



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2025 – 08:10 PM JST

PDB ID : 9IMO
Title : Crystal structure of Tubulin-RB3-TTL-Y12
Authors : Yan, W.; Yang, J.H.
Deposited on : 2024-07-04
Resolution : 2.75 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

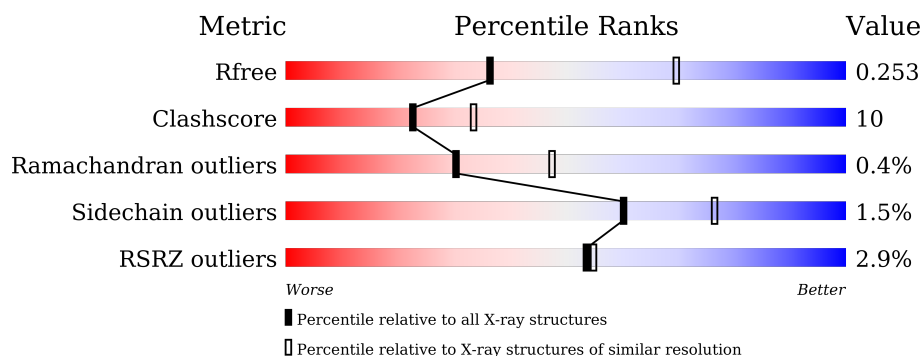
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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>0%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>
1	C	451	<div> <div>2%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
2	B	431	<div> <div>2%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
2	D	431	<div> <div>3%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
3	E	189	<div> <div>4%</div> <div>52%</div> <div>12%</div> <div>36%</div> </div>
4	F	384	<div> <div>5%</div> <div>66%</div> <div>16%</div> <div>17%</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17121 atoms, of which 68 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	6	0
			3409	2165	573	649	22			
1	C	440	Total	C	N	O	S	0	7	0
			3443	2185	577	659	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	3	0
			3275	2066	551	634	24			
2	D	421	Total	C	N	O	S	0	2	0
			3224	2032	543	624	25			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			943	586	171	181	5			

- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	320	Total	C	N	O	S	0	3	0
			2478	1609	409	449	11			

There are 39 discrepancies between the modelled and reference sequences:

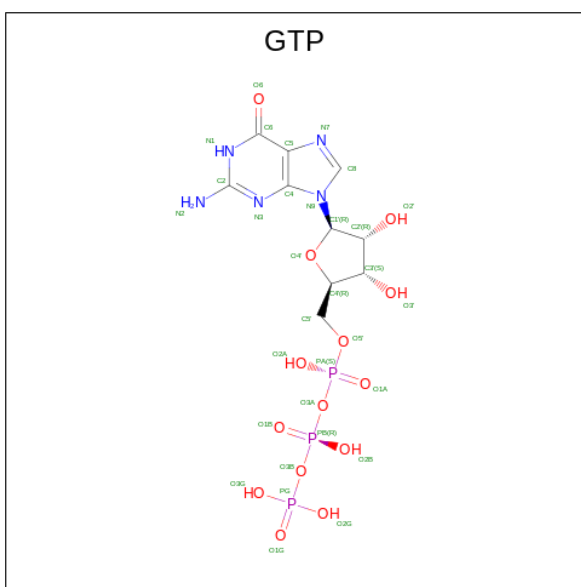
Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	MET	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	GLN	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	LEU	deletion	UNP A0A8V0Z8P0
F	?	-	ALA	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	THR	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	PRO	deletion	UNP A0A8V0Z8P0
F	?	-	GLU	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	VAL	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	SER	deletion	UNP A0A8V0Z8P0
F	?	-	ASP	deletion	UNP A0A8V0Z8P0
F	?	-	LYS	deletion	UNP A0A8V0Z8P0
F	?	-	ASN	deletion	UNP A0A8V0Z8P0
F	?	-	HIS	deletion	UNP A0A8V0Z8P0
F	?	-	GLY	deletion	UNP A0A8V0Z8P0
F	?	-	PHE	deletion	UNP A0A8V0Z8P0
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

- 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	
			32	10	5	14	3	0
5	C	1	Total	C	N	O	P	
			32	10	5	14	3	0

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

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

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

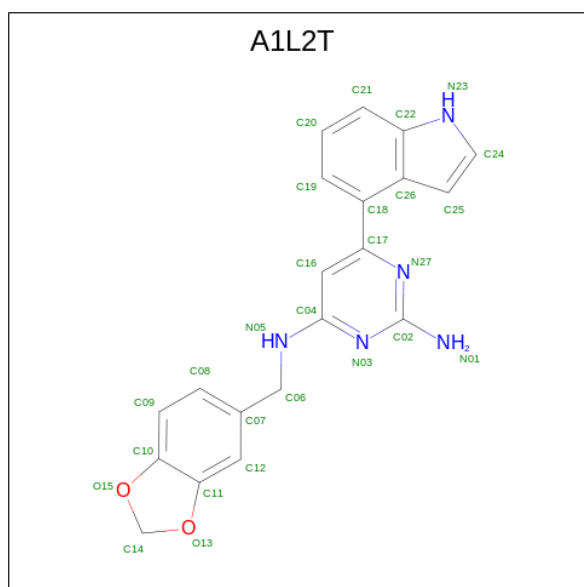
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca		
			1	1	0	0
7	B	1	Total	Ca		
			1	1	0	0

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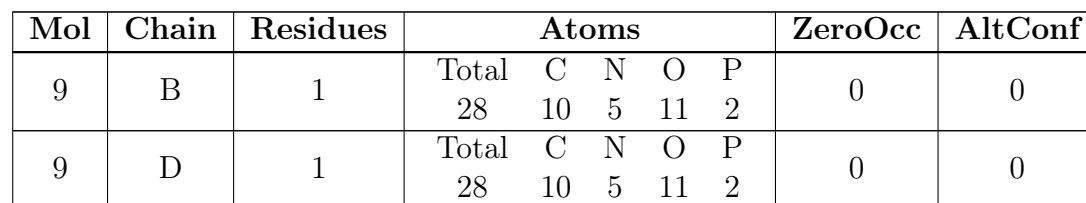
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is {N}4-(1,3-benzodioxol-5-ylmethyl)-6-(1 {H}-indol-4-yl)pyrimidine-2,4-diamine (three-letter code: A1L2T) (formula: C₂₀H₁₇N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	0	0
			44	20	17	5	2		
8	B	1	Total	C	H	N	O	0	0
			44	20	17	5	2		
8	B	1	Total	C	H	N	O	0	0
			44	20	17	5	2		
8	D	1	Total	C	H	N	O	0	0
			44	20	17	5	2		

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



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- The chemical structure of Adenosine 3'-phosphate (AdP) is shown. It consists of an adenine base (a purine ring system with an amino group at the 6-position) connected to a ribose sugar (a five-membered ring with hydroxyl groups at the 2' and 3' positions). The ribose sugar is linked to a triphosphate chain (three phosphate groups connected in series) via a phosphodiester bond at the 3' position. The structure is labeled with atom names (N1, N3, N7, C2, C4, C5, C6, C8, 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, O806, O807

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

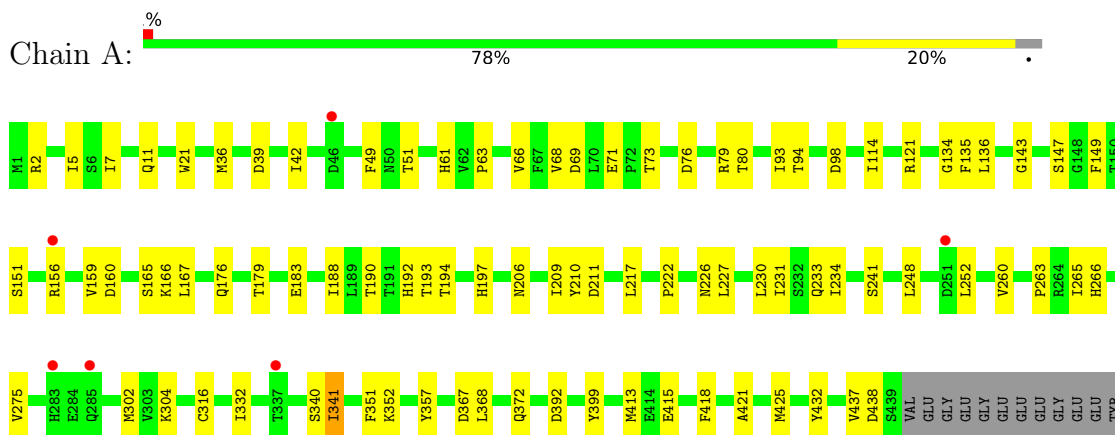
- Molecule 11 is water.

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

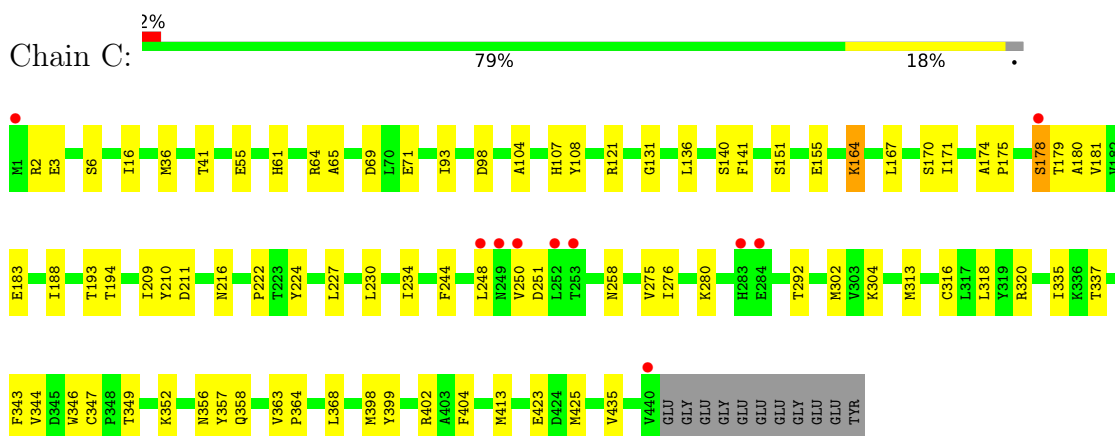
3 Residue-property plots [i](#)

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.

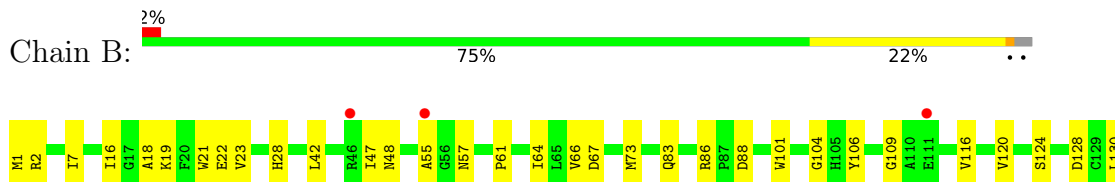
- Molecule 1: Tubulin alpha-1B chain

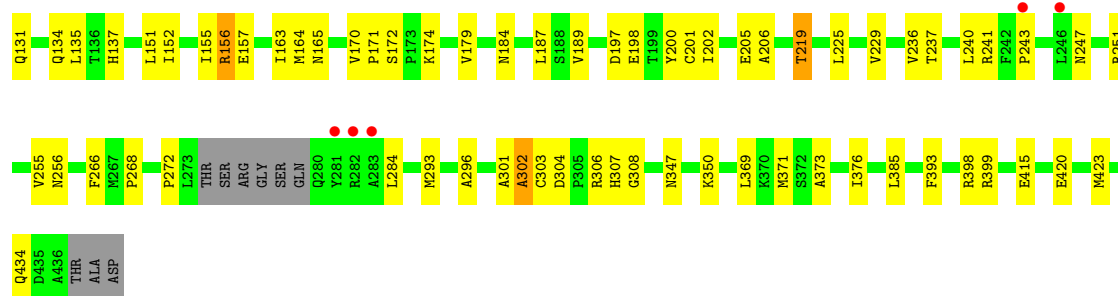


- Molecule 1: Tubulin alpha-1B chain

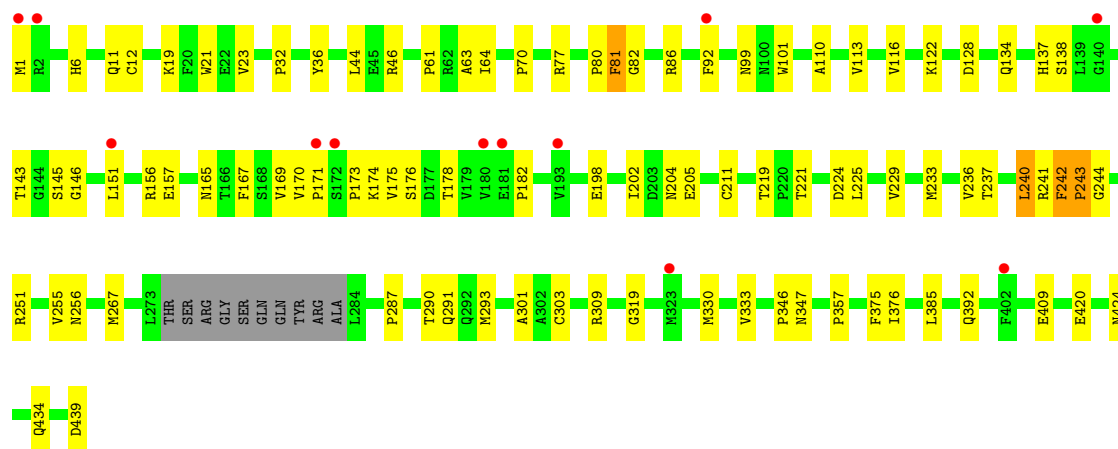
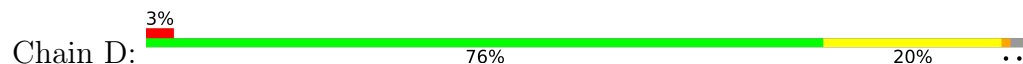


- Molecule 2: Tubulin beta chain

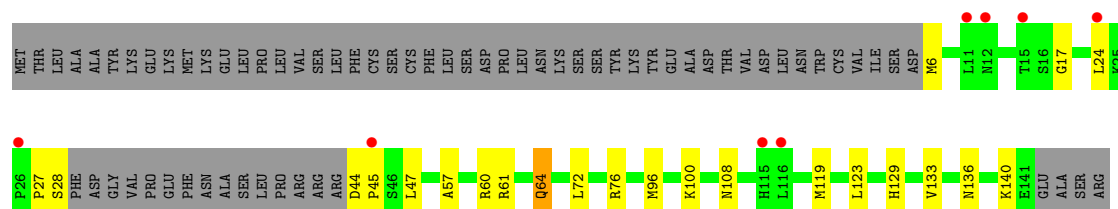




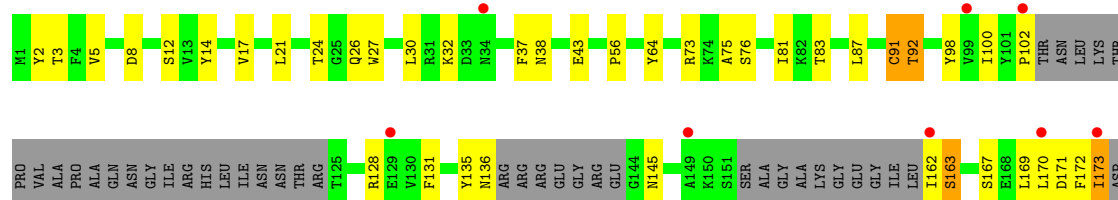
• Molecule 2: Tubulin beta chain

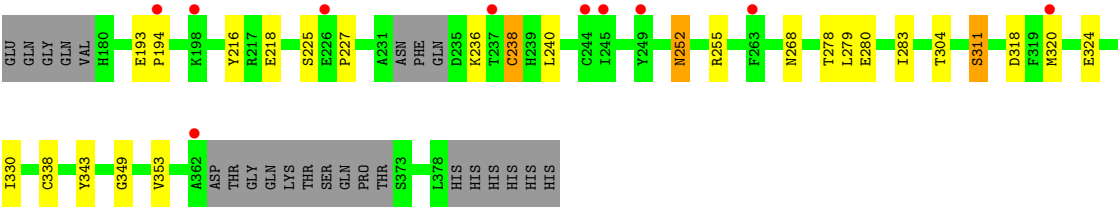


• Molecule 3: Stathmin-4



• 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	105.27Å 158.14Å 179.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.35 – 2.75 41.35 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.35-2.75) 99.8 (41.35-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.211 , 0.255 0.211 , 0.253	Depositor DCC
R_{free} test set	76633 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	79.1	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17121	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, A1L2T, CA, GTP, ACP, MG

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	0.32	0/3504	0.57	0/4767
1	C	0.35	0/3542	0.60	0/4814
2	B	0.35	0/3358	0.61	0/4561
2	D	0.31	0/3303	0.57	0/4496
3	E	0.35	0/951	0.58	0/1269
4	F	0.29	0/2543	0.55	0/3463
All	All	0.33	0/17201	0.58	0/23370

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

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	3409	0	3300	75	0
1	C	3443	0	3352	69	0
2	B	3275	0	3110	75	0
2	D	3224	0	3030	74	0
3	E	943	0	928	19	0
4	F	2478	0	2352	47	0
5	A	32	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	27	17	0	0	0
8	B	54	34	0	2	0
8	D	27	17	0	2	0
9	B	28	0	12	0	0
9	D	28	0	12	4	0
10	F	31	0	14	2	0
11	A	1	0	0	0	0
11	B	2	0	0	1	0
11	C	9	0	0	3	0
11	D	2	0	0	1	0
All	All	17053	68	16134	343	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 10.

The worst 5 of 343 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:A:188:ILE:HD12	1:A:425:MET:HG3	1.30	1.06
4:F:81:ILE:HD13	4:F:87:LEU:HD13	1.38	1.03
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.43	0.99
2:D:101:TRP:HD1	2:D:145:SER:HG	1.14	0.96
2:B:16[B]:ILE:HD13	2:B:229:VAL:HG11	1.47	0.96

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	443/451 (98%)	433 (98%)	10 (2%)	0	100	100
1	C	445/451 (99%)	434 (98%)	9 (2%)	2 (0%)	30	47
2	B	421/431 (98%)	410 (97%)	10 (2%)	1 (0%)	44	63
2	D	419/431 (97%)	406 (97%)	10 (2%)	3 (1%)	19	32
3	E	117/189 (62%)	113 (97%)	3 (3%)	1 (1%)	14	26
4	F	309/384 (80%)	287 (93%)	20 (6%)	2 (1%)	22	36
All	All	2154/2337 (92%)	2083 (97%)	62 (3%)	9 (0%)	30	47

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	302	ALA
2	D	243	PRO
3	E	27	PRO
4	F	92	THR
1	C	178	SER

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	363/379 (96%)	362 (100%)	1 (0%)	91	95
1	C	372/379 (98%)	368 (99%)	4 (1%)	70	83
2	B	352/370 (95%)	346 (98%)	6 (2%)	56	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	342/370 (92%)	339 (99%)	3 (1%)	75	86
3	E	95/171 (56%)	92 (97%)	3 (3%)	34	55
4	F	256/342 (75%)	246 (96%)	10 (4%)	27	48
All	All	1780/2011 (88%)	1753 (98%)	27 (2%)	60	76

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	28	SER
4	F	12	SER
4	F	238	CYS
3	E	64	GLN
4	F	136	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	285	GLN
2	B	256	ASN
2	D	256	ASN
3	E	64	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 8 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	$\# Z > 2$
5	GTP	A	501	6	26,34,34	1.14	2 (7%)	32,54,54	1.40	5 (15%)
8	A1L2T	A	504	-	29,31,31	1.31	5 (17%)	39,44,44	1.31	6 (15%)
8	A1L2T	D	502	-	29,31,31	1.71	5 (17%)	39,44,44	1.70	9 (23%)
9	GDP	D	503	6	24,30,30	1.00	1 (4%)	30,47,47	1.24	4 (13%)
9	GDP	B	505	6	24,30,30	0.93	1 (4%)	30,47,47	1.12	3 (10%)
5	GTP	C	501	6	26,34,34	1.17	2 (7%)	32,54,54	1.45	5 (15%)
8	A1L2T	B	503	-	29,31,31	1.58	3 (10%)	39,44,44	1.68	9 (23%)
8	A1L2T	B	504	-	29,31,31	1.36	4 (13%)	39,44,44	1.56	8 (20%)
10	ACP	F	402	-	27,33,33	1.56	6 (22%)	32,52,52	1.24	4 (12%)

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	A	501	6	-	4/18/38/38	0/3/3/3
8	A1L2T	A	504	-	-	1/9/15/15	0/5/5/5
8	A1L2T	D	502	-	-	2/9/15/15	0/5/5/5
9	GDP	D	503	6	-	4/12/32/32	0/3/3/3
9	GDP	B	505	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
8	A1L2T	B	503	-	-	2/9/15/15	0/5/5/5
8	A1L2T	B	504	-	-	1/9/15/15	0/5/5/5
10	ACP	F	402	-	-	6/15/38/38	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	502	A1L2T	C04-N05	5.63	1.44	1.36
8	B	503	A1L2T	C04-N05	5.21	1.44	1.36
5	C	501	GTP	C5-C6	-4.11	1.39	1.47
10	F	402	ACP	PB-O3A	3.83	1.62	1.58
5	A	501	GTP	C5-C6	-3.80	1.39	1.47

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	502	A1L2T	C18-C17-N27	-4.96	109.65	116.14
8	B	503	A1L2T	C06-N05-C04	3.93	131.13	123.40
8	D	502	A1L2T	C06-N05-C04	3.93	131.13	123.40
8	B	504	A1L2T	C06-N05-C04	3.88	131.04	123.40
8	D	502	A1L2T	C16-C17-C18	3.59	127.93	121.05

There are no chirality outliers.

5 of 30 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
8	B	503	A1L2T	C16-C04-N05-C06

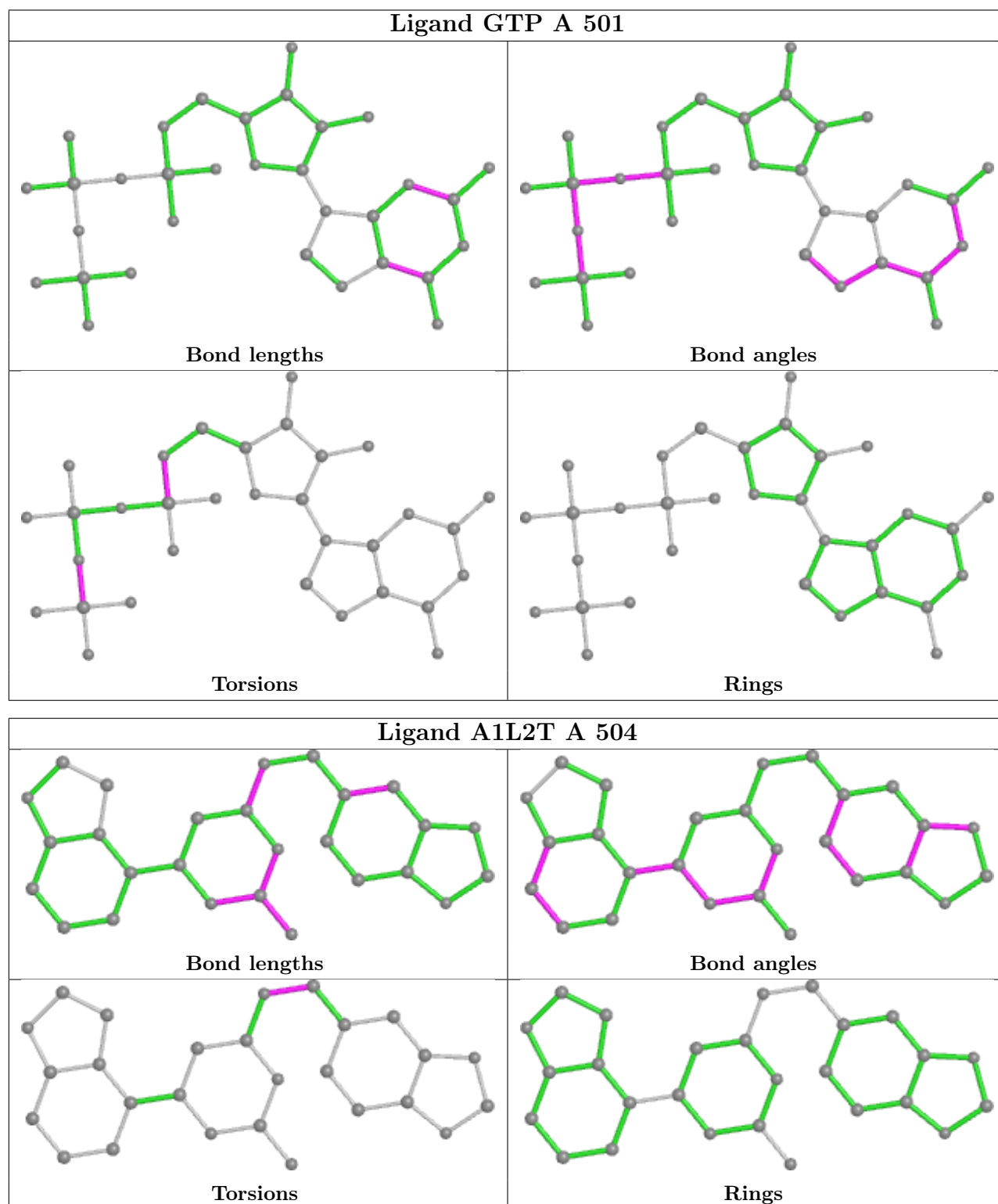
There are no ring outliers.

6 monomers are involved in 12 short contacts:

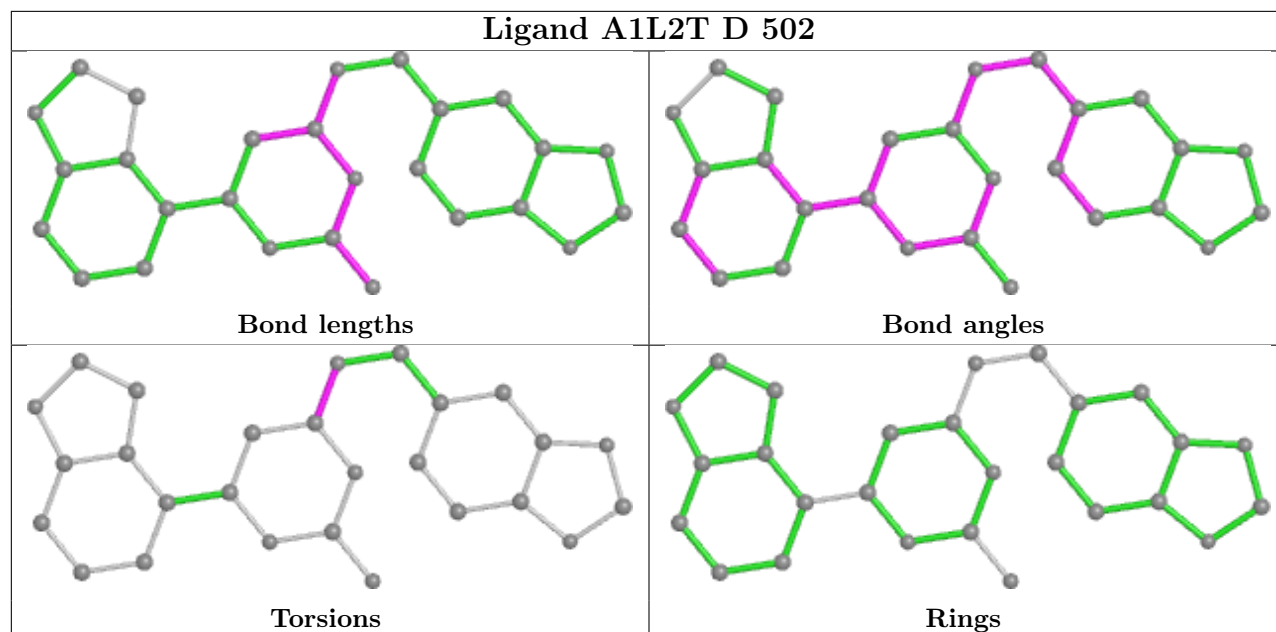
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	2	0
8	D	502	A1L2T	2	0
9	D	503	GDP	4	0
8	B	503	A1L2T	1	0
8	B	504	A1L2T	1	0
10	F	402	ACP	2	0

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

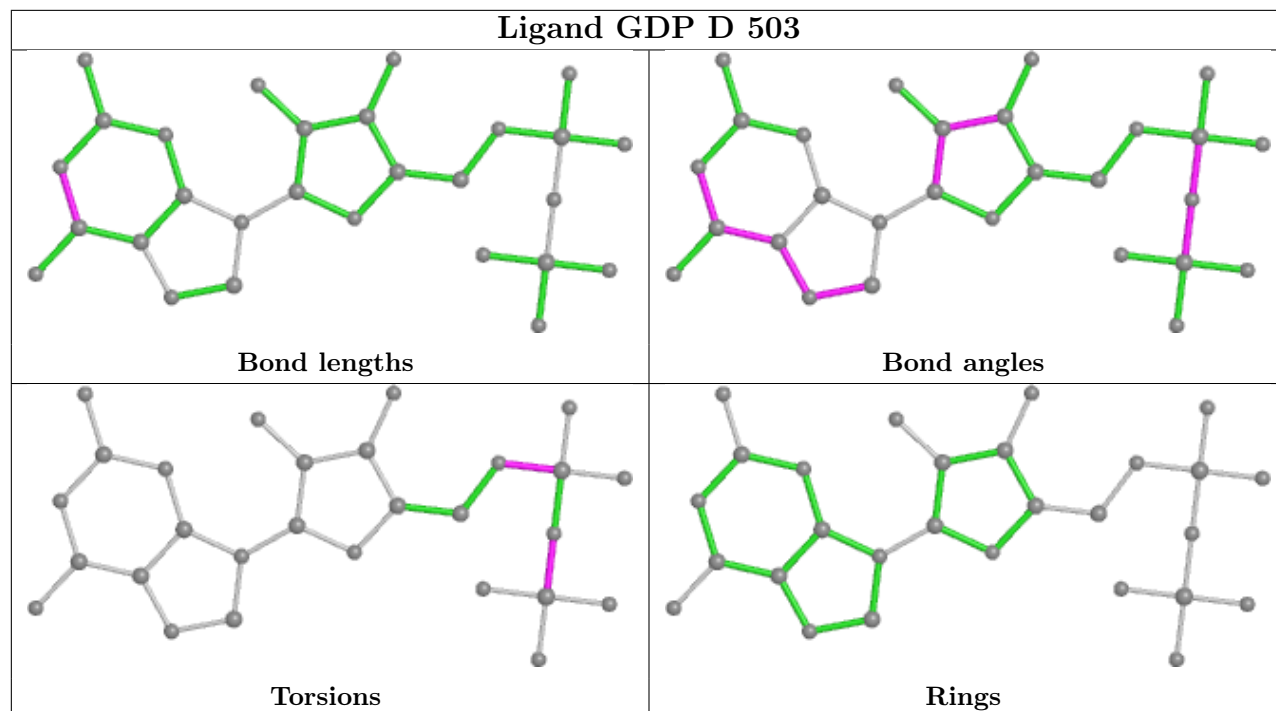
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

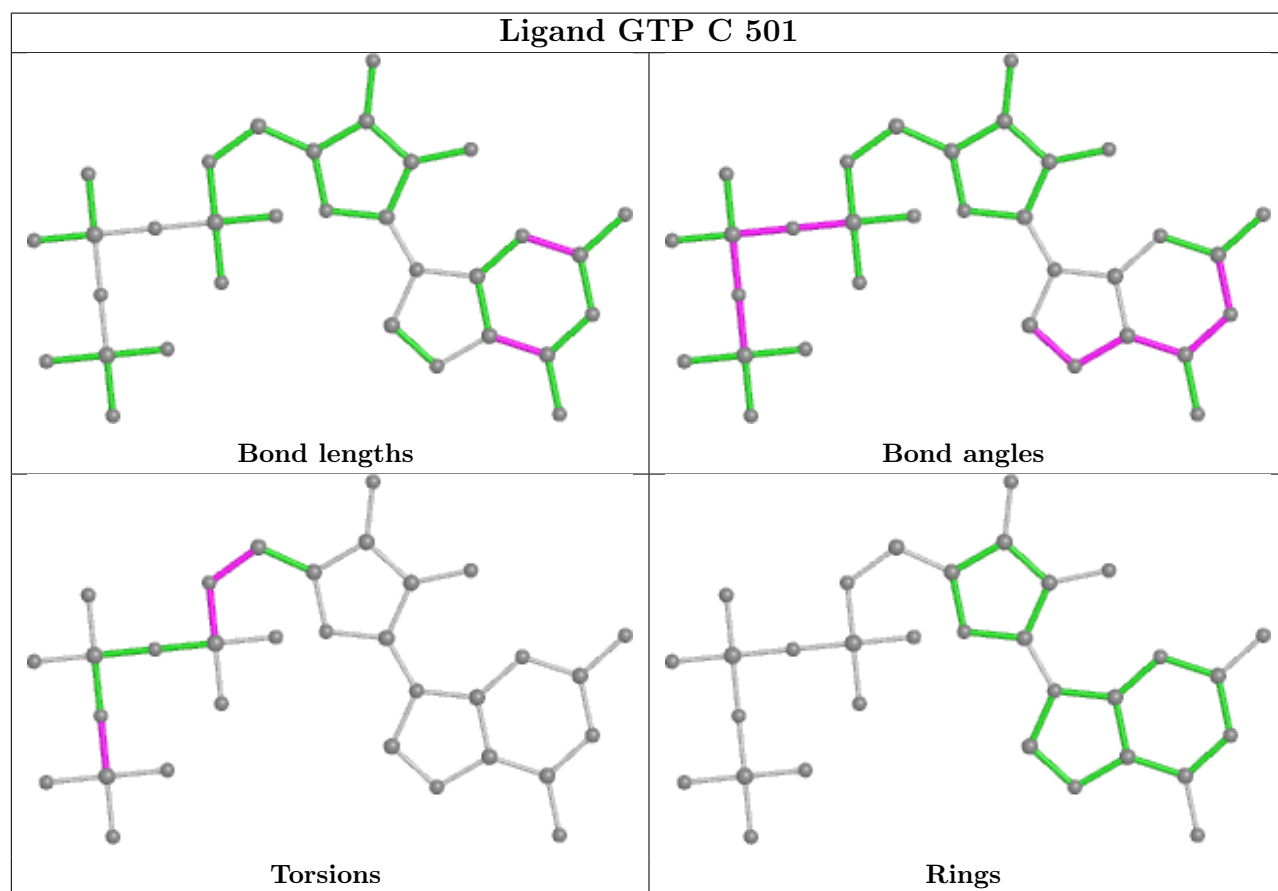
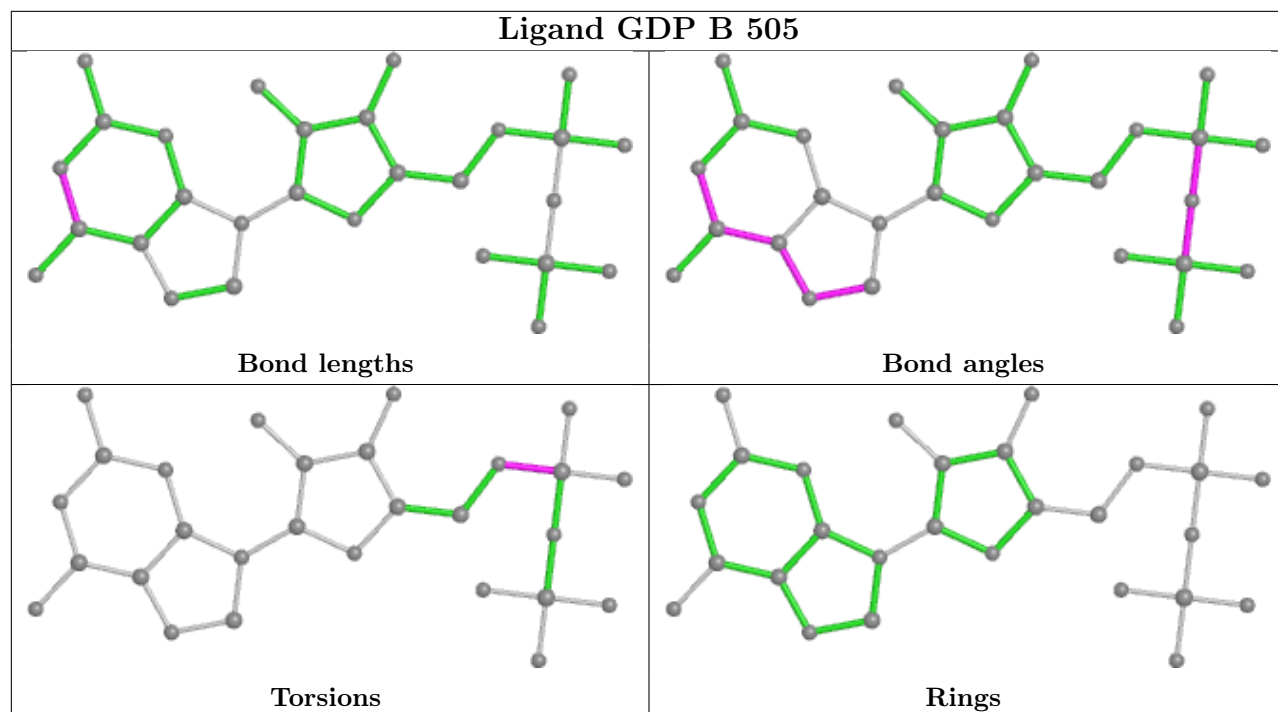


Ligand A1L2T D 502

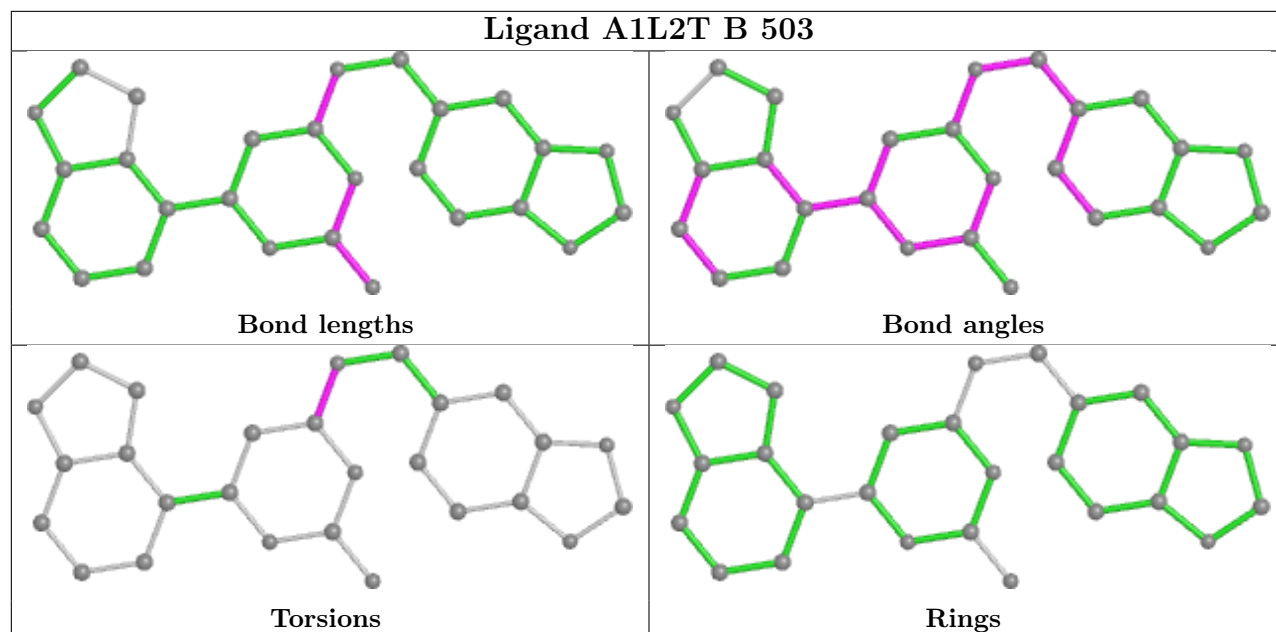


Ligand GDP D 503

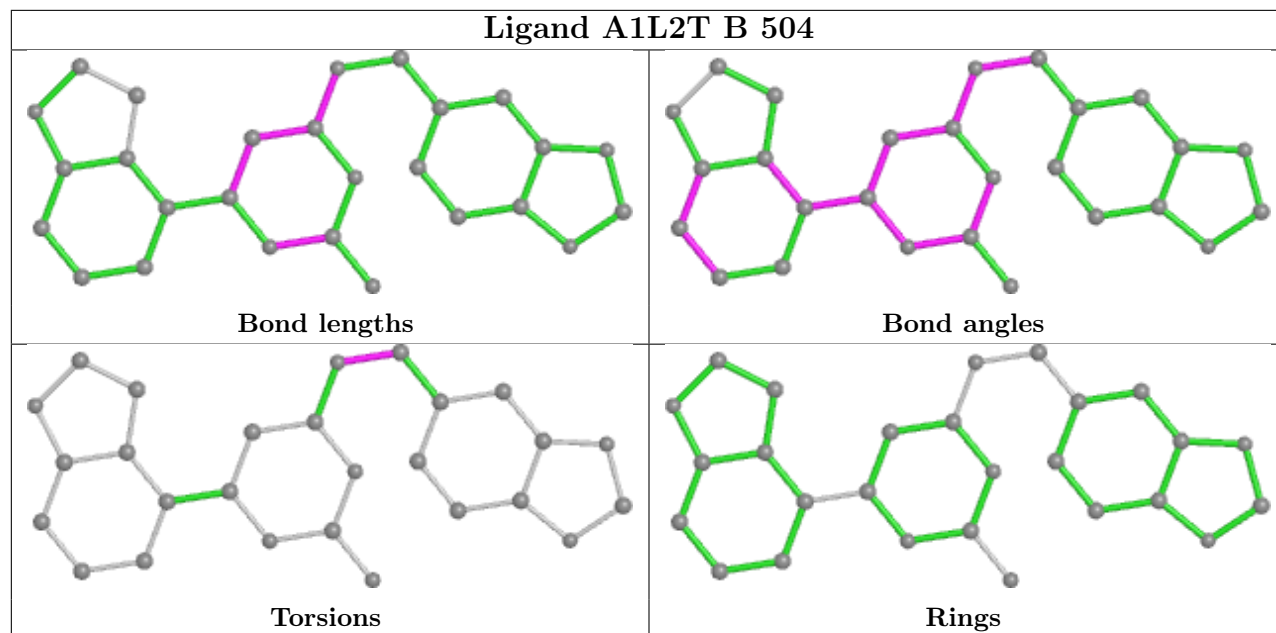




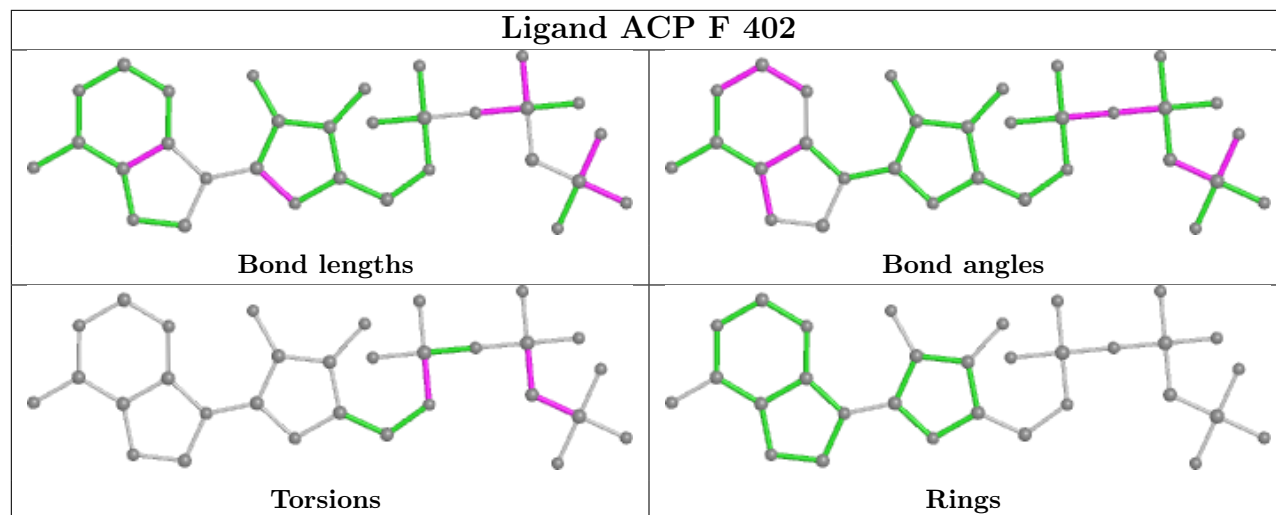
Ligand A1L2T B 503



Ligand A1L2T B 504



Ligand ACP F 402



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	439/451 (97%)	0.19	6 (1%) 73 75	39, 75, 106, 136	6 (1%)
1	C	440/451 (97%)	-0.02	10 (2%) 61 61	33, 64, 92, 115	7 (1%)
2	B	422/431 (97%)	0.15	8 (1%) 66 67	39, 73, 106, 128	4 (0%)
2	D	421/431 (97%)	0.45	12 (2%) 54 55	47, 91, 115, 132	3 (0%)
3	E	121/189 (64%)	0.44	8 (6%) 26 29	60, 88, 126, 137	0
4	F	320/384 (83%)	0.61	18 (5%) 31 33	59, 105, 139, 154	3 (0%)
All	All	2163/2337 (92%)	0.27	62 (2%) 54 55	33, 81, 120, 154	23 (1%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	178	SER	5.0
4	F	149	ALA	4.2
1	C	249	ASN	4.0
4	F	170	LEU	3.6
1	C	1	MET	3.6

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

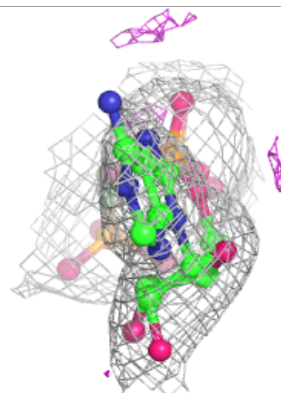
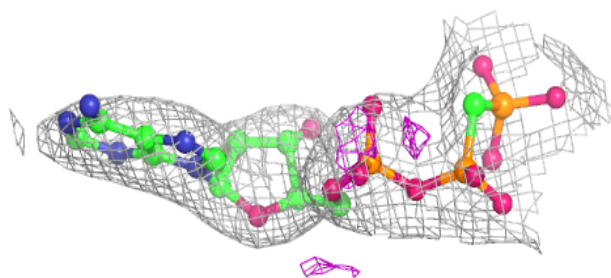
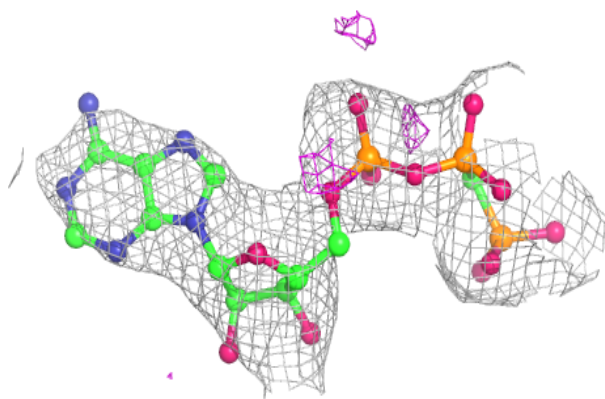
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	A	502	1/1	0.71	0.39	71,71,71,71	0
6	MG	F	401	1/1	0.72	0.14	123,123,123,123	0
6	MG	C	502	1/1	0.76	0.34	71,71,71,71	0
7	CA	C	503	1/1	0.83	0.12	129,129,129,129	0
10	ACP	F	402	31/31	0.84	0.10	116,127,152,158	0
6	MG	B	501	1/1	0.85	0.26	88,88,88,88	0
9	GDP	D	503	28/28	0.86	0.12	71,80,96,107	0
8	A1L2T	B	504	27/27	0.88	0.13	66,83,103,110	0
6	MG	D	501	1/1	0.90	0.28	68,68,68,68	0
8	A1L2T	A	504	27/27	0.91	0.10	64,78,93,103	0
8	A1L2T	D	502	27/27	0.93	0.10	58,77,97,101	0
8	A1L2T	B	503	27/27	0.94	0.11	51,68,98,109	0
9	GDP	B	505	28/28	0.94	0.08	50,59,74,76	0
7	CA	B	502	1/1	0.95	0.11	121,121,121,121	0
5	GTP	A	501	32/32	0.95	0.08	49,62,71,82	0
7	CA	A	503	1/1	0.95	0.05	117,117,117,117	0
5	GTP	C	501	32/32	0.96	0.08	49,57,65,69	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.

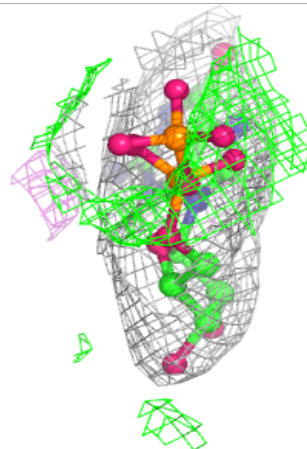
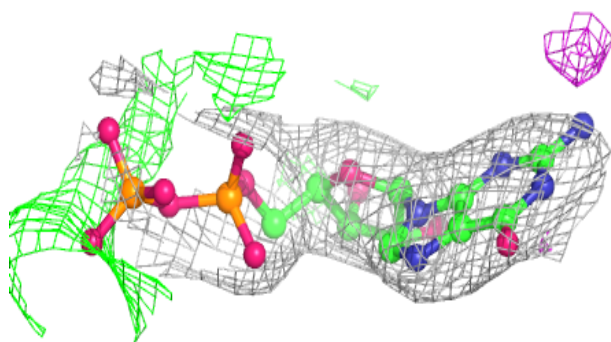
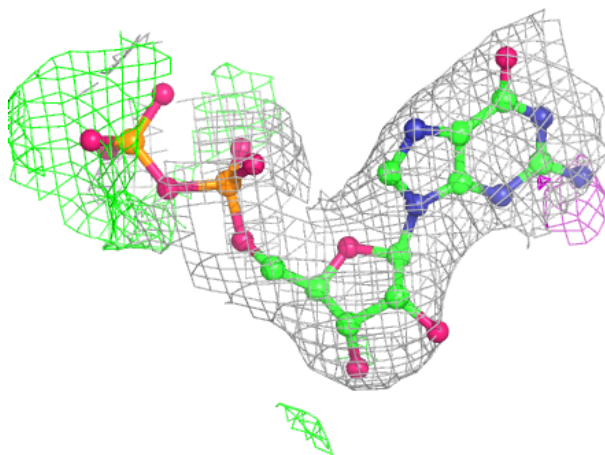
Electron density around ACP F 402:

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



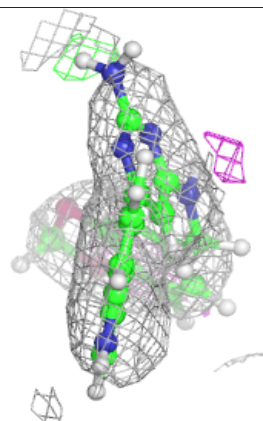
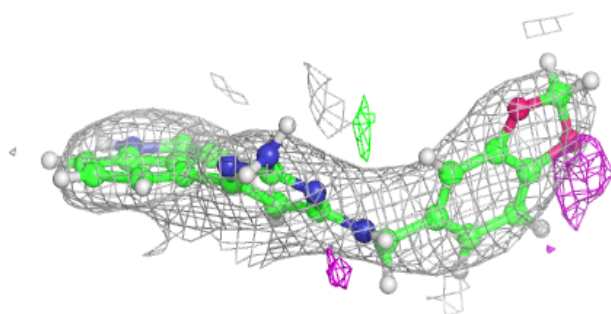
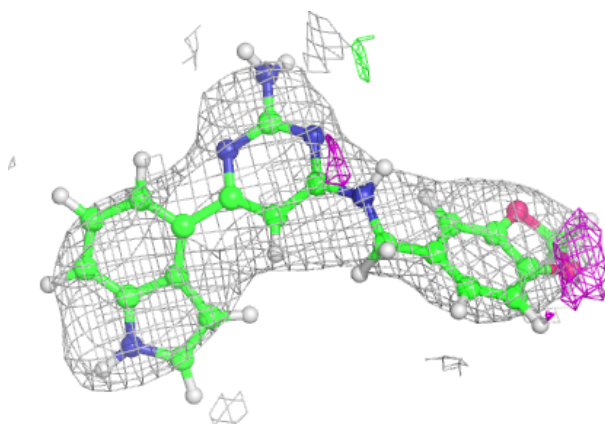
Electron density around GDP D 503:

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and green (positive)

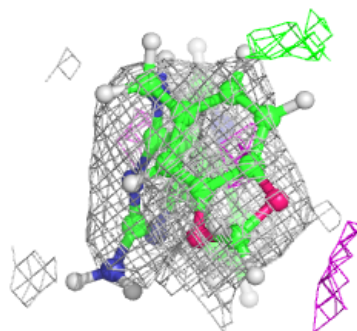
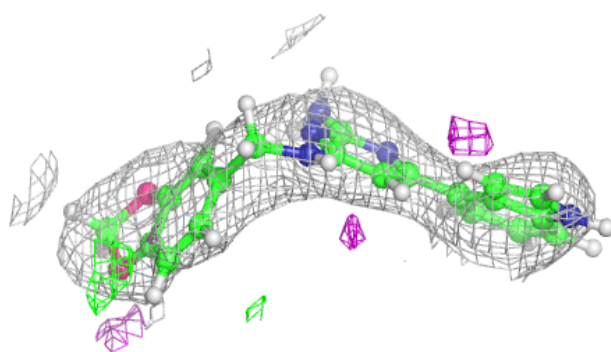
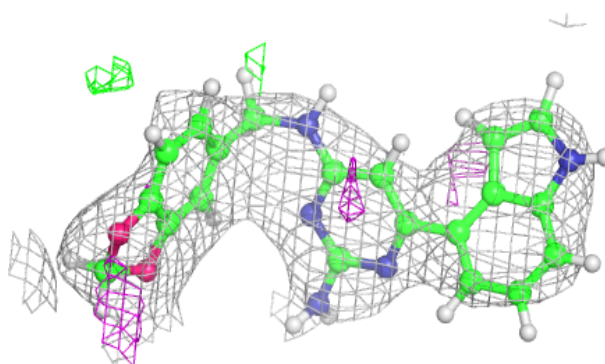


Electron density around A1L2T B 504:

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and green (positive)

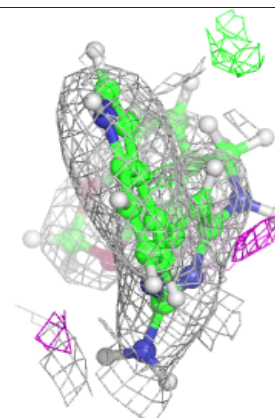
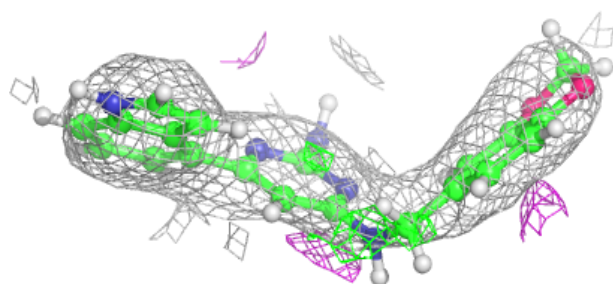
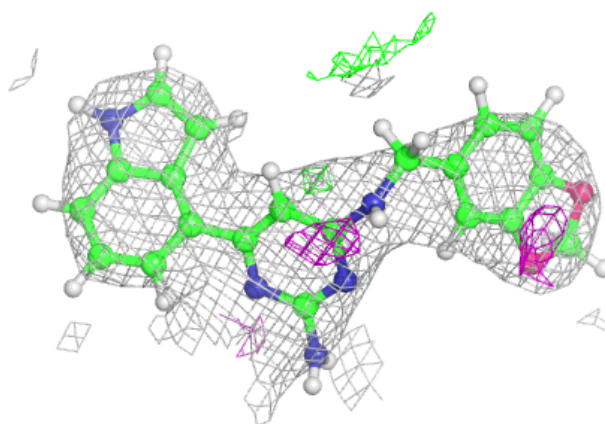
**Electron density around A1L2T A 504:**

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and green (positive)

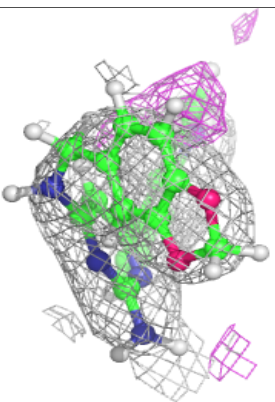
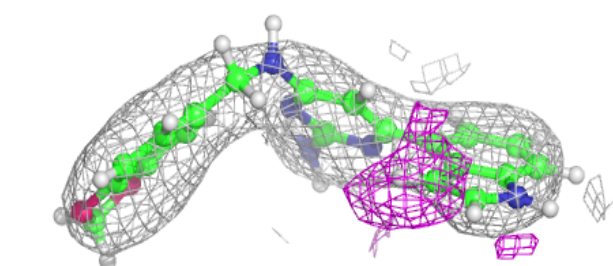
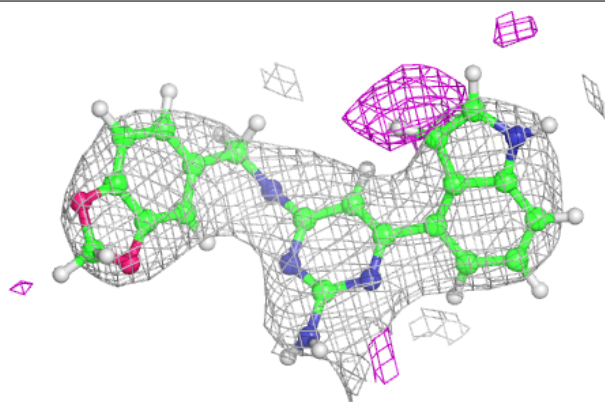


Electron density around A1L2T D 502:

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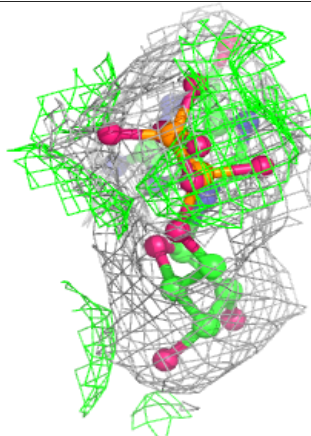
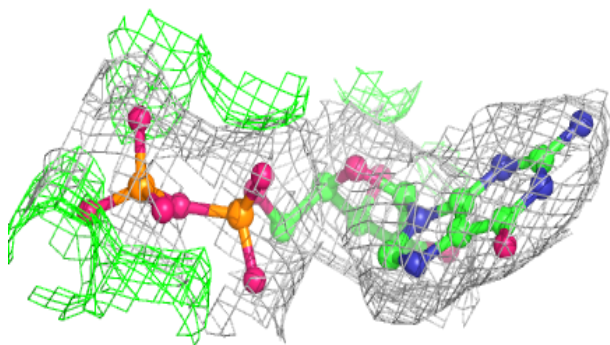
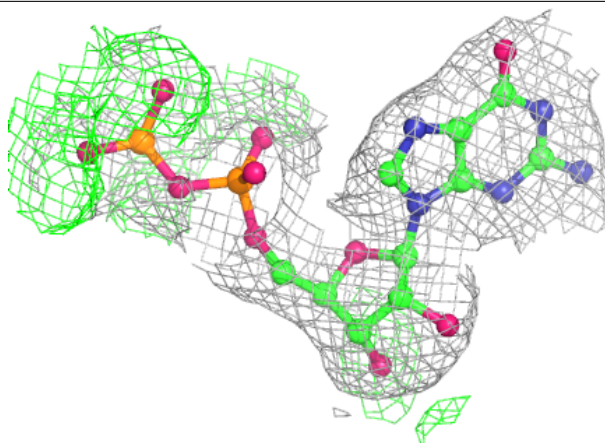
**Electron density around A1L2T B 503:**

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

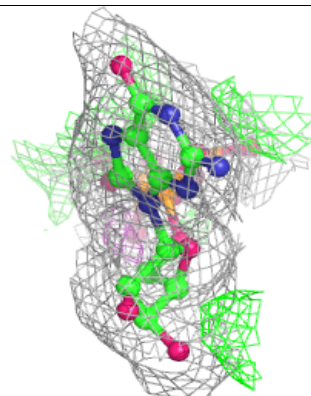
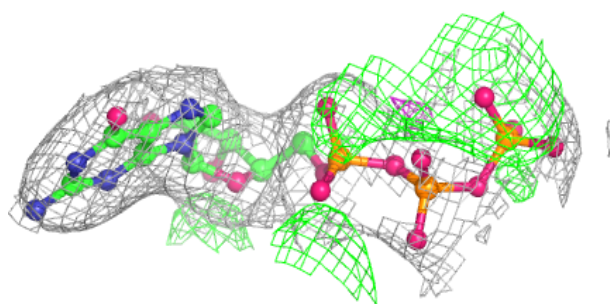
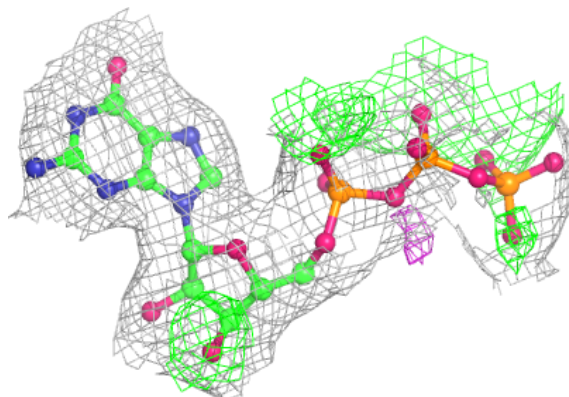


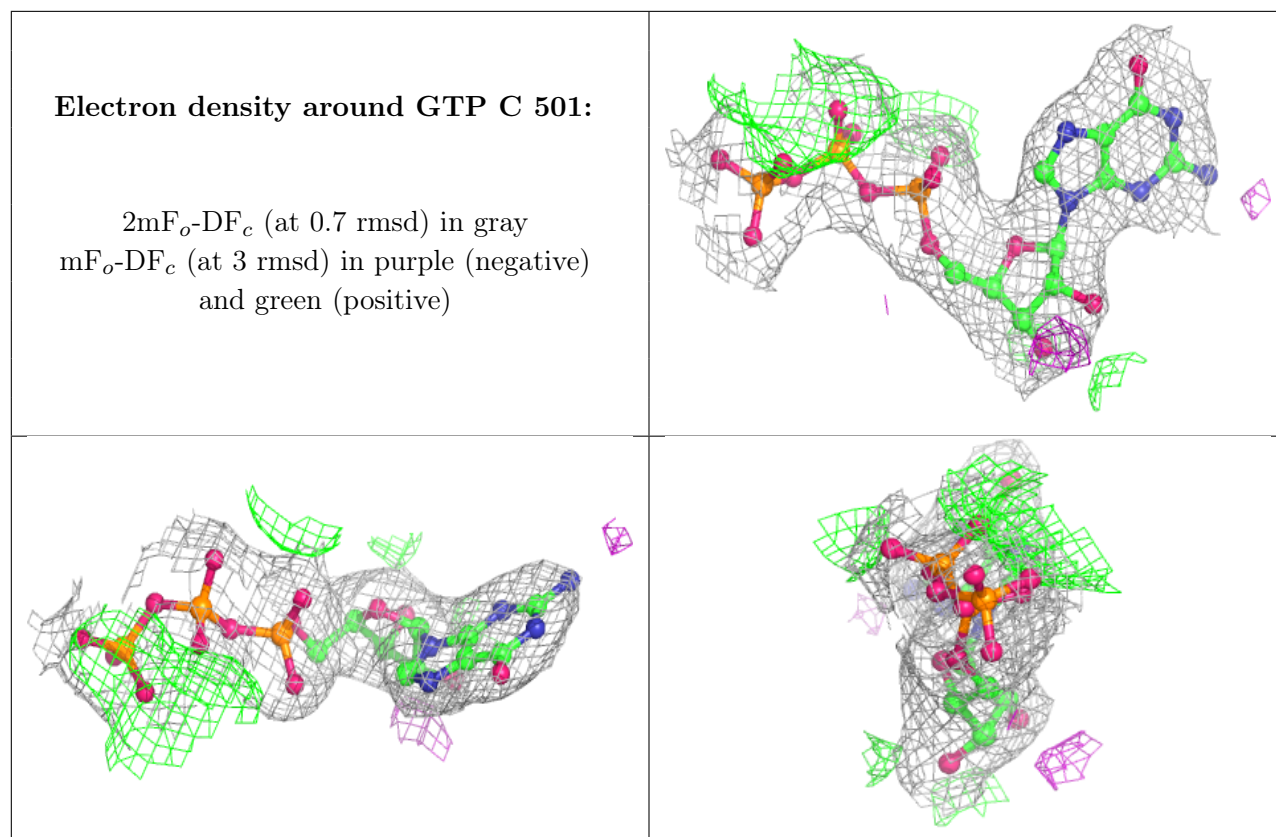
Electron density around GDP B 505:

$2mF_o-DF_c$ (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.