1.30
13	F	401	ACP	O4'-C1'	8.94	1.62	1.42
11	B	504	MES	C8-S	-7.93	1.66	1.77
11	B	503	MES	C8-S	-7.49	1.67	1.77

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	D	503	M5U	C37-N36-C35	11.14	112.81	103.69
12	D	503	M5U	C21-N20-C19	10.98	112.67	103.69
12	D	503	M5U	O39-C38-C37	9.54	115.16	108.12
12	D	503	M5U	O39-C35-N36	-9.51	104.28	114.79
12	D	503	M5U	O23-C22-C21	9.38	115.04	108.12

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

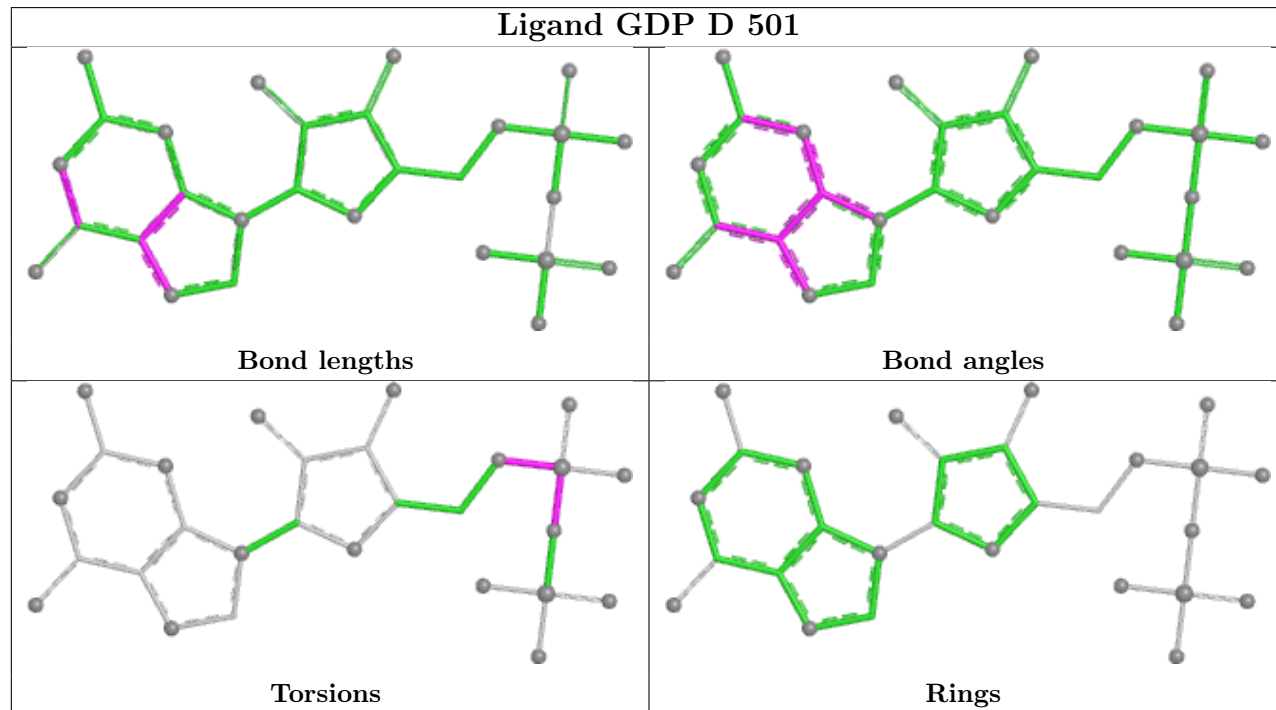
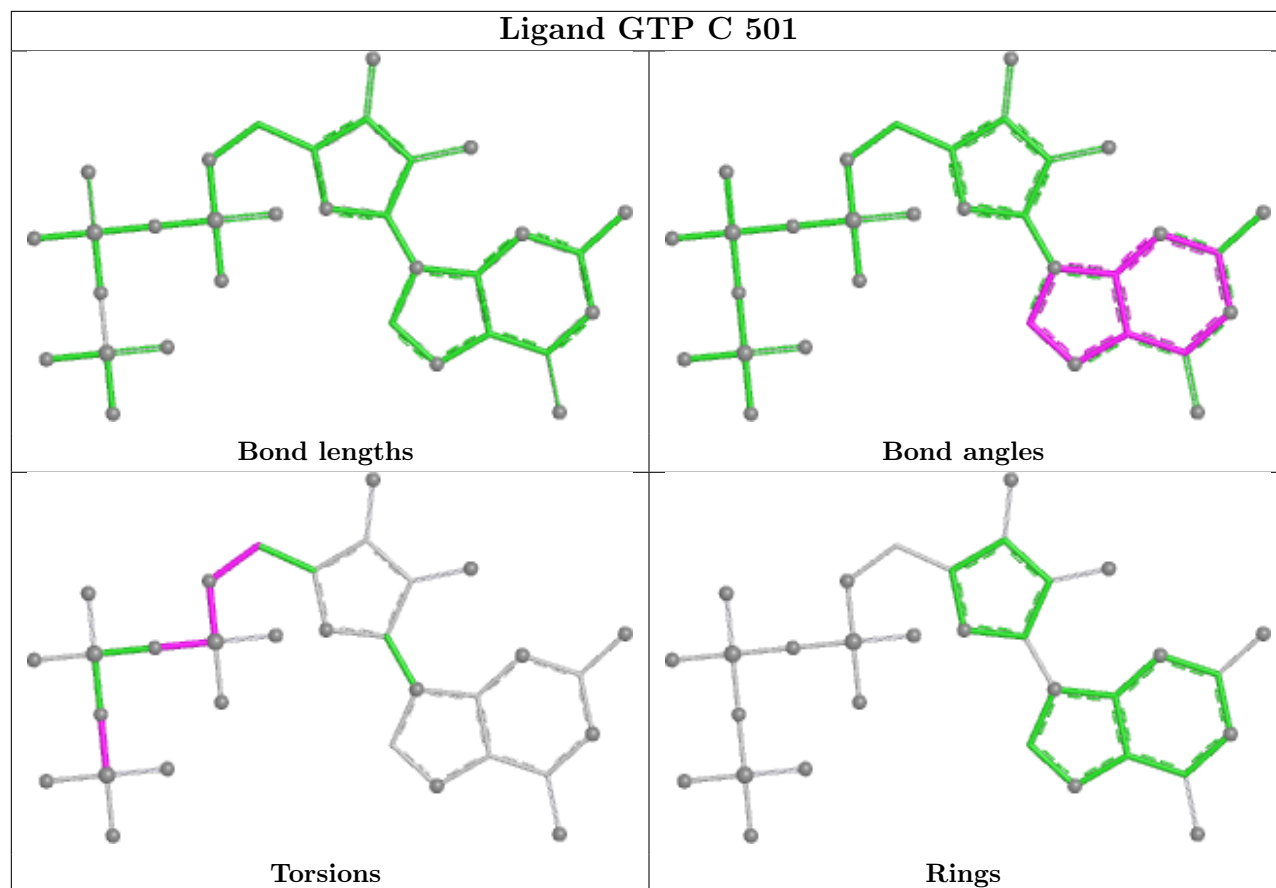
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A

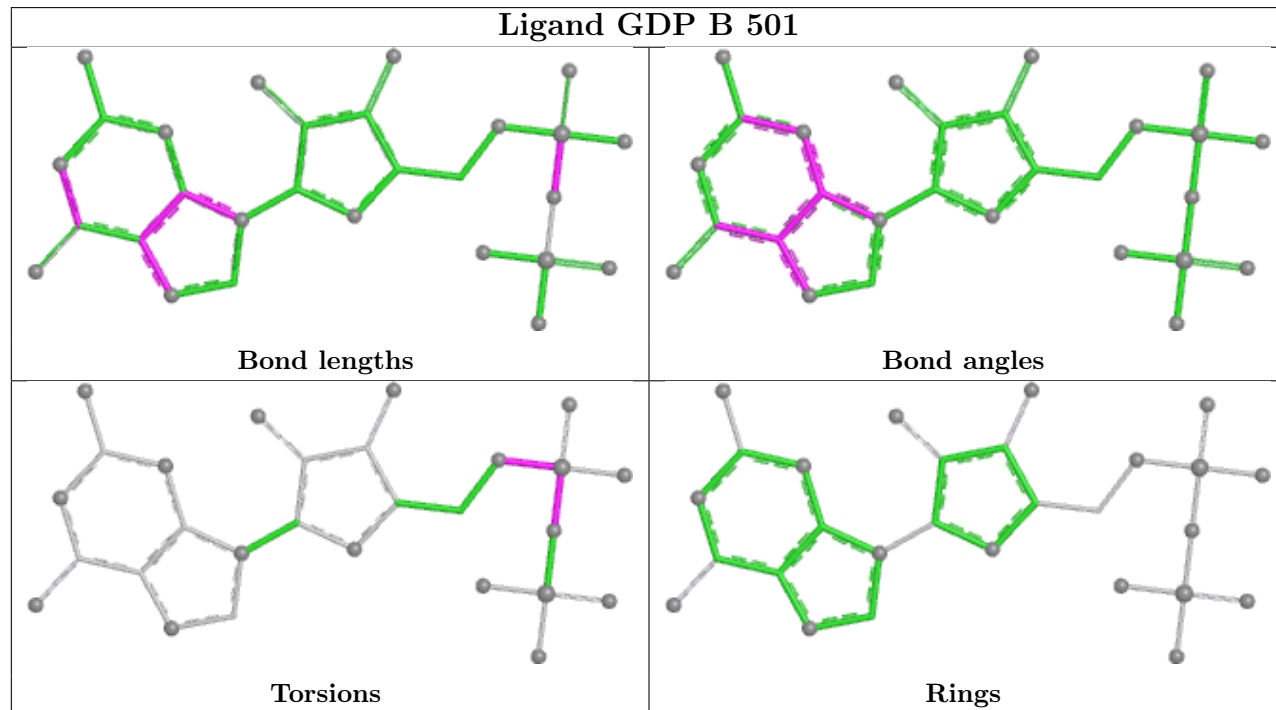
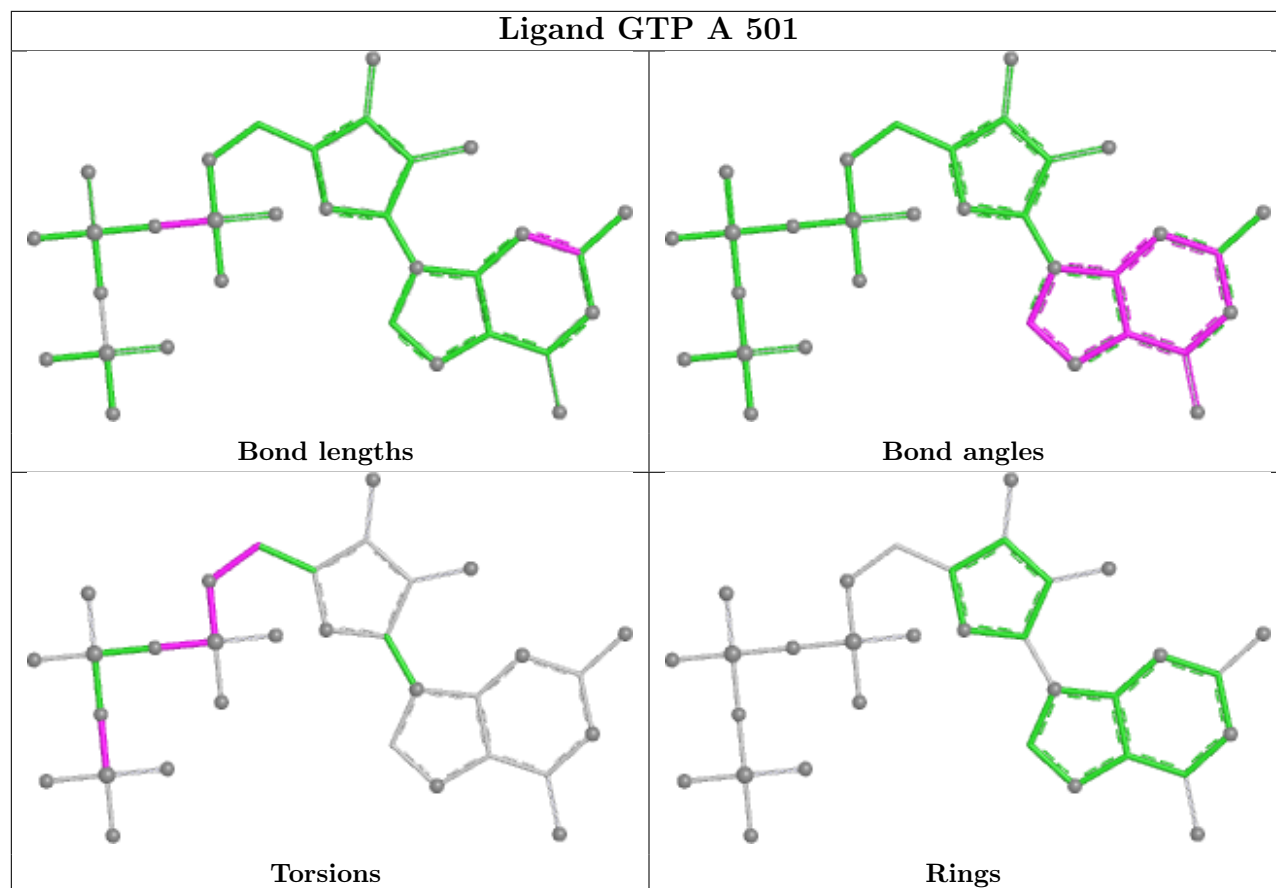
There are no ring outliers.

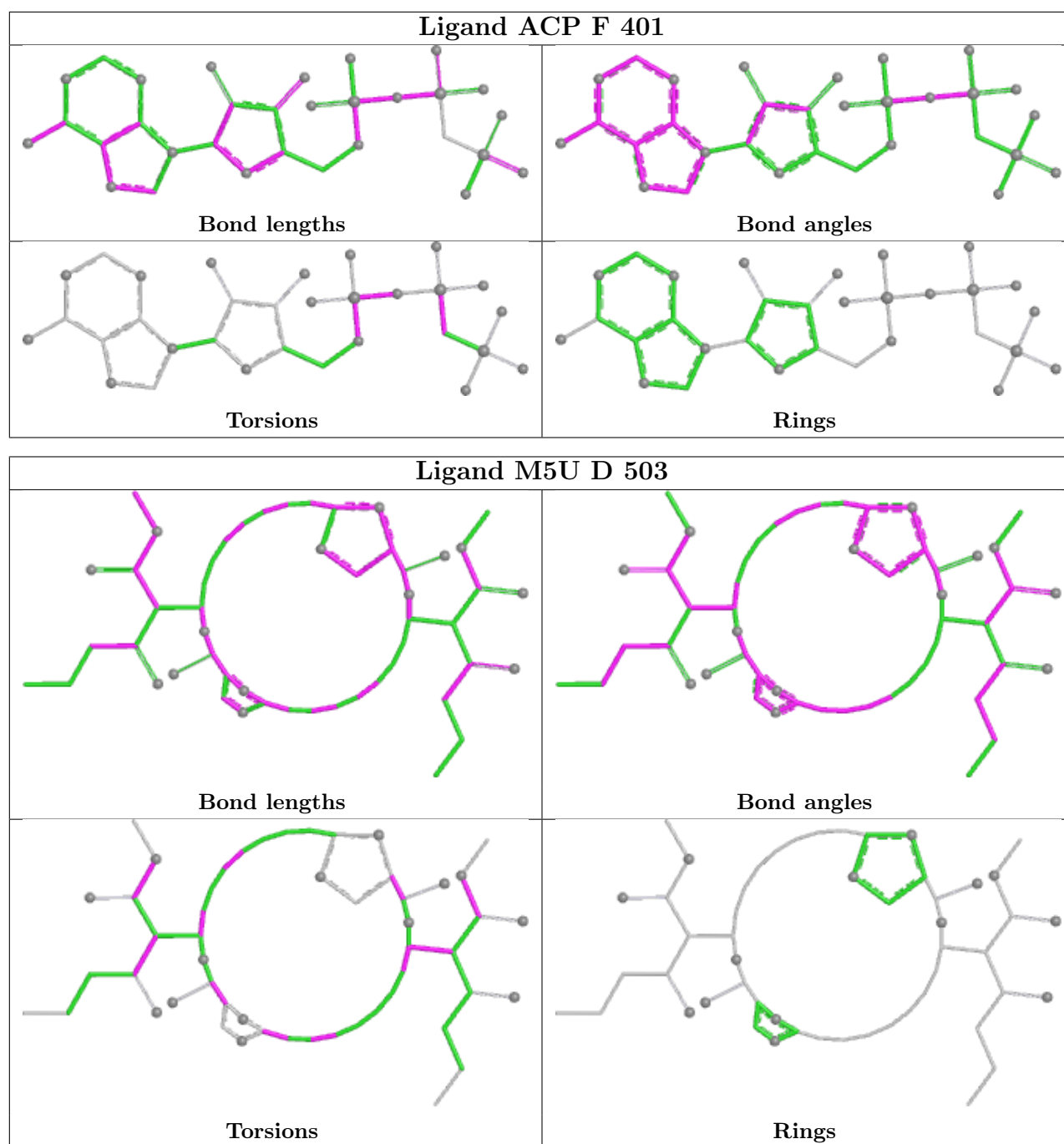
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	504	MES	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	0.30	9 (2%) 63 60	29, 59, 93, 141	4 (0%)
1	C	440/451 (97%)	-0.05	8 (1%) 67 64	22, 47, 80, 120	10 (2%)
2	B	425/445 (95%)	0.14	9 (2%) 63 60	26, 55, 94, 165	5 (1%)
2	D	420/445 (94%)	0.51	17 (4%) 42 38	41, 71, 103, 138	3 (0%)
3	E	121/189 (64%)	0.53	10 (8%) 17 14	30, 72, 109, 125	1 (0%)
4	F	315/384 (82%)	0.60	29 (9%) 14 11	34, 78, 129, 154	1 (0%)
All	All	2158/2365 (91%)	0.29	82 (3%) 44 40	22, 62, 104, 165	24 (1%)

The worst 5 of 82 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	440	VAL	6.4
1	C	88[A]	HIS	4.8
4	F	237	THR	4.8
2	D	276	THR	4.6
4	F	91	CYS	4.3

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

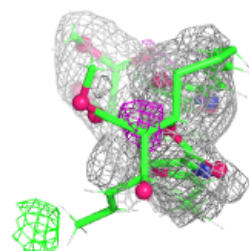
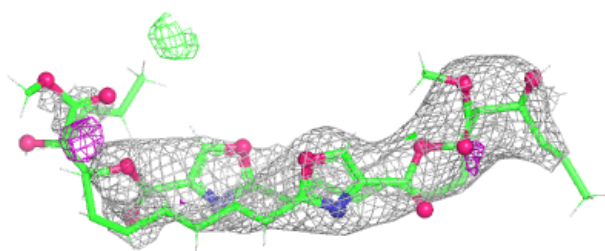
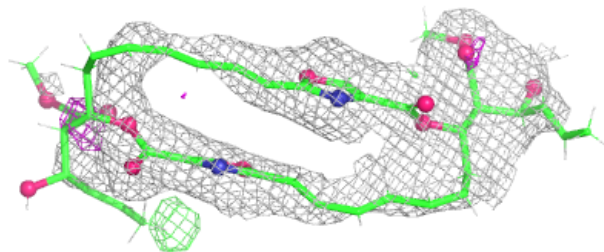
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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	DMS	A	505	4/4	0.60	0.22	67,72,84,116	0
12	M5U	D	503	52/52	0.72	0.18	80,96,132,142	0
8	CA	B	506	1/1	0.79	0.10	87,87,87,87	0
6	MG	F	402	1/1	0.82	0.09	80,80,80,80	0
11	MES	B	504	12/12	0.88	0.13	67,77,85,93	25
7	GOL	A	503	6/6	0.89	0.12	60,67,86,86	0
13	ACP	F	401	31/31	0.90	0.10	77,89,110,127	0
9	DMS	C	504	4/4	0.91	0.13	48,67,69,78	0
11	MES	B	503	12/12	0.92	0.12	45,55,66,73	0
8	CA	B	505	1/1	0.93	0.09	102,102,102,102	0
10	GDP	D	501	28/28	0.93	0.10	50,61,80,88	0
6	MG	D	502	1/1	0.94	0.06	59,59,59,59	0
10	GDP	B	501	28/28	0.97	0.07	30,39,49,58	0
5	GTP	A	501	32/32	0.97	0.06	33,43,50,56	0
6	MG	B	502	1/1	0.98	0.04	44,44,44,44	0
5	GTP	C	501	32/32	0.98	0.06	30,36,43,46	0
8	CA	A	504	1/1	0.99	0.04	72,72,72,72	0
8	CA	C	503	1/1	0.99	0.03	61,61,61,61	0
6	MG	C	502	1/1	1.00	0.02	33,33,33,33	0
6	MG	A	502	1/1	1.00	0.02	40,40,40,40	0

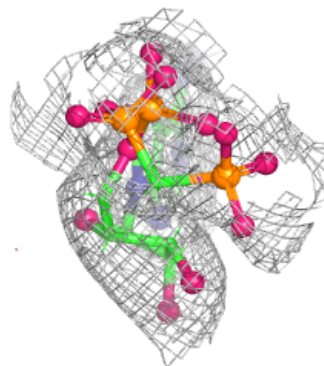
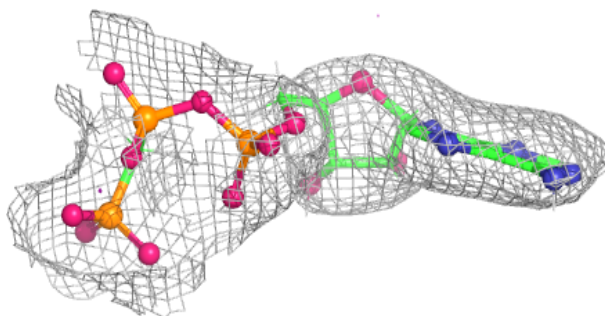
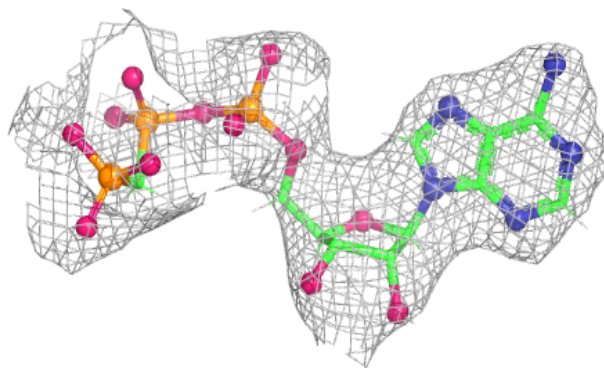
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around M5U 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)

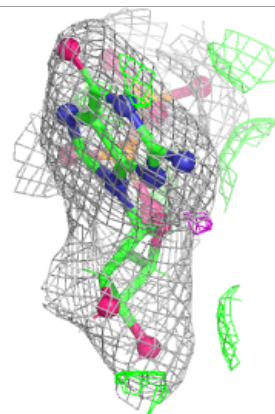
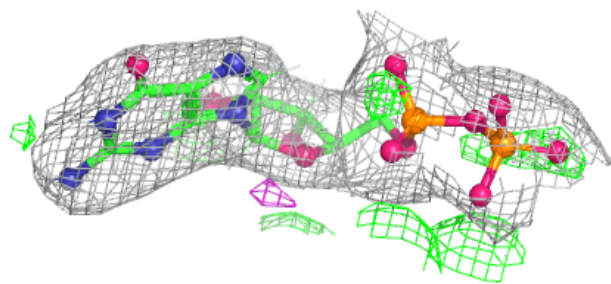
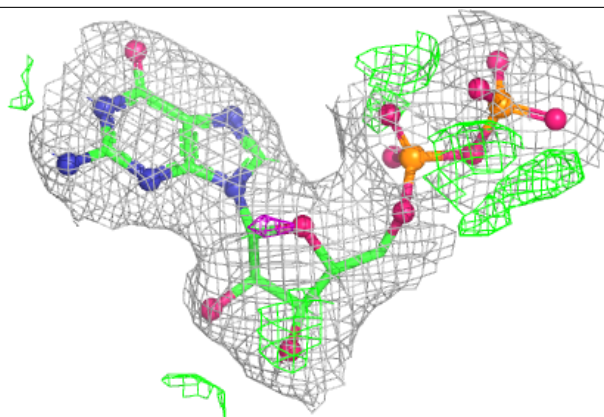
**Electron density around ACP F 401:**

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



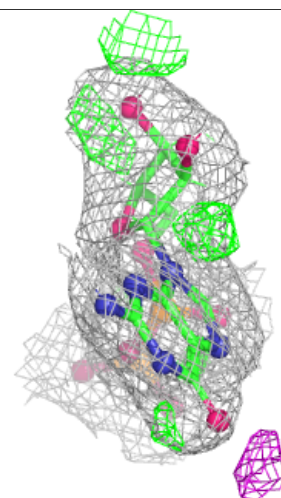
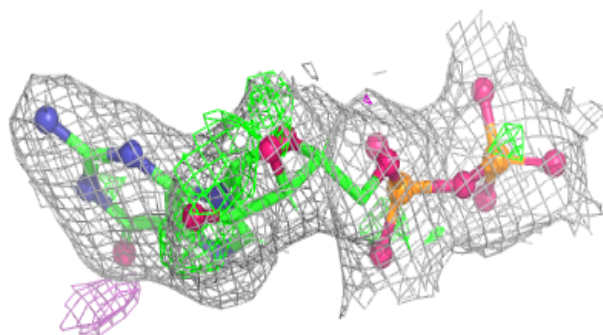
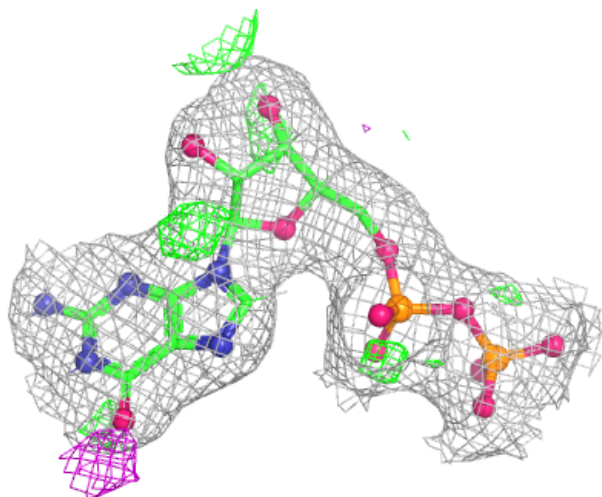
Electron density around GDP D 501:

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



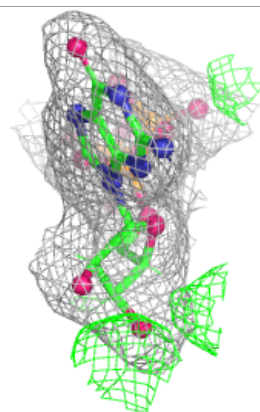
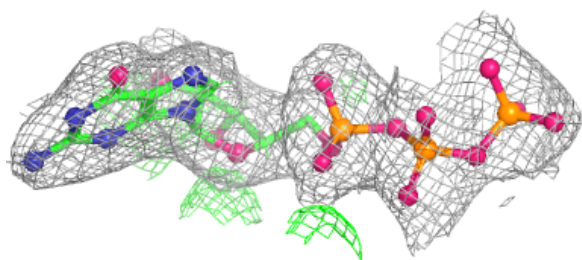
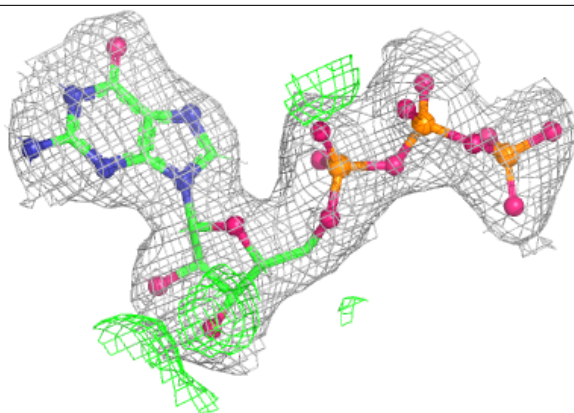
Electron density around GDP B 501:

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

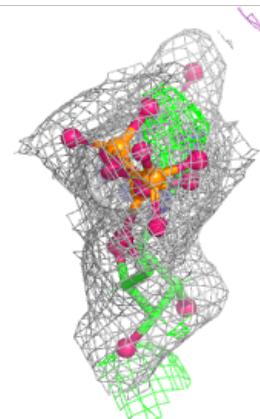
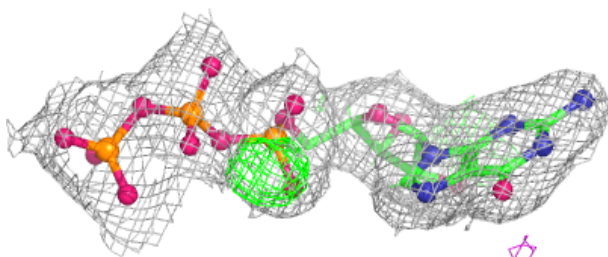
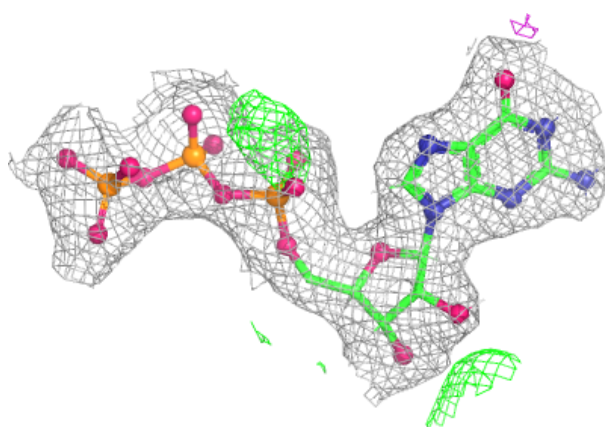


Electron density around GTP A 501:

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

**Electron density around 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.