



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:41 am BST

PDB ID : 5M8G
Title : Tubulin-MTD265 complex
Authors : Bohnacker, T.; Protá, A.E.; Steinmetz, M.O.; Wymann, M.P.
Deposited on : 2016-10-28
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

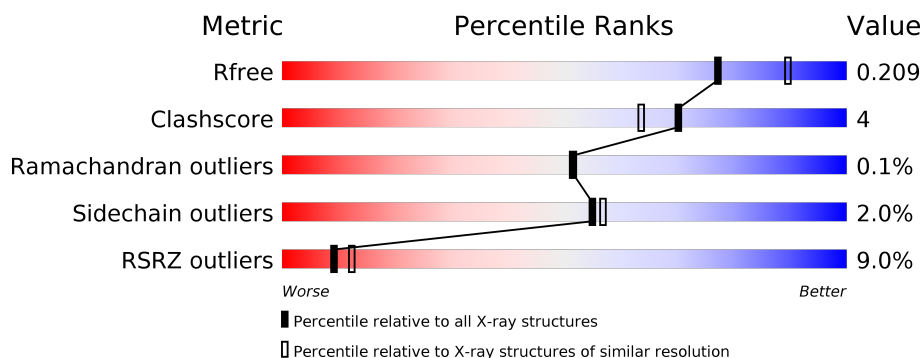
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 on 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>5%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>•</div> </div> </div>
1	C	451	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>••</div> </div> </div>
2	B	445	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>5%</div> </div> </div>
2	D	445	<div> <div>9%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>•</div> </div> </div>
3	E	143	<div> <div>10%</div> <div> <div></div> <div>77%</div> <div>9%</div> <div>14%</div> </div> </div>
4	F	384	<div> <div>24%</div> <div> <div></div> <div>79%</div> <div>7%</div> <div>•</div> <div>14%</div> </div> </div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 18016 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	1	0
			3436	2172	584	657	23			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	0	0
			3331	2094	568	643	26			
2	D	427	Total	C	N	O	S	0	0	0
			3349	2101	572	650	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	331	Total	C	N	O	S	0	0	0
			2724	1756	461	493	14			

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

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

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

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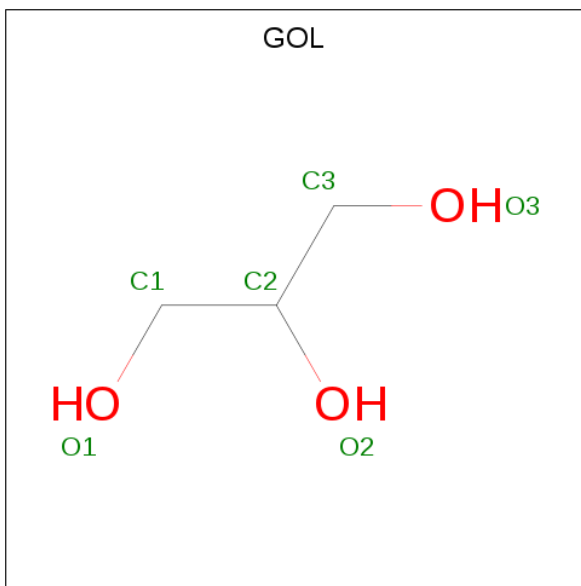
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

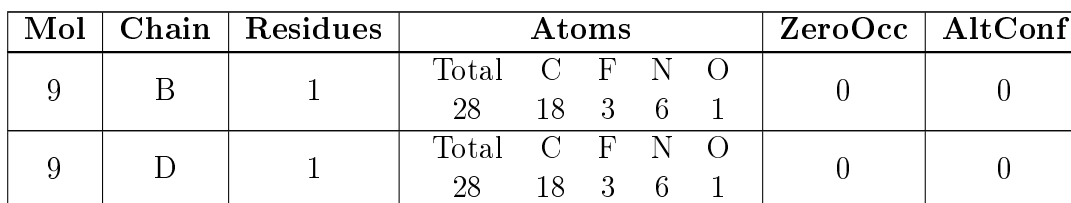
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	2	Total	Ca	0	0
			2	2		
7	A	2	Total	Ca	0	0
			2	2		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is 5-(2-morpholin-4-yl-6-pyrrolidin-1-yl-pyrimidin-4-yl)-4-(trifluoromethyl)pyridine-2-amine (three-letter code: 918) (formula: C₁₈H₂₁F₃N₆O).



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- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine ring system with an amino group at C2) linked to a ribose sugar (a five-membered ring with hydroxyl groups at C2' and C3'). The ribose is further linked to two phosphate groups (P4(S) and P3(S)) via phosphodiester bonds. The structure is labeled with atom names and numbers, including C1, C2, C3, C4, C5, C6, C7, C8, C9, C10, C11, C12, C13, C14, C15, C16, C17, C18, C19, C20, C21, C22, C23, C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34, C35, C36, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, C52, C53, C54, C55, C56, C57, C58, C59, C60, C61, C62, C63, C64, C65, C66, C67, C68, C69, C70, C71, C72, C73, C74, C75, C76, C77, C78, C79, C80, C81, C82, C83, C84, C85, C86, C87, C88, C89, C90, C91, C92, C93, C94, C95, C96, C97, C98, C99, C100, C101, C102, C103, C104, C105, C106, C107, C108, C109, C110, C111, C112, C113, C114, C115, C116, C117, C118, C119, C120, C121, C122, C123, C124, C125, C126, C127, C128, C129, C130, C131, C132, C133, C134, C135, C136, C137, C138, C139, C140, C141, C142, C143, C144, C145, C146, C147, C148, C149, C150, C151, C152, C153, C154, C155, C156, C157, C158, C159, C160, C161, C162, C163, C164, C165, C166, C167, C168, C169, C170, C171, C172, C173, C174, C175, C176, C177, C178, C179, C180, C181, C182, C183, C184, C185, C186, C187, C188, C189, C190, C191, C192, C193, C194, C195, C196, C197, C198, C199, C200, C201, C202, C203, C204, C205, C206, C207, C208, C209, C210, C211, C212, C213, C214, C215, C216, C217, C218, C219, C220, C221, C222, C223, C224, C225, C226, C227, C228, C229, C230, C231, C232, C233, C234, C235, C236, C237, C238, C239, C240, C241, C242, C243, C244, C245, C246, C247, C248, C249, C250, C251, C252, C253, C254, C255, C256, C257, C258, C259, C260, C261, C262, C263, C264, C265, C266, C267, C268, C269, C270, C271, C272, C273, C274, C275, C276, C277, C278, C279, C280, C281, C282, C283, C284, C285, C286, C287, C288, C289, C290, C291, C292, C293, C294, C295, C296, C297, C298, C299, C300, C301, C302, C303, C304, C305, C306, C307, C308, C309, C310, C311, C312, C313, C314, C315, C316, C317, C318, C319, C320, C321, C322, C323, C324, C325, C326, C327, C328, C329, C330, C331, C332, C333, C334, C335, C336, C337, C338, C339, C340, C341, C342, C343, C344, C345, C346, C347, C348, C349, C350, C351, C352, C353, C354, C355, C356, C357, C358, C359, C360, C361, C362, C363, C364, C365, C366, C367, C368, C369, C370, C371, C372, C373, C374, C375, C376, C377, C378, C379, C380, C381, C382, C383, C384, C385, C386, C387, C388, C389, C390, C391, C392, C393, C394, C395, C396, C397, C398, C399, C400, C401, C402, C403, C404, C405, C406, C407, C408, C409, C410, C411, C412, C413, C414, C415, C416, C417, C418, C419, C420, C421, C422, C423, C424, C425, C426, C427, C428, C429, C430, C431, C432, C433, C434, C435, C436, C437, C438, C439, C440, C441, C442, C443, C444, C445, C446, C447, C448, C449, C450, C451, C452, C453, C454, C455, C456, C457, C458, C459, C460, C461, C462, C463, C464, C465, C466, C467, C468, C469, C470, C471, C472, C473, C474, C475, C476, C477, C478, C479, C480, C481, C482, C483, C484, C485, C486, C487, C488, C489, C490, C491, C492, C493, C494, C495, C496, C497, C498, C499, C500, C501, C502, C503, C504, C505, C506, C507, C508, C509, C510, C511, C512, C513, C514, C515, C516, C517, C518, C519, C520, C521, C522, C523, C524, C525, C526, C527, C528, C529, C530, C531, C532, C533, C534, C535, C536, C537, C538, C539, C540, C541, C542, C543, C544, C545, C546, C547, C548, C549, C550, C551, C552, C553, C554, C555, C556, C557, C558, C559, C560, C561, C562, C563, C564, C565, C566, C567, C568, C569, C570, C571, C572, C573, C574, C575, C576, C577, C578, C579, C580, C581, C582, C583, C584, C585, C586, C587, C588, C589, C590, C591, C592, C593, C594, C595, C596, C597, C598, C599, C600, C601, C602, C603, C604, C605, C606, C607, C608, C609, C610, C611, C612, C613, C614, C615, C616, C617, C618, C619, C620, C621, C622, C623, C624, C625, C626, C627, C628, C629, C630, C631, C632, C633, C634, C635, C636, C637, C638, C639, C640, C641, C642, C643, C644, C645, C646, C647, C648, C649, C650, C651, C652, C653, C654, C655, C656, C657, C658, C659, C660, C661, C662, C663, C664, C665, C666, C667, C668, C669, C670, C671, C672, C673, C674, C675, C676, C677, C678, C679, C680, C681, C682, C683, C684, C685, C686, C687, C688, C689, C690, C691, C692, C693, C694, C695, C696, C697, C698, C699, C700, C701, C702, C703, C704, C705, C706, C707, C708, C709, C710, C711, C712, C713, C714, C715, C716, C717, C718, C719, C720, C721, C722, C723, C724, C725, C726, C727, C728, C729, C730, C731, C732, C733, C734, C735, C736, C737, C738, C739, C740, C741, C742, C743, C744, C745, C746, C747, C748, C749, C750, C751, C752, C753, C754, C755, C756, C757, C758, C759, C760, C761, C762, C763, C764, C765, C766, C767, C768, C769, C770, C771, C772, C773, C774, C775, C776, C777, C778, C779, C780, C781, C782, C783, C784, C785, C786, C787, C788, C789, C790, C791, C792, C793, C794, C795, C796, C797, C798, C799, C800, C801, C802, C803, C804, C805, C806, C807, C808, C809, C810, C811, C812, C813, C814

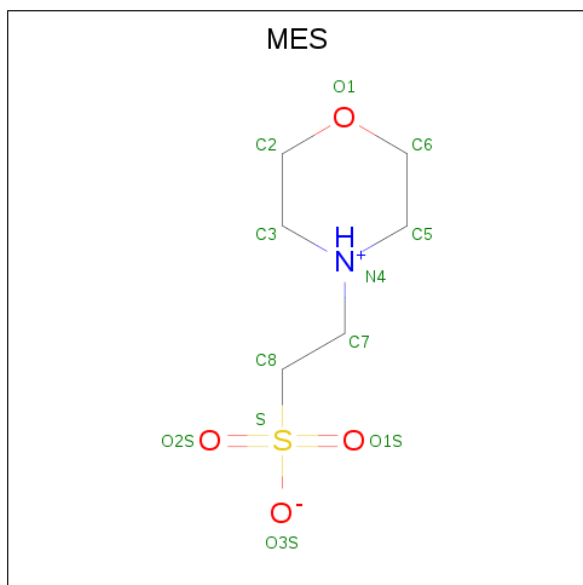
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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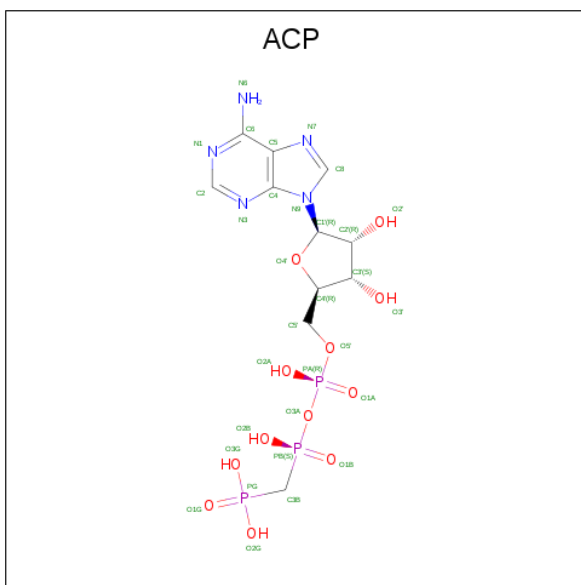
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 11 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

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



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

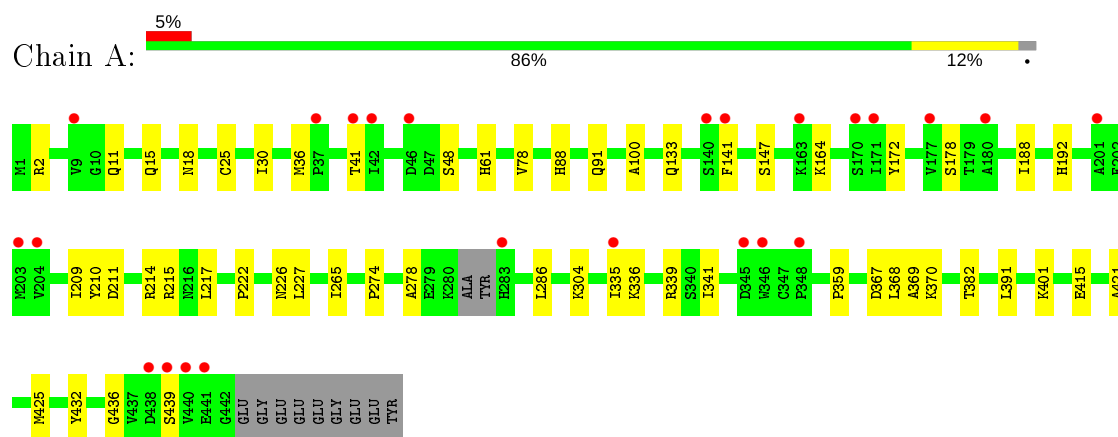
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	95	Total O 95 95	0	0
13	B	93	Total O 93 93	0	0
13	C	186	Total O 186 186	0	0
13	D	51	Total O 51 51	0	0
13	E	17	Total O 17 17	0	0
13	F	36	Total O 36 36	0	0

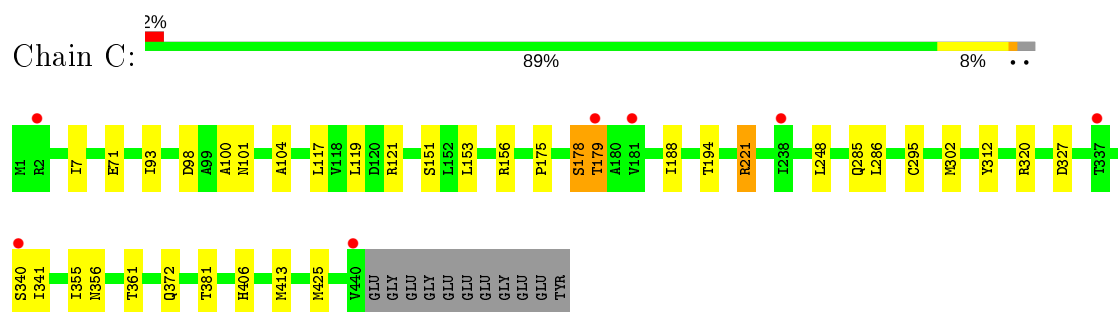
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

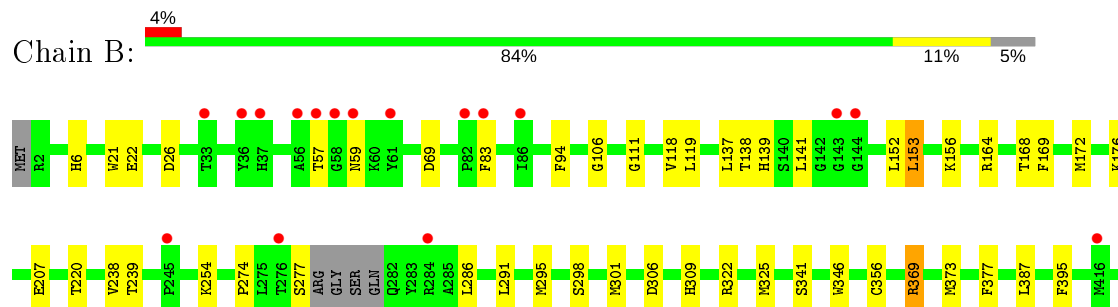
- Molecule 1: Tubulin alpha-1B chain

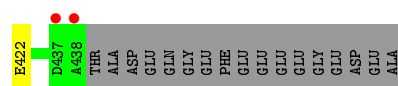


- Molecule 1: Tubulin alpha-1B chain

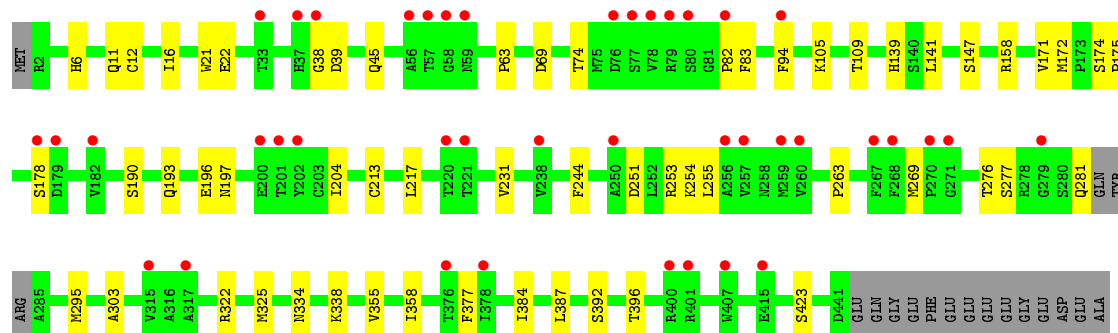
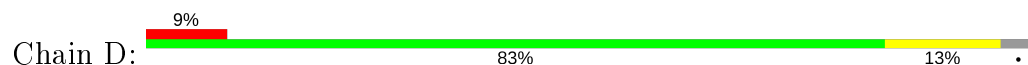


- Molecule 2: Tubulin beta-2B chain

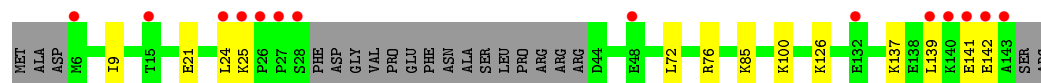
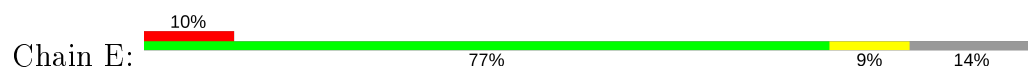




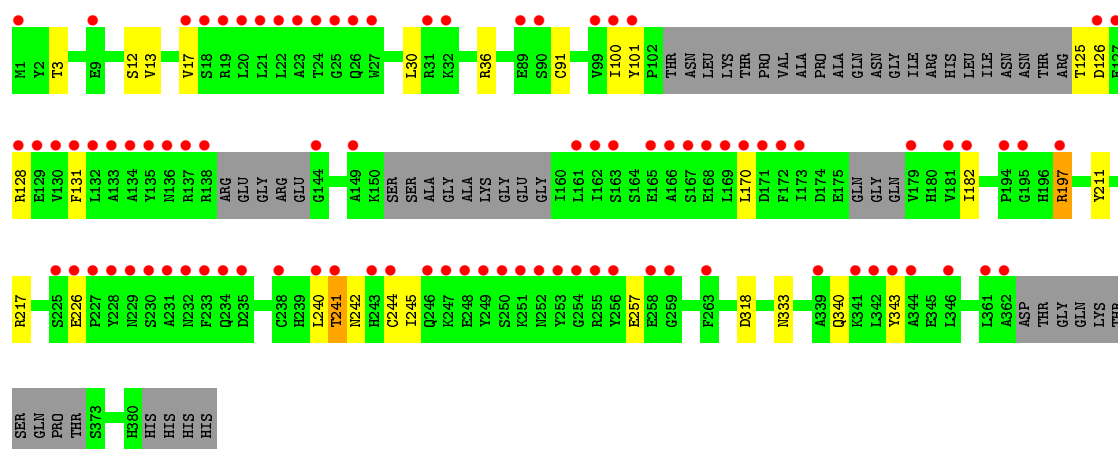
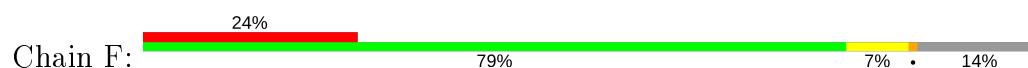
• Molecule 2: Tubulin beta-2B chain



• 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	104.77Å 157.51Å 179.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 2.15 49.29 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.29-2.15) 99.7 (49.29-2.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.14Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.171 , 0.208 0.172 , 0.209	Depositor DCC
R_{free} test set	8071 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	18016	wwPDB-VP
Average B, all atoms (Å ²)	64.0	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, GOL, MG, CA, GTP, ACP, 918, MES

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	0.39	0/3515	0.53	0/4769
1	C	0.48	1/3515 (0.0%)	0.58	0/4772
2	B	0.41	0/3405	0.56	0/4612
2	D	0.36	0/3422	0.52	0/4635
3	E	0.37	0/1022	0.48	0/1356
4	F	0.33	0/2786	0.50	0/3763
All	All	0.40	1/17665 (0.0%)	0.54	0/23907

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	295	CYS	CB-SG	-8.23	1.68	1.82

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	3436	0	3348	29	0
1	C	3437	0	3349	19	0
2	B	3331	0	3208	26	0
2	D	3349	0	3223	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1014	0	1029	9	0
4	F	2724	0	2698	15	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
9	B	28	0	0	0	0
9	D	28	0	0	0	0
10	B	28	0	12	0	0
10	D	28	0	12	1	0
11	B	12	0	12	0	0
11	D	12	0	12	1	0
12	F	31	0	14	1	0
13	A	95	0	0	0	0
13	B	93	0	0	2	0
13	C	186	0	0	1	0
13	D	51	0	0	1	0
13	E	17	0	0	1	0
13	F	36	0	0	0	0
All	All	18016	0	16949	124	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 4.

All (124) 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:158:ARG:NH1	2:D:197:ASN:OD1	2.22	0.73
4:F:318:ASP:OD2	12:F:402:ACP:O3G	2.06	0.72
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.79	0.65
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.79	0.64
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.80	0.64
2:B:176:LYS:HD3	2:B:207:GLU:HG3	1.81	0.63
4:F:101:TYR:O	4:F:128:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:253:ARG:NH1	11:D:504:MES:O3S	2.33	0.62
2:D:11:GLN:HA	2:D:74:THR:HG21	1.83	0.61
4:F:101:TYR:HD1	4:F:126:ASP:HB2	1.67	0.60
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.84	0.60
3:E:85:LYS:NZ	13:E:201:HOH:O	2.28	0.59
1:A:88:HIS:N	1:A:91:GLN:OE1	2.27	0.59
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.84	0.58
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.85	0.58
2:B:152:LEU:HD11	2:B:156:LYS:HZ1	1.69	0.58
1:C:285:GLN:OE1	1:C:372:GLN:NE2	2.37	0.58
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.84	0.58
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.34	0.57
2:B:69:ASP:O	2:B:94:PHE:HA	2.05	0.57
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.85	0.56
1:A:210:TYR:CE2	1:A:214:ARG:HD2	2.40	0.56
1:C:221:ARG:HD2	2:D:325:MET:HB3	1.87	0.56
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.88	0.55
3:E:137:LYS:O	3:E:141:GLU:HG2	2.07	0.55
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.88	0.55
3:E:139:LEU:O	3:E:142:GLU:HG2	2.08	0.54
2:B:106:GLY:O	2:B:111:GLY:HA3	2.08	0.54
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.43	0.54
2:D:325:MET:SD	2:D:355:VAL:HG21	2.48	0.53
1:C:175:PRO:HA	1:C:179:THR:OG1	2.08	0.53
2:B:220:THR:O	13:B:601:HOH:O	2.19	0.53
2:B:26:ASP:OD2	2:B:369:ARG:HD2	2.08	0.52
2:D:193:GLN:OE1	3:E:126:LYS:HE2	2.09	0.52
2:D:16:ILE:HD13	2:D:231:VAL:HG11	1.91	0.52
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.46	0.51
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.29	0.50
2:B:118:VAL:HG11	2:B:153:LEU:HD21	1.94	0.49
2:D:12:CYS:HB2	10:D:502:GDP:C8	2.47	0.49
1:C:101:ASN:ND2	2:D:254:LYS:HE2	2.26	0.49
1:A:336:LYS:NZ	1:A:341:ILE:O	2.46	0.49
3:E:24:LEU:O	3:E:25:LYS:HD2	2.13	0.48
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.28	0.48
4:F:241:THR:O	4:F:241:THR:OG1	2.30	0.48
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.48	0.48
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.95	0.48
1:A:336:LYS:HG2	3:E:24:LEU:HD23	1.95	0.48
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:9:ILE:HG12	3:E:21:GLU:HB3	1.95	0.48
1:C:327:ASP:OD2	13:C:601:HOH:O	2.19	0.47
1:A:2:ARG:HB3	1:A:133:GLN:HG2	1.97	0.47
3:E:72:LEU:O	3:E:76:ARG:HG2	2.15	0.47
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.95	0.47
1:A:359:PRO:HB2	1:A:370:LYS:HE2	1.96	0.46
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.32	0.46
2:D:325:MET:CE	2:D:355:VAL:HG21	2.45	0.46
4:F:240:LEU:HB3	4:F:242:ASN:HD22	1.80	0.46
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.50	0.46
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.98	0.46
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.42	0.46
1:A:192:HIS:CG	1:A:421:ALA:HA	2.51	0.46
2:D:171:VAL:HA	2:D:204:ILE:O	2.16	0.46
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.51	0.45
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.97	0.45
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.48	0.45
2:B:137:LEU:HB3	2:B:168:THR:HG22	1.99	0.44
2:D:82:PRO:O	2:D:83:PHE:HB2	2.18	0.44
4:F:128:ARG:HH11	4:F:170:LEU:HD23	1.82	0.44
1:A:211:ASP:HB3	1:A:215:ARG:NH2	2.32	0.44
1:C:320:ARG:HA	1:C:356:ASN:O	2.17	0.44
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.98	0.44
2:D:174:SER:O	2:D:178:SER:N	2.51	0.44
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.18	0.44
2:B:141:LEU:HD12	2:B:172:MET:SD	2.57	0.44
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.53	0.44
2:B:176:LYS:HD3	2:B:207:GLU:CG	2.47	0.44
2:B:298:SER:HA	2:B:301:MET:HG3	2.00	0.43
1:A:188:ILE:HG13	1:A:425:MET:HG3	2.00	0.43
1:A:11:GLN:O	1:A:15:GLN:HG3	2.18	0.43
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.33	0.43
2:B:138:THR:HG22	2:B:169:PHE:HB2	2.00	0.43
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.54	0.43
4:F:240:LEU:HB3	4:F:242:ASN:ND2	2.34	0.43
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.01	0.43
4:F:244:CYS:SG	4:F:245:ILE:N	2.92	0.43
1:C:151:SER:HA	1:C:194:THR:HG22	2.01	0.43
2:D:392:SER:O	2:D:396:THR:HG22	2.19	0.43
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.54	0.42
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ILE:HG13	1:C:425:MET:HG3	2.00	0.42
2:D:251:ASP:O	2:D:255:LEU:HG	2.18	0.42
2:D:105:LYS:HA	2:D:109:THR:OG1	2.20	0.42
1:A:141:PHE:O	1:A:147:SER:HB3	2.20	0.42
1:A:336:LYS:HA	1:A:336:LYS:HD2	1.87	0.42
2:D:22:GLU:OE1	2:D:82:PRO:HG2	2.19	0.42
3:E:100:LYS:HB2	3:E:100:LYS:HE3	1.85	0.42
4:F:126:ASP:OD2	4:F:128:ARG:HB2	2.19	0.42
2:D:175:PRO:HA	2:D:178:SER:HB3	2.02	0.42
1:A:25:CYS:HB3	1:A:30:ILE:O	2.19	0.42
1:A:211:ASP:HB3	1:A:215:ARG:HH22	1.85	0.42
2:B:238:VAL:HG23	2:B:239:THR:HG23	2.01	0.41
2:D:147:SER:HB2	2:D:190:SER:OG	2.20	0.41
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.02	0.41
4:F:13:VAL:O	4:F:17:VAL:HG23	2.20	0.41
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.55	0.41
2:D:334:ASN:HD21	2:D:338:LYS:NZ	2.18	0.41
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.86	0.41
2:B:322:ARG:O	2:B:373:MET:HE1	2.20	0.41
1:A:382:THR:HG21	1:A:436:GLY:HA3	2.01	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.56	0.41
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.55	0.41
2:B:164:ARG:HD2	13:B:685:HOH:O	2.20	0.41
2:D:39:ASP:N	2:D:39:ASP:OD1	2.54	0.41
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.03	0.41
1:C:104:ALA:HB2	1:C:413:MET:SD	2.61	0.41
2:D:281:GLN:NE2	13:D:602:HOH:O	2.39	0.40
4:F:3:THR:HB	4:F:30:LEU:HD11	2.02	0.40
2:B:295:MET:HE2	2:B:377:PHE:HB2	2.02	0.40
2:D:141:LEU:HD12	2:D:172:MET:SD	2.62	0.40
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.20	0.40
2:B:286:LEU:HD23	2:B:291:LEU:HG	2.04	0.40
1:C:286:LEU:HA	1:C:286:LEU:HD23	1.80	0.40
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.03	0.40
2:D:69:ASP:O	2:D:94:PHE:HA	2.21	0.40

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	437/451 (97%)	427 (98%)	9 (2%)	1 (0%)	47	45
1	C	438/451 (97%)	431 (98%)	6 (1%)	1 (0%)	47	45
2	B	419/445 (94%)	409 (98%)	10 (2%)	0	100	100
2	D	423/445 (95%)	416 (98%)	7 (2%)	0	100	100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	319/384 (83%)	314 (98%)	5 (2%)	0	100	100
All	All	2155/2319 (93%)	2115 (98%)	38 (2%)	2 (0%)	51	51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER
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	372/379 (98%)	367 (99%)	5 (1%)	69	73
1	C	371/379 (98%)	364 (98%)	7 (2%)	57	59
2	B	366/383 (96%)	357 (98%)	9 (2%)	47	47
2	D	368/383 (96%)	361 (98%)	7 (2%)	57	59
3	E	110/127 (87%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	300/342 (88%)	290 (97%)	10 (3%)	38	35
All	All	1887/1993 (95%)	1849 (98%)	38 (2%)	55	57

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	48	SER
1	A	164	LYS
1	A	415	GLU
1	A	439	SER
2	B	57	THR
2	B	59	ASN
2	B	139	HIS
2	B	153	LEU
2	B	277	SER
2	B	325	MET
2	B	341	SER
2	B	356	CYS
2	B	369	ARG
1	C	178	SER
1	C	179	THR
1	C	221	ARG
1	C	302	MET
1	C	340	SER
1	C	361	THR
1	C	381	THR
2	D	139	HIS
2	D	196	GLU
2	D	276	THR
2	D	277	SER
2	D	322	ARG
2	D	384	ILE
2	D	423	SER
4	F	12	SER
4	F	36	ARG
4	F	91	CYS
4	F	125	THR
4	F	197	ARG
4	F	211	TYR
4	F	217	ARG
4	F	226	GLU

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Mol	Chain	Res	Type
4	F	241	THR
4	F	333	ASN

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

Mol	Chain	Res	Type
4	F	242	ASN
4	F	252	ASN
4	F	348	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
11	MES	B	506	-	12,12,12	1.89	1 (8%)	14,16,16	1.98	4 (28%)
11	MES	D	504	-	12,12,12	2.12	1 (8%)	14,16,16	1.91	4 (28%)
12	ACP	F	402	6	27,33,33	1.72	6 (22%)	32,52,52	1.34	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	A	505	-	5,5,5	0.33	0	5,5,5	0.37	0
5	GTP	C	501	6	26,34,34	0.94	1 (3%)	33,54,54	1.81	7 (21%)
5	GTP	A	501	6	26,34,34	0.95	1 (3%)	33,54,54	1.68	6 (18%)
9	918	D	501	-	31,31,31	1.25	4 (12%)	41,45,45	1.91	9 (21%)
10	GDP	B	502	6	24,30,30	1.12	2 (8%)	31,47,47	2.03	7 (22%)
10	GDP	D	502	6	24,30,30	1.18	2 (8%)	31,47,47	1.98	8 (25%)
9	918	B	501	-	31,31,31	1.34	3 (9%)	41,45,45	1.74	11 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MES	B	506	-	-	0/6/14/14	0/1/1/1
11	MES	D	504	-	-	1/6/14/14	0/1/1/1
12	ACP	F	402	6	-	5/15/38/38	0/3/3/3
8	GOL	A	505	-	-	2/4/4/4	-
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
5	GTP	A	501	6	-	9/18/38/38	0/3/3/3
9	918	D	501	-	-	0/18/33/33	0/4/4/4
10	GDP	B	502	6	-	5/12/32/32	0/3/3/3
10	GDP	D	502	6	-	4/12/32/32	0/3/3/3
9	918	B	501	-	-	0/18/33/33	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	504	MES	C8-S	-7.04	1.67	1.77
11	B	506	MES	C8-S	-6.16	1.68	1.77
12	F	402	ACP	PB-O1B	4.04	1.61	1.51
10	D	502	GDP	C6-C5	3.97	1.48	1.41
9	D	501	918	CAO-CAN	-3.96	1.41	1.50
12	F	402	ACP	PB-O3A	3.79	1.62	1.58
9	B	501	918	CAO-CAN	-3.70	1.42	1.50
9	B	501	918	C6-NAI	-3.61	1.30	1.37
10	B	502	GDP	C6-C5	3.35	1.47	1.41
9	B	501	918	CAH-C4	-3.33	1.40	1.48
9	D	501	918	CAH-C4	-3.20	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	402	ACP	PB-O2B	-3.17	1.48	1.56
12	F	402	ACP	PG-O2G	2.94	1.61	1.54
5	A	501	GTP	C6-N1	2.84	1.38	1.33
5	C	501	GTP	C6-N1	2.79	1.37	1.33
12	F	402	ACP	PG-O3G	2.74	1.61	1.54
12	F	402	ACP	C5-C4	2.48	1.47	1.40
10	D	502	GDP	C5-C4	2.43	1.47	1.40
9	D	501	918	CAJ-NAK	2.22	1.39	1.34
10	B	502	GDP	O4'-C1'	2.10	1.44	1.41
9	D	501	918	C6-NAI	-2.09	1.33	1.37

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	N3-C2-N1	-5.63	119.71	127.22
11	B	506	MES	C5-N4-C3	5.21	120.56	108.83
10	B	502	GDP	C2-N3-C4	5.07	121.14	115.36
10	B	502	GDP	C6-C5-C4	-4.79	116.22	120.80
5	A	501	GTP	N3-C2-N1	-4.66	121.01	127.22
10	B	502	GDP	C6-N1-C2	4.47	123.03	115.93
9	B	501	918	CAU-NAG-CAQ	4.44	121.33	111.52
10	D	502	GDP	C5-C6-N1	-4.36	117.47	123.43
11	D	504	MES	C5-N4-C3	4.33	118.58	108.83
10	B	502	GDP	N3-C2-N1	-4.26	121.53	127.22
5	A	501	GTP	C5-C6-N1	-4.21	117.67	123.43
9	D	501	918	CAU-NAG-CAQ	4.18	120.75	111.52
10	D	502	GDP	C6-N1-C2	4.14	122.51	115.93
9	D	501	918	CAJ-CAH-C4	-4.13	114.16	121.16
5	C	501	GTP	C2-N3-C4	4.12	120.06	115.36
10	D	502	GDP	C2-N3-C4	4.11	120.05	115.36
10	D	502	GDP	C6-C5-C4	-4.00	116.98	120.80
9	B	501	918	N3-C2-N1	-3.95	119.78	126.31
9	D	501	918	N3-C2-N1	-3.84	119.96	126.31
9	B	501	918	CAJ-CAH-C4	-3.83	114.67	121.16
9	B	501	918	CAY-NAI-C6	3.73	128.17	123.60
10	B	502	GDP	C5-C6-N1	-3.71	118.36	123.43
9	D	501	918	CAY-NAI-C6	3.67	128.09	123.60
9	D	501	918	C2-N1-C6	3.65	121.70	115.03
5	A	501	GTP	C6-N1-C2	3.50	121.49	115.93
11	B	506	MES	O1S-S-C8	3.44	111.06	106.92
12	F	402	ACP	C3'-C2'-C1'	3.40	106.10	100.98
5	C	501	GTP	C5-C6-N1	-3.36	118.84	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C6-N1-C2	3.30	121.18	115.93
9	D	501	918	N3-C2-NAG	3.28	121.16	117.11
10	D	502	GDP	C4-C5-N7	-3.26	106.00	109.40
9	D	501	918	C5-C4-N3	-3.23	118.52	122.35
12	F	402	ACP	C4-C5-N7	-2.98	106.30	109.40
12	F	402	ACP	N3-C2-N1	-2.95	124.07	128.68
11	D	504	MES	O3S-S-C8	2.90	110.46	105.77
9	D	501	918	CAT-CAU-NAG	2.87	115.31	110.02
11	D	504	MES	O1S-S-C8	2.86	110.35	106.92
9	B	501	918	C2-N1-C6	2.85	120.25	115.03
10	D	502	GDP	PA-O3A-PB	-2.84	123.08	132.83
5	A	501	GTP	C2-N3-C4	2.73	118.47	115.36
10	B	502	GDP	C4-C5-N7	-2.72	106.56	109.40
10	D	502	GDP	N3-C2-N1	-2.70	123.63	127.22
9	B	501	918	C5-C4-N3	-2.68	119.16	122.35
9	B	501	918	N1-C2-NAG	2.45	120.14	117.11
12	F	402	ACP	PA-O3A-PB	-2.44	124.83	132.56
9	B	501	918	N3-C2-NAG	2.40	120.07	117.11
10	D	502	GDP	O2B-PB-O3A	2.36	112.56	104.64
11	B	506	MES	O3S-S-C8	2.35	109.57	105.77
11	B	506	MES	O3S-S-O1S	-2.32	105.62	111.27
5	C	501	GTP	C6-C5-C4	-2.31	118.59	120.80
5	A	501	GTP	C4-C5-N7	-2.26	107.04	109.40
9	B	501	918	CAV-NAI-C6	-2.23	120.87	123.60
5	A	501	GTP	PB-O3B-PG	-2.22	125.20	132.83
5	C	501	GTP	PB-O3B-PG	-2.22	125.20	132.83
9	B	501	918	CAM-CAN-CAH	-2.15	117.18	119.77
9	B	501	918	CAH-CAJ-NAK	-2.12	121.15	124.49
5	C	501	GTP	N2-C2-N1	2.10	120.52	117.25
9	D	501	918	CAW-CAV-NAI	2.04	106.04	103.45
11	D	504	MES	C7-N4-C5	2.01	116.39	111.23
10	B	502	GDP	C1'-N9-C4	-2.01	123.12	126.64

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	F	402	ACP	PG-C3B-PB-O1B
12	F	402	ACP	PG-C3B-PB-O2B
12	F	402	ACP	PG-C3B-PB-O3A
12	F	402	ACP	C5'-O5'-PA-O1A
10	B	502	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
10	B	502	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
8	A	505	GOL	O1-C1-C2-O2
8	A	505	GOL	O1-C1-C2-C3
10	D	502	GDP	C5'-O5'-PA-O1A
11	D	504	MES	C8-C7-N4-C3
5	A	501	GTP	PB-O3B-PG-O1G
10	D	502	GDP	C5'-O5'-PA-O3A
10	D	502	GDP	C5'-O5'-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
12	F	402	ACP	PB-O3A-PA-O2A
10	B	502	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
10	B	502	GDP	PB-O3A-PA-O1A
10	B	502	GDP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
10	D	502	GDP	PB-O3A-PA-O2A

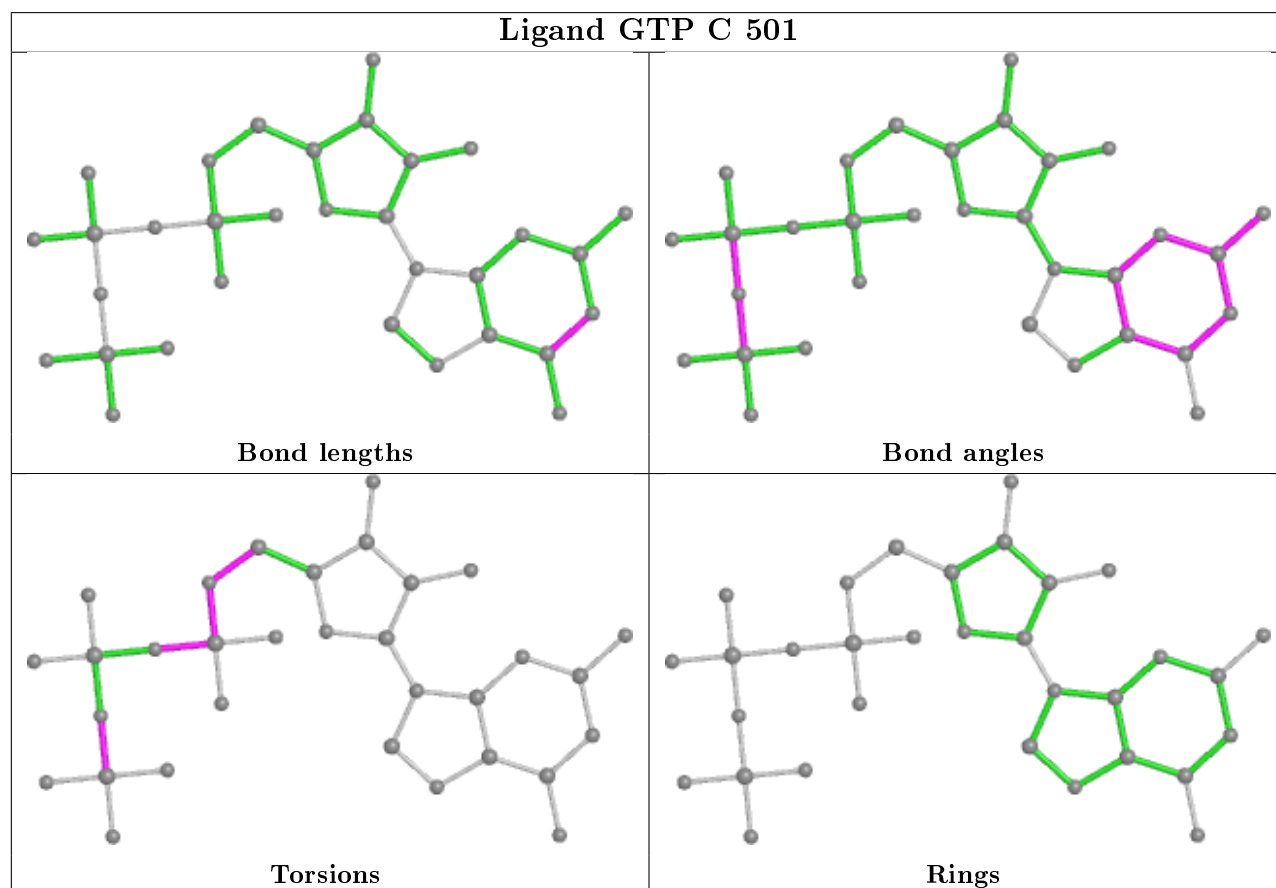
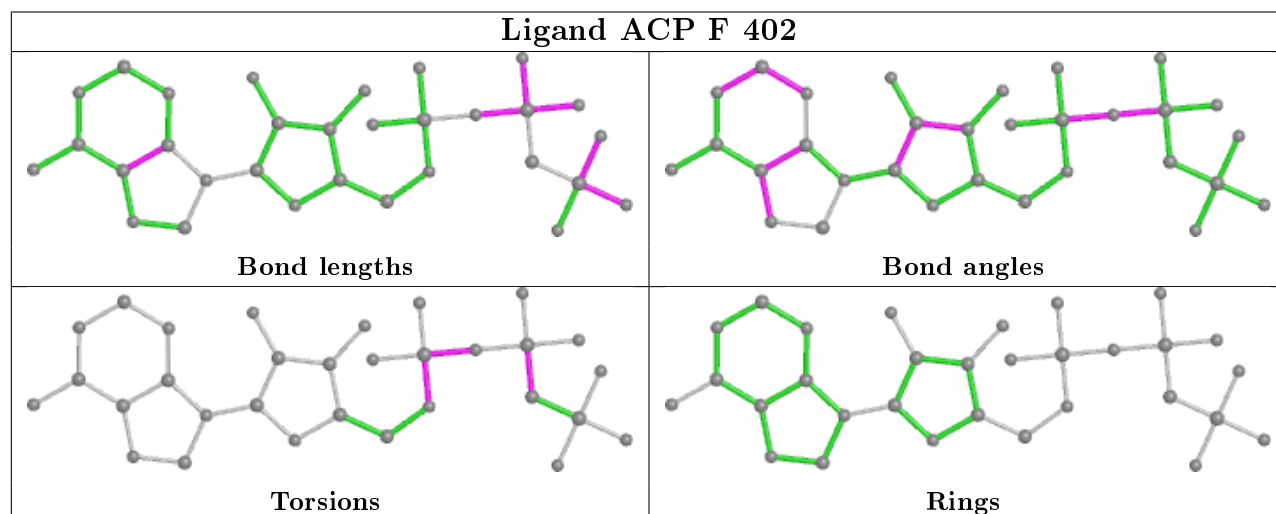
There are no ring outliers.

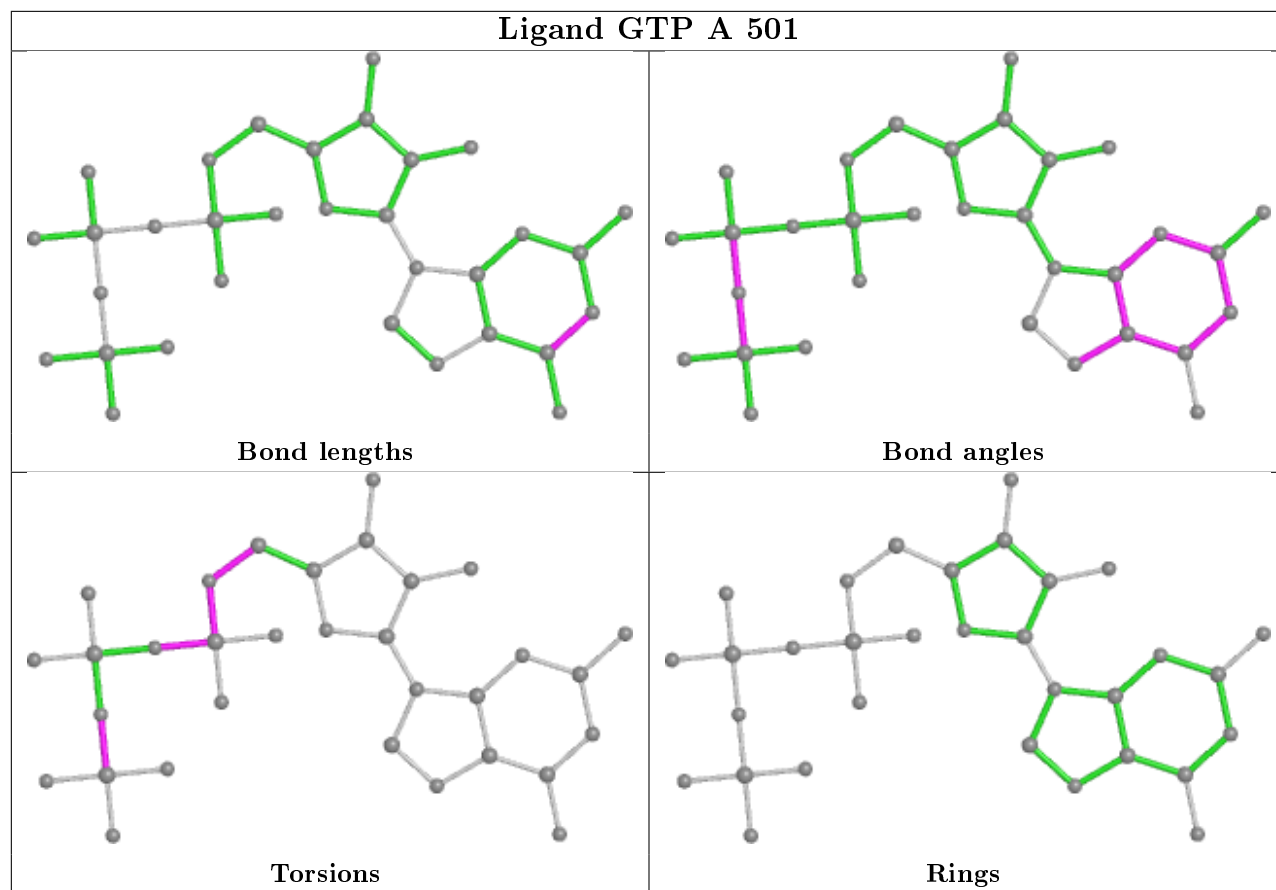
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	504	MES	1	0
12	F	402	ACP	1	0
10	D	502	GDP	1	0

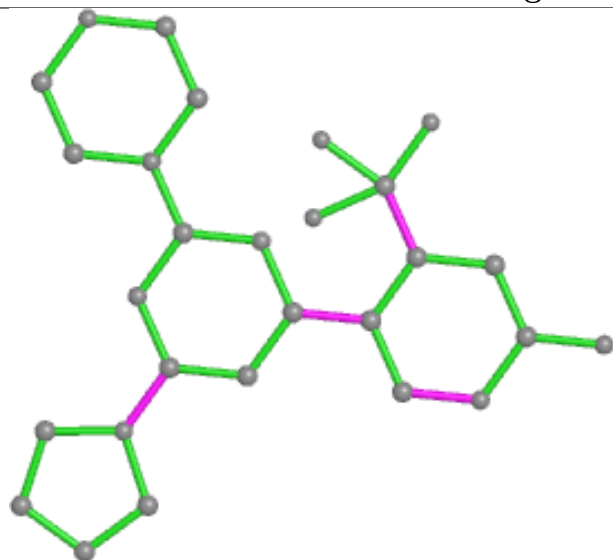
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

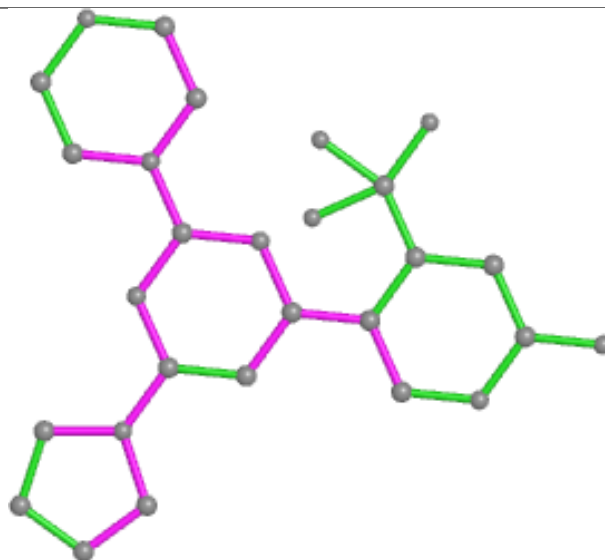




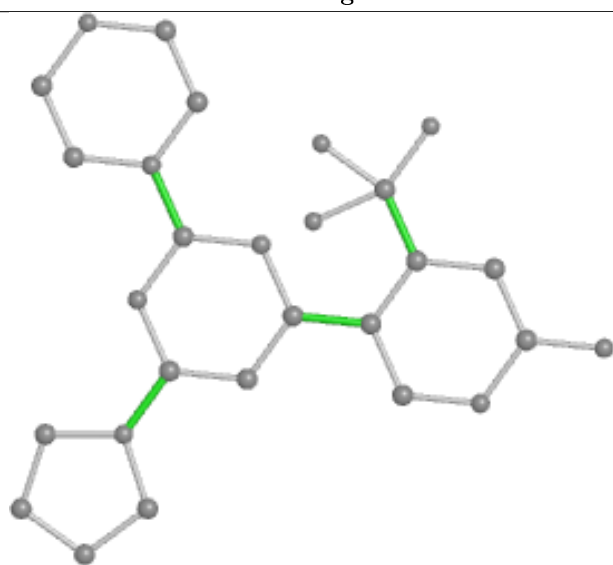
Ligand 918 D 501



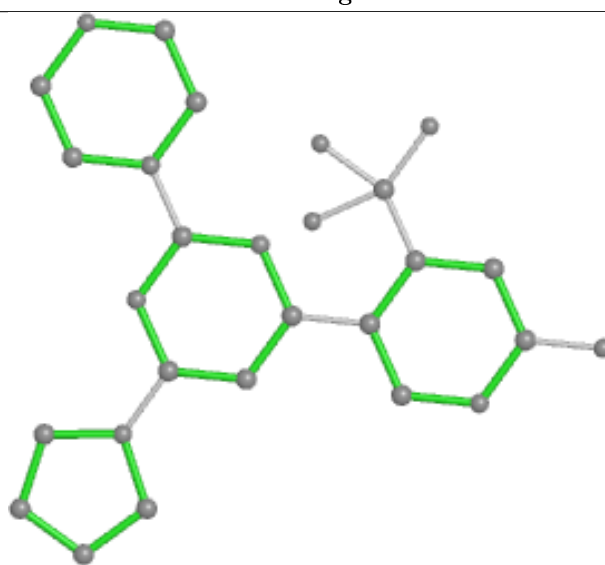
Bond lengths



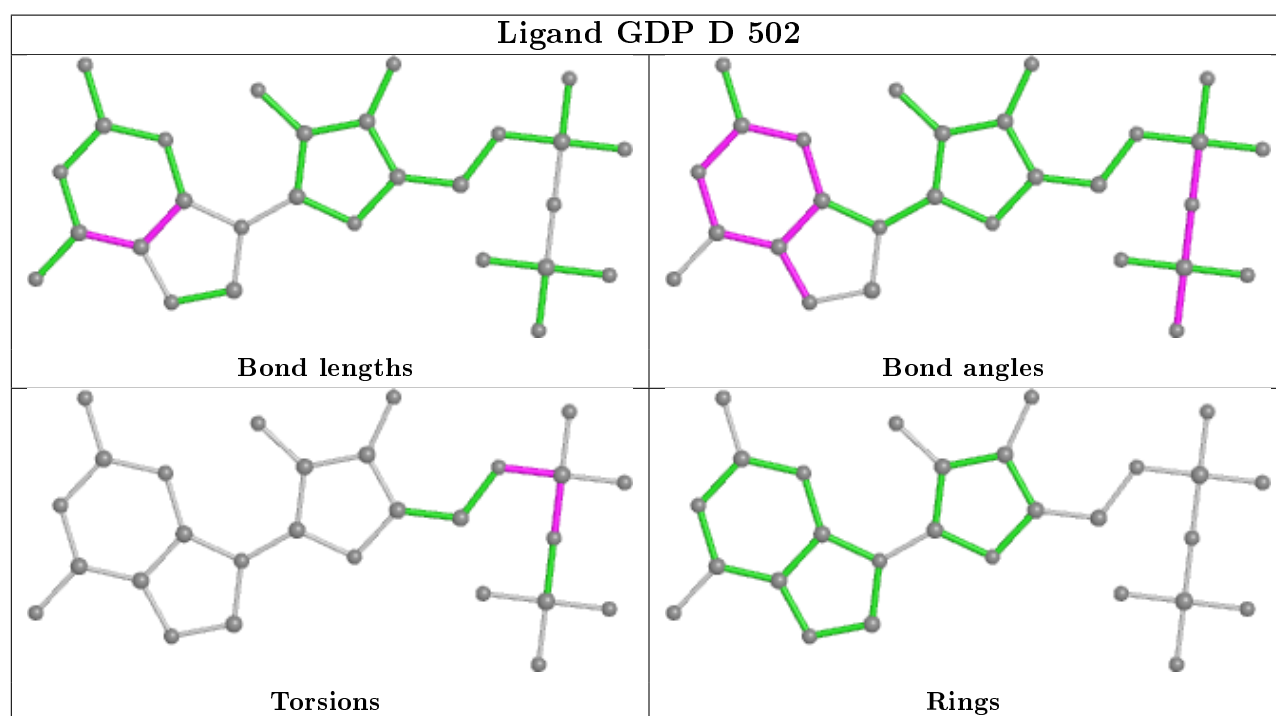
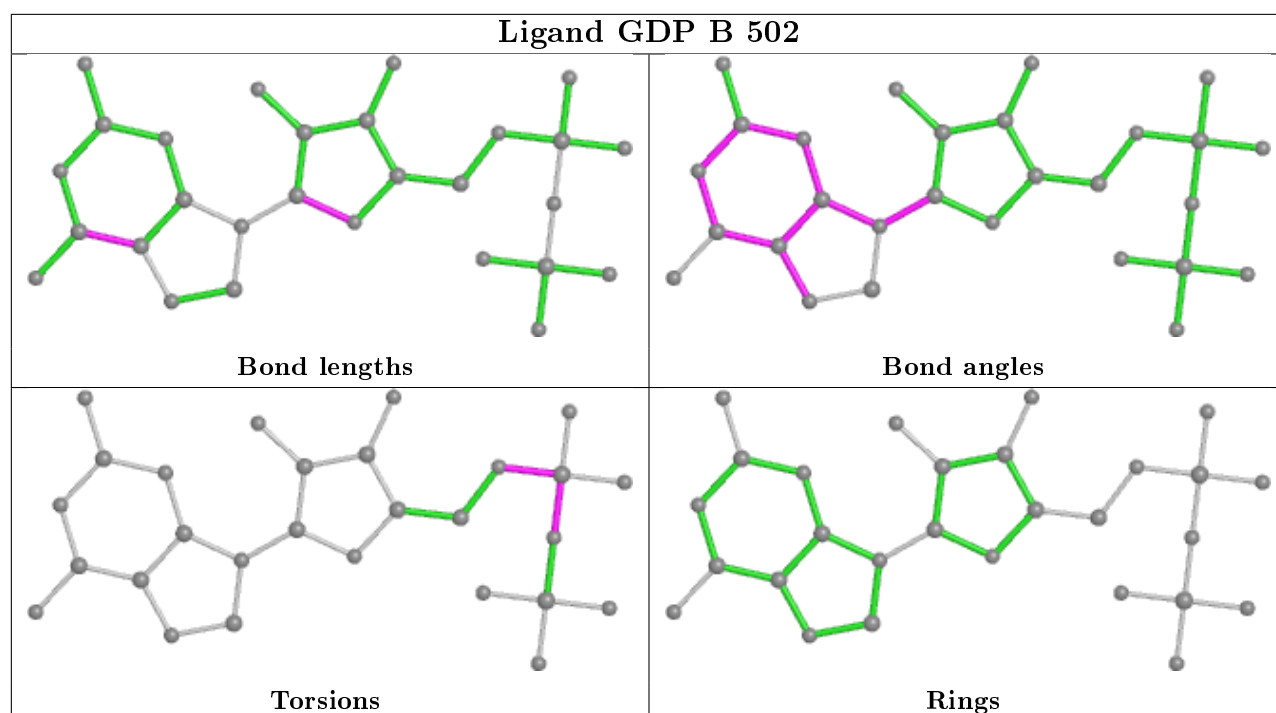
Bond angles

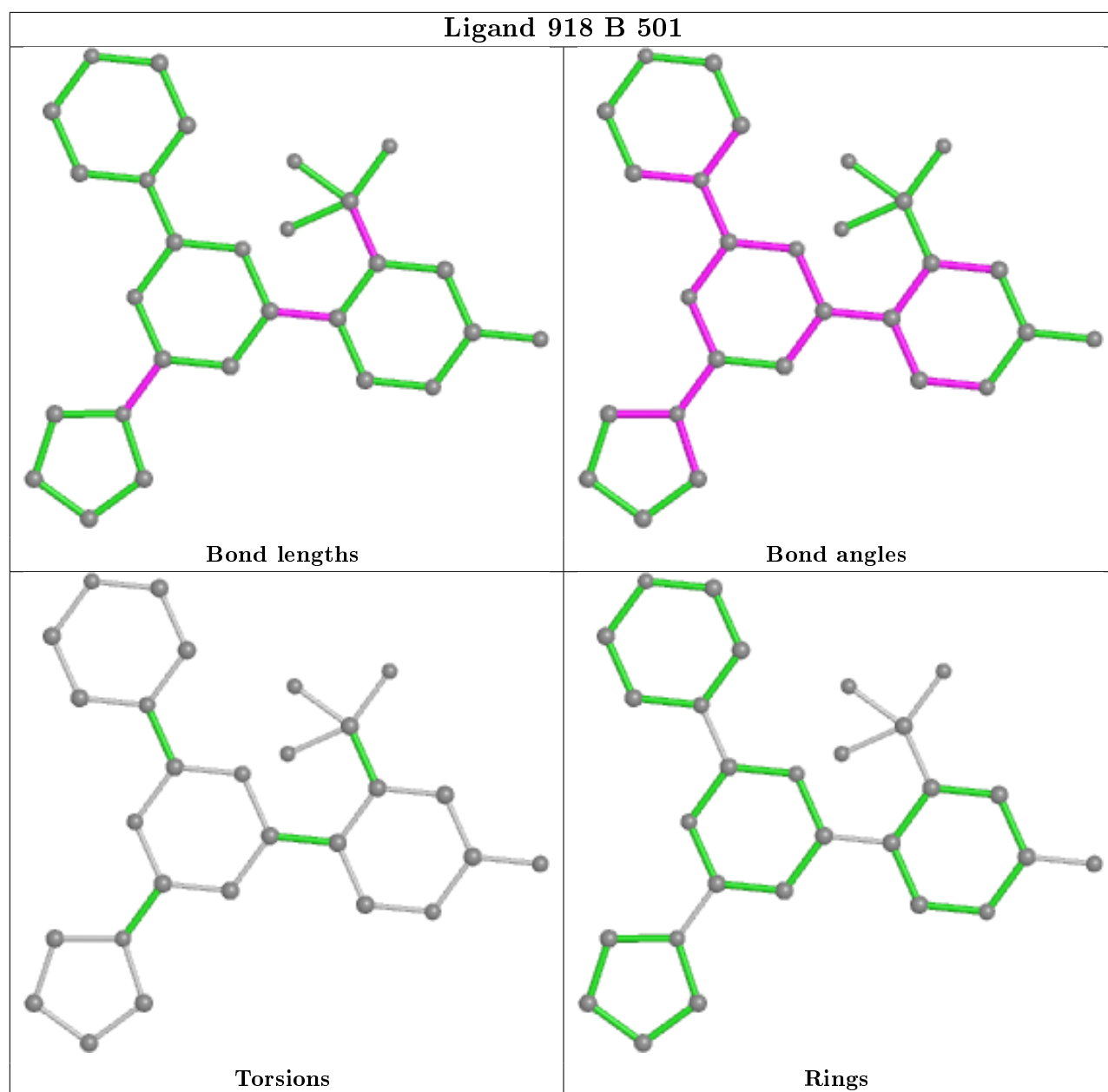


Torsions



Rings





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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	440/451 (97%)	0.37	24 (5%)	25 31	37, 56, 95, 136	0
1	C	440/451 (97%)	0.03	7 (1%)	72 77	31, 44, 77, 119	0
2	B	423/445 (95%)	0.25	19 (4%)	33 40	32, 52, 88, 132	2 (0%)
2	D	427/445 (95%)	0.47	41 (9%)	8 10	38, 65, 100, 132	4 (0%)
3	E	123/143 (86%)	0.38	14 (11%)	5 6	40, 70, 113, 131	0
4	F	331/384 (86%)	1.18	91 (27%)	0 0	47, 83, 141, 168	0
All	All	2184/2319 (94%)	0.42	196 (8%)	9 12	31, 59, 110, 168	6 (0%)

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	231	ALA	8.7
4	F	173	ILE	8.3
4	F	249	TYR	7.2
4	F	130	VAL	6.9
4	F	169	LEU	6.9
4	F	132	LEU	6.5
4	F	233	PHE	6.4
4	F	161	LEU	6.3
4	F	250	SER	6.2
4	F	100	ILE	6.1
2	D	57	THR	5.9
4	F	179	VAL	5.8
1	A	440	VAL	5.7
3	E	26	PRO	5.6
4	F	252	ASN	5.5
4	F	253	TYR	5.5
2	B	57	THR	5.4
2	D	82	PRO	5.3
4	F	20	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
4	F	182	ILE	5.2
4	F	133	ALA	5.1
3	E	27	PRO	5.1
4	F	101	TYR	5.1
4	F	227	PRO	5.0
1	A	439	SER	4.9
4	F	134	ALA	4.9
4	F	99	VAL	4.8
4	F	248	GLU	4.8
2	D	58	GLY	4.7
2	B	245	PRO	4.7
4	F	251	LYS	4.6
1	C	340	SER	4.6
4	F	170	LEU	4.6
4	F	244	CYS	4.5
4	F	232	ASN	4.4
3	E	143	ALA	4.4
4	F	362	ALA	4.4
2	D	56	ALA	4.4
4	F	17	VAL	4.3
4	F	166	ALA	4.3
4	F	167	SER	4.3
4	F	263	PHE	4.3
3	E	142	GLU	4.1
3	E	139	LEU	4.1
3	E	24	LEU	4.1
2	D	407	TRP	4.0
1	A	441	GLU	4.0
4	F	259	GLY	3.9
2	B	37	HIS	3.8
4	F	137	ARG	3.8
4	F	361	LEU	3.8
4	F	194	PRO	3.7
1	A	346	TRP	3.7
2	B	284	ARG	3.7
2	B	59	ASN	3.7
2	D	37	HIS	3.7
4	F	22	LEU	3.7
1	A	171	ILE	3.7
4	F	163	SER	3.7
4	F	172	PHE	3.7
4	F	129	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
4	F	25	GLY	3.6
1	A	42	ILE	3.6
2	B	36	TYR	3.5
1	C	440	VAL	3.5
4	F	234	GLN	3.5
4	F	256	TYR	3.5
4	F	165	GLU	3.5
2	B	58	GLY	3.5
2	B	33	THR	3.4
4	F	131	PHE	3.4
4	F	135	TYR	3.4
4	F	24	THR	3.4
4	F	32	LYS	3.3
4	F	255	ARG	3.3
2	D	268	PHE	3.2
4	F	344	ALA	3.2
4	F	31	ARG	3.2
1	A	163	LYS	3.2
4	F	144	GLY	3.1
2	D	279	GLY	3.1
3	E	6	MET	3.1
4	F	168	GLU	3.1
4	F	171	ASP	3.1
4	F	149	ALA	3.1
2	D	220	THR	3.0
2	B	56	ALA	3.0
4	F	18	SER	3.0
1	A	201	ALA	3.0
4	F	341	LYS	3.0
4	F	162	ILE	2.9
4	F	27	TRP	2.9
4	F	136	ASN	2.9
2	B	61	TYR	2.9
2	D	317	ALA	2.9
4	F	247	LYS	2.9
2	D	260	VAL	2.8
3	E	25	LYS	2.8
2	B	438	ALA	2.8
2	D	202	TYR	2.8
3	E	15	THR	2.8
4	F	342	LEU	2.8
3	E	140	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	345	ASP	2.8
4	F	346	LEU	2.8
2	D	77	SER	2.8
4	F	126	ASP	2.7
4	F	181	VAL	2.7
4	F	128	ARG	2.7
2	D	79	ARG	2.7
3	E	28	SER	2.7
2	D	33	THR	2.7
2	D	59	ASN	2.7
4	F	229	ASN	2.7
1	A	283	HIS	2.7
2	D	378	ILE	2.7
2	D	94	PHE	2.7
2	B	437	ASP	2.7
4	F	1	MET	2.7
4	F	21	LEU	2.7
4	F	195	GLY	2.6
1	A	438	ASP	2.6
2	D	80	SER	2.6
2	B	83	PHE	2.6
4	F	90	SER	2.6
4	F	238	CYS	2.6
1	C	2	ARG	2.6
3	E	141	GLU	2.6
2	D	221	THR	2.5
4	F	138	ARG	2.5
2	B	276	THR	2.5
2	D	401	ARG	2.5
2	D	182	VAL	2.5
2	D	259	MET	2.5
4	F	241	THR	2.5
4	F	9	GLU	2.5
4	F	89	GLU	2.5
4	F	225	SER	2.5
4	F	339	ALA	2.5
1	A	9	VAL	2.5
2	D	38	GLY	2.5
4	F	230	SER	2.4
4	F	235	ASP	2.4
4	F	254	GLY	2.4
4	F	26	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	335	ILE	2.4
2	D	400	ARG	2.4
4	F	246	GLN	2.4
4	F	23	ALA	2.4
2	D	178	SER	2.4
2	D	201	THR	2.4
2	B	86	ILE	2.4
2	D	267	PHE	2.3
2	D	415	GLU	2.3
4	F	127	GLU	2.3
4	F	226	GLU	2.3
4	F	197	ARG	2.3
2	B	82	PRO	2.3
2	D	76	ASP	2.3
2	D	250	ALA	2.3
2	B	143	GLY	2.3
1	C	179	THR	2.2
1	C	181	VAL	2.2
2	B	144	GLY	2.2
2	B	416	MET	2.2
1	A	348	PRO	2.2
1	A	141	PHE	2.2
1	A	41	THR	2.2
2	D	315	VAL	2.2
4	F	228	TYR	2.2
3	E	48	GLU	2.2
1	C	238	ILE	2.1
2	D	78	VAL	2.1
4	F	258	GLU	2.1
1	A	203	MET	2.1
4	F	240	LEU	2.1
1	A	204	VAL	2.1
1	A	37	PRO	2.1
4	F	19	ARG	2.1
1	A	177	VAL	2.1
4	F	343	TYR	2.1
1	C	337	THR	2.1
2	D	200	GLU	2.1
2	D	238	VAL	2.1
2	D	179	ASP	2.1
1	A	170	SER	2.1
1	A	46	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	257	VAL	2.1
3	E	132	GLU	2.1
2	D	271	GLY	2.1
2	D	270	PRO	2.0
2	D	376	THR	2.0
2	D	256	ALA	2.0
1	A	140	SER	2.0
4	F	243	HIS	2.0
1	A	180	ALA	2.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

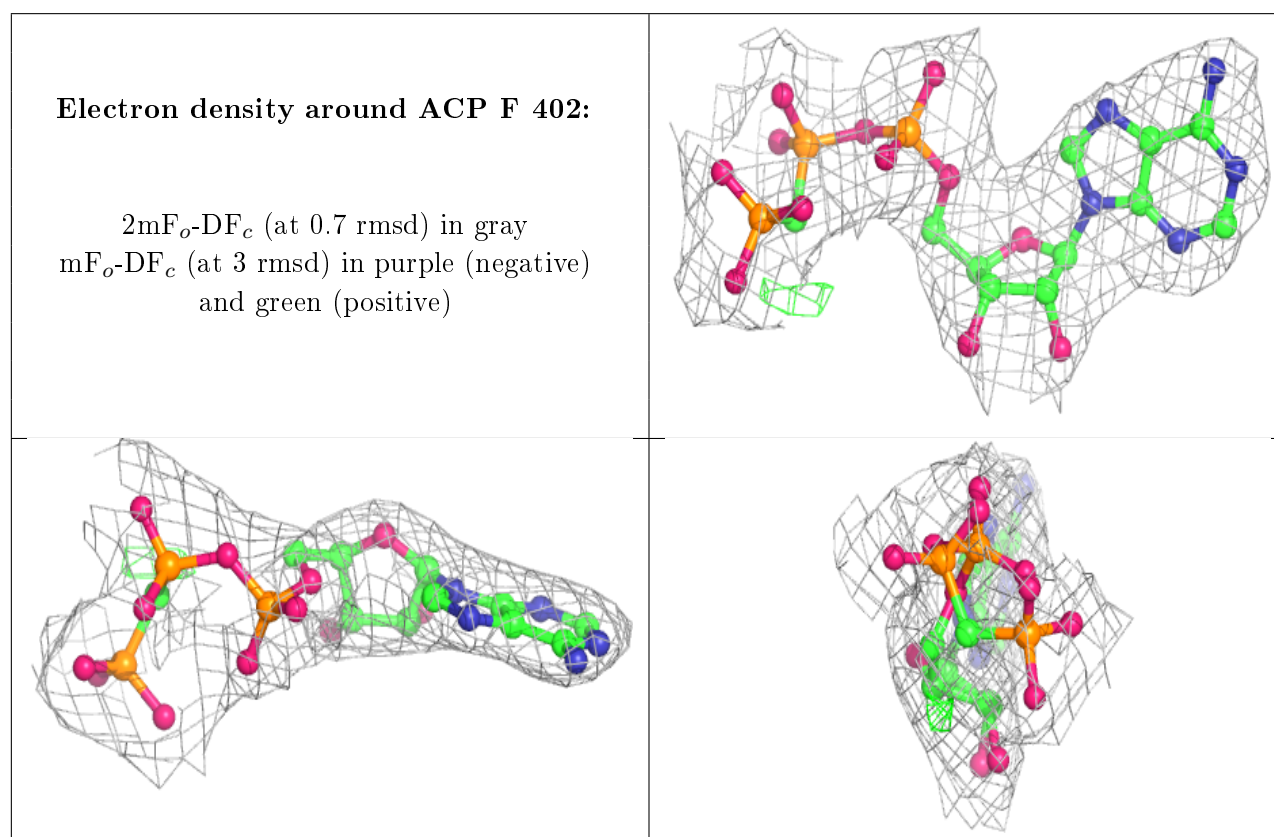
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	B	504	1/1	0.82	0.09	112,112,112,112	0
6	MG	F	401	1/1	0.83	0.06	71,71,71,71	0
7	CA	A	504	1/1	0.85	0.11	114,114,114,114	0
11	MES	D	504	12/12	0.89	0.22	89,100,103,107	0
8	GOL	A	505	6/6	0.89	0.19	78,81,88,89	0
7	CA	B	505	1/1	0.90	0.24	92,92,92,92	0
12	ACP	F	402	31/31	0.91	0.12	82,96,119,130	0
9	918	D	501	28/28	0.92	0.16	44,50,57,60	0
6	MG	D	503	1/1	0.93	0.05	61,61,61,61	0
9	918	B	501	28/28	0.95	0.15	34,44,55,60	0
6	MG	A	502	1/1	0.96	0.17	38,38,38,38	0
11	MES	B	506	12/12	0.97	0.12	36,47,67,75	0
7	CA	A	503	1/1	0.97	0.04	75,75,75,75	0
10	GDP	D	502	28/28	0.97	0.10	46,56,66,72	0

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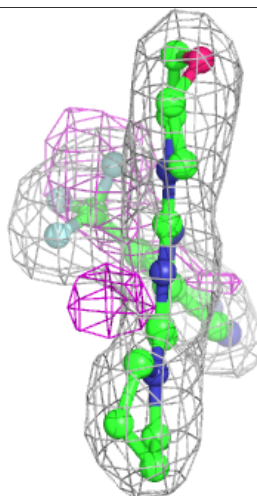
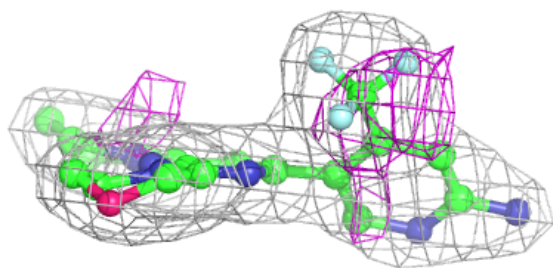
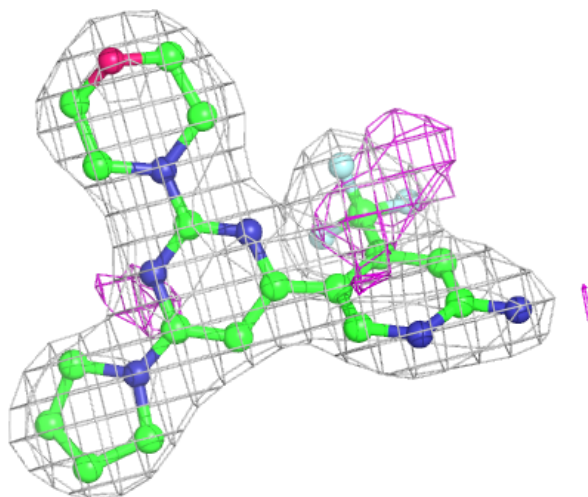
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	C	502	1/1	0.97	0.12	39,39,39,39	0
5	GTP	C	501	32/32	0.98	0.14	27,34,40,44	0
5	GTP	A	501	32/32	0.98	0.19	32,40,44,54	0
7	CA	C	503	1/1	0.99	0.05	59,59,59,59	0
10	GDP	B	502	28/28	0.99	0.18	31,37,43,43	0
6	MG	B	503	1/1	0.99	0.25	30,30,30,30	0

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.



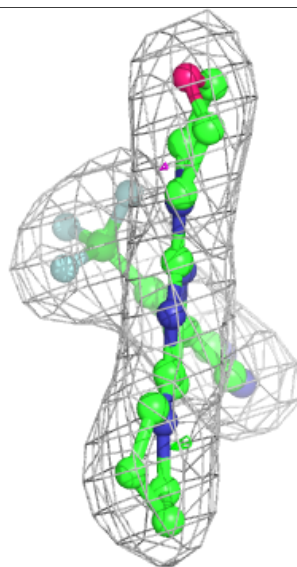
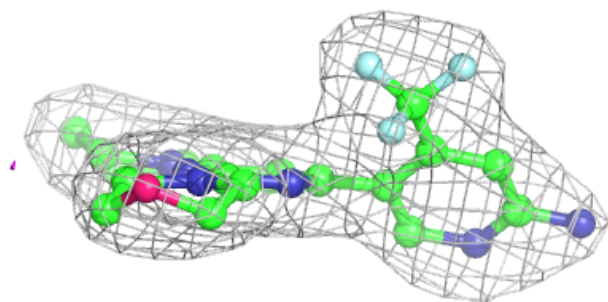
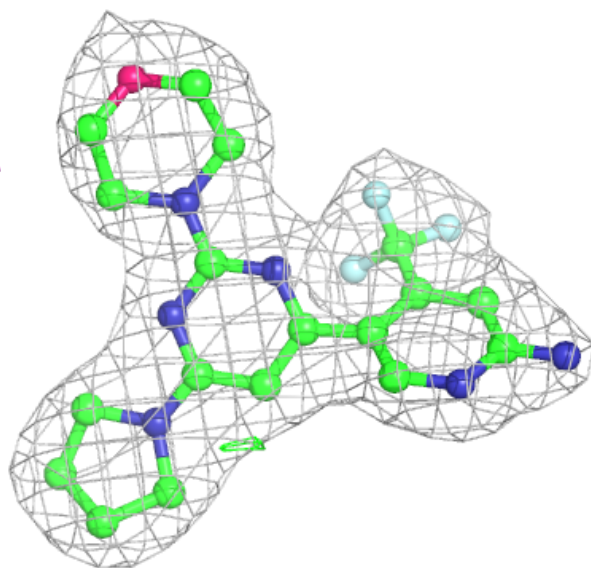
Electron density around 918 D 501:

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



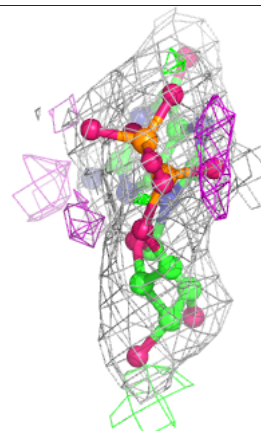
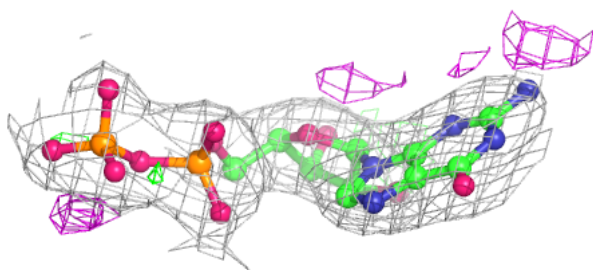
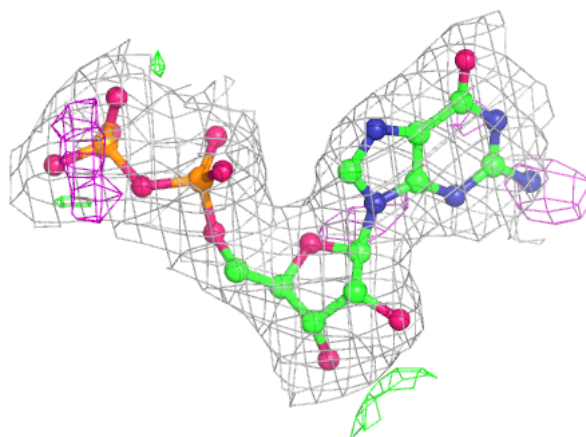
Electron density around 918 B 501:

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

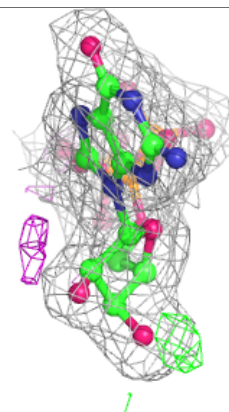
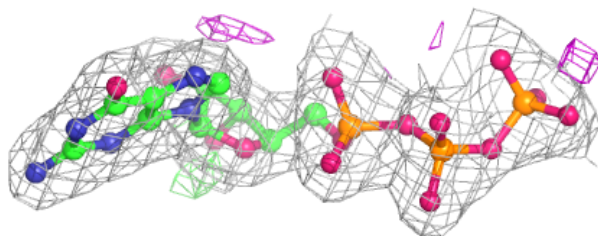
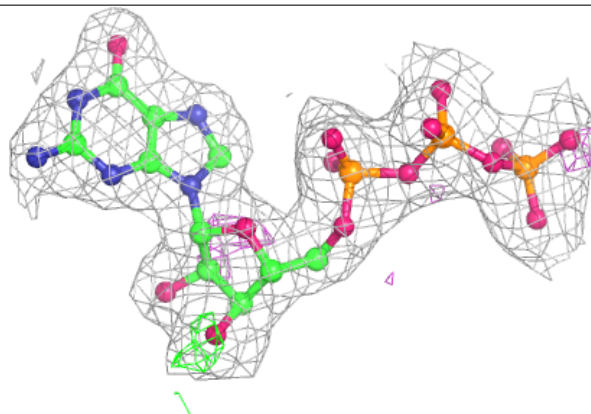


Electron density around GDP D 502:

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

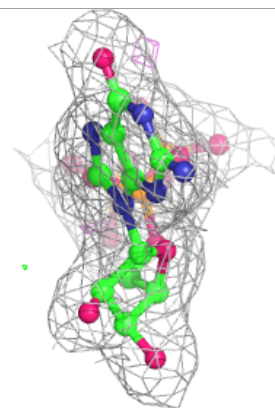
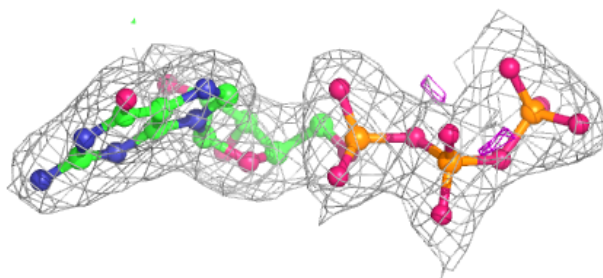
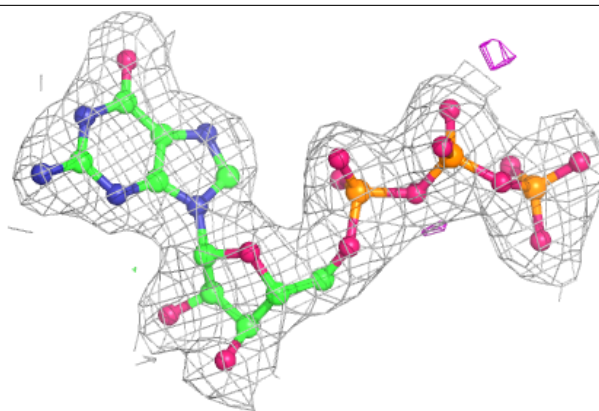
**Electron density around GTP C 501:**

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

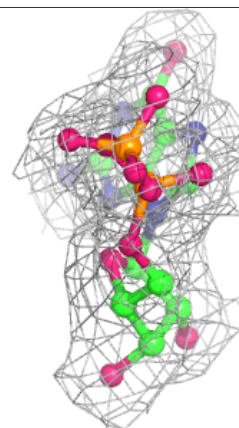
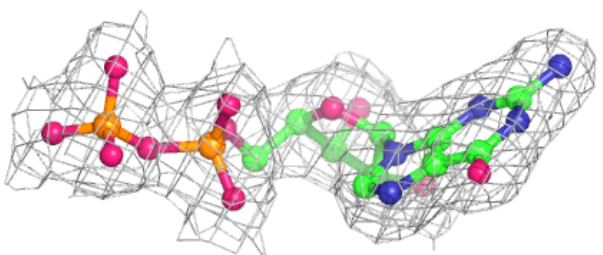
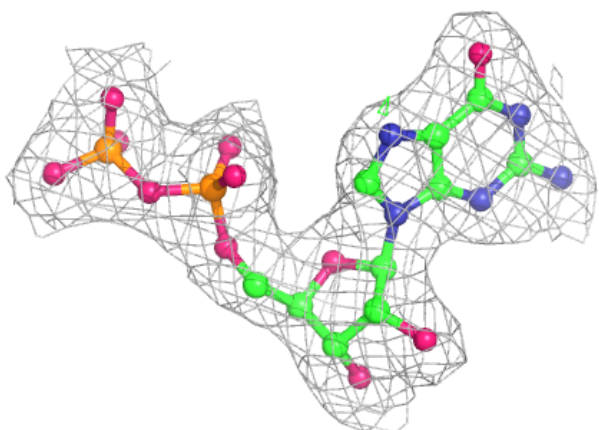


Electron density around GTP A 501:

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

**Electron density around GDP B 502:**

$2mF_o-DF_c$ (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.