



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 01:08 AM UTC

PDB ID : 9KBN / pdb_00009kbn
Title : Crystal structure of T2R-TTL-IKP104-Colchicine
Authors : Yan, W.; Yang, J.H.
Deposited on : 2024-10-31
Resolution : 2.56 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

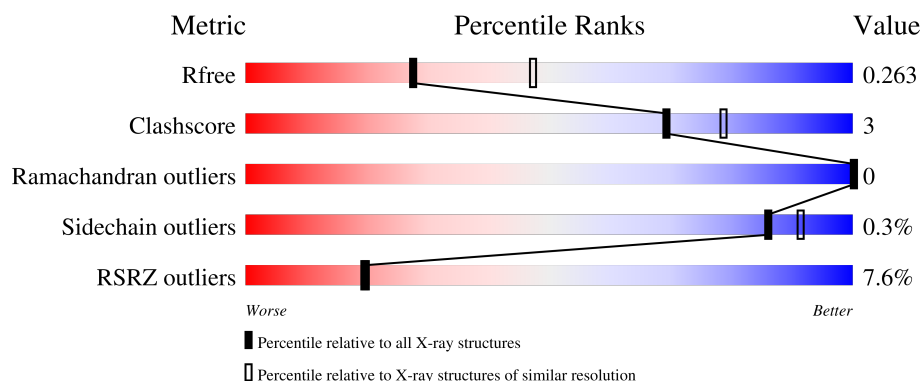
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	450	6% 89% 8% .
1	C	450	3% 89% 8% .
2	B	431	6% 90% 7% .
2	D	431	6% 93% 6% .
3	E	143	10% 81% 14% .

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Mol	Chain	Length	Quality of chain
4	F	384	15% 82% 9% 9%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 33462 atoms, of which 16135 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 Detyrosinated tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	438	Total	C	H	N	O	S	0	2	0
			6451	2107	3122	559	640	23			
1	C	440	Total	C	H	N	O	S	0	4	0
			6651	2160	3245	573	652	21			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	418	Total	C	H	N	O	S	0	1	0
			6265	2032	3037	545	626	25			
2	D	426	Total	C	H	N	O	S	0	0	0
			6336	2052	3069	554	637	24			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	123	Total	C	H	N	O	S	0	0	0
			1919	598	942	179	195	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	351	Total	C	H	N	O	S	0	0	0
			5326	1750	2583	464	515	14			

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
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 (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

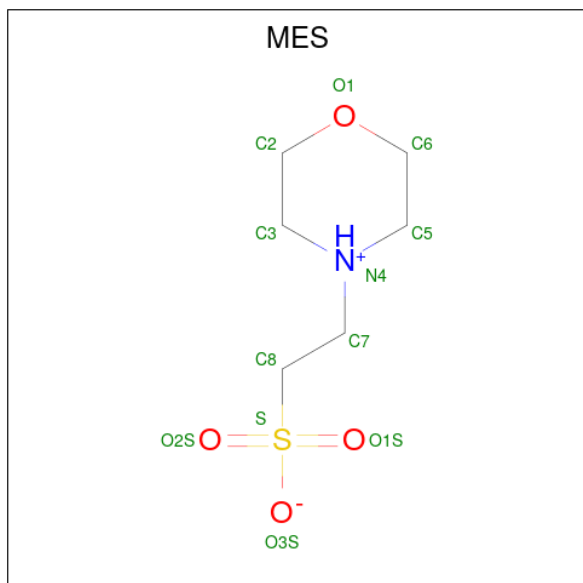
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	2	Total	Ca	0	0
			2	2		

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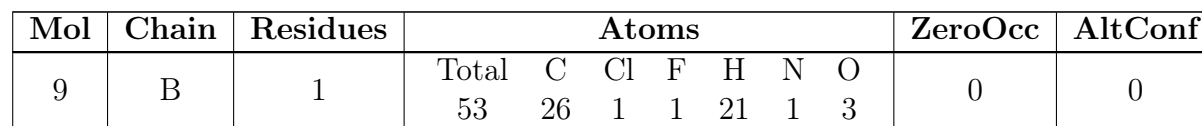
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	2	Total	Ca	0	0
			2	2		
7	D	1	Total	Ca	0	0
			1	1		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 9 is 1-(2-chloranyl-3,5-dimethoxy-phenyl)-2-(4-fluorophenyl)-3-methyl-6-phenyl-pyridin-4-one (CCD ID: W4Q) (formula: $C_{26}H_{21}ClFNO_3$) (labeled as "Ligand of Interest" by depositor).



- # LOC
-
- Chemical structure of Locin, a tricyclic alkaloid. The structure is labeled with atom names: C1 through C22, N1, O1 through O6, and O4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total 54	C 22	H 25	N 1	O 6	0	0
10	D	1	Total 54	C 22	H 25	N 1	O 6	0	0

-
- 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 and a carbonyl group at C6) linked to a ribose sugar via a glycosidic bond at the N9 position. The ribose sugar is further linked to two phosphate groups (P1 and P2) via phosphodiester bonds. The structure is labeled with atom names (N1, N2, N3, N7, N9, C2, C4, C5, C6, C8, O1, O2, O3, O4, O5, O6, O7, O8, O9, O10, O11, O12, O13, O14, O15, O16, O17, O18, O19, O20, O21, O22, O23, O24, O25, O26, O27, O28, O29, O30, O31, O32, O33, O34, O35, O36, O37, O38, O39, O40, O41, O42, O43, O44, O45, O46, O47, O48, O49, O50, O51, O52, O53, O54, O55, O56, O57, O58, O59, O60, O61, O62, O63, O64, O65, O66, O67, O68, O69, O70, O71, O72, O73, O74, O75, O76, O77, O78, O79, O80, O81, O82, O83, O84, O85, O86, O87, O88, O89, O90, O91, O92, O93, O94, O95, O96, O97, O98, O99, O100, O101, O102, O103, O104, O105, O106, O107, O108, O109, O110, O111, O112, O113, O114, O115, O116, O117, O118, O119, O120, O121, O122, O123, O124, O125, O126, O127, O128, O129, O130, O131, O132, O133, O134, O135, O136, O137, O138, O139, O140, O141, O142, O143, O144, O145, O146, O147, O148, O149, O150, O151, O152, O153, O154, O155, O156, O157, O158, O159, O160, O161, O162, O163, O164, O165, O166, O167, O168, O169, O170, O171, O172, O173, O174, O175, O176, O177, O178, O179, O180, O181, O182, O183, O184, O185, O186, O187, O188, O189, O190, O191, O192, O193, O194, O195, O196, O197, O198, O199, O200, O201, O202, O203, O204, O205, O206, O207, O208, O209, O210, O211, O212, O213, O214, O215, O216, O217, O218, O219, O220, O221, O222, O223, O224, O225, O226, O227, O228, O229, O230, O231, O232, O233, O234, O235, O236, O237, O238, O239, O240, O241, O242, O243, O244, O245, O246, O247, O248, O249, O250, O251, O252, O253, O254, O255, O256, O257, O258, O259, O260, O261, O262, O263, O264, O265, O266, O267, O268, O269, O270, O271, O272, O273, O274, O275, O276, O277, O278, O279, O280, O281, O282, O283, O284, O285, O286, O287, O288, O289, O290, O291, O292, O293, O294, O295, O296, O297, O298, O299, O300, O301, O302, O303, O304, O305, O306, O307, O308, O309, O310, O311, O312, O313, O314, O315, O316, O317, O318, O319, O320, O321, O322, O323, O324, O325, O326, O327, O328, O329, O330, O331, O332, O333, O334, O335, O336, O337, O338, O339, O340, O341, O342, O343, O344, O345, O346, O347, O348, O349, O350, O351, O352, O353, O354, O355, O356, O357, O358, O359, O360, O361, O362, O363, O364, O365, O366, O367, O368, O369, O370, O371, O372, O373, O374, O375, O376, O377, O378, O379, O380, O381, O382, O383, O384, O385, O386, O387, O388, O389, O390, O391, O392, O393, O394, O395, O396, O397, O398, O399, O400, O401, O402, O403, O404, O405, O406, O407, O408, O409, O410, O411, O412, O413, O414, O415, O416, O417, O418, O419, O420, O421, O422, O423, O424, O425, O426, O427, O428, O429, O430, O431, O432, O433, O434, O435, O436, O437, O438, O439, O440, O441, O442, O443, O444, O445, O446, O447, O448, O449, O450, O451, O452, O453, O454, O455, O456, O457, O458, O459, O460, O461, O462, O463, O464, O465, O466, O467, O468, O469, O470, O471, O472, O473, O474, O475, O476, O477, O478, O479, O480, O481, O482, O483, O484, O485, O486, O487, O488, O489, O490, O491, O492, O493, O494, O495, O496, O497, O498, O499, O500, O501, O502, O503, O504, O505, O506, O507, O508, O509, O510, O511, O512, O513, O514, O515, O516, O517, O518, O519, O520, O521, O522, O523, O524, O525, O526, O527, O528, O529, O530, O531, O532, O533, O534, O535, O536, O537, O538, O539, O540, O541, O542, O543, O544, O545, O546, O547, O548, O549, O550, O551, O552, O553, O554, O555, O556, O557, O558, O559, O560, O561, O562, O563, O564, O565, O566, O567, O568, O569, O570, O571, O572, O573, O574, O575, O576, O577, O578, O579, O580, O581, O582, O583, O584, O585, O586, O587, O588, O589, O590, O591, O592, O593, O594, O595, O596, O597, O598, O599, O600, O601, O602, O603, O604, O605, O606, O607, O608, O609, O610, O611, O612, O613, O614, O615, O616, O617, O618, O619, O620, O621, O622, O623, O624, O625, O626, O627, O628, O629, O630, O631, O632, O633, O634, O635, O636, O637, O638, O639, O640, O641, O642, O643, O644, O645, O646, O647, O648, O649, O650, O651, O652, O653, O654, O655, O656, O657, O658, O659, O660, O661, O662, O663, O664, O665, O666, O667, O668, O669, O670, O671, O672, O673, O674, O675, O676, O677, O678, O679, O680, O681, O682, O683, O684, O685, O686, O687, O688, O689, O690, O691, O692, O693, O694, O695, O696, O697, O698, O699, O700, O701, O702, O703, O704, O705, O706, O707, O708, O709, O710, O711, O712, O713, O714, O715, O716, O717, O718, O719, O720, O721, O722, O723, O724, O725, O726, O727, O728, O729, O730, O731, O732, O733, O734, O735, O736, O737, O738, O739, O740, O741, O742, O743, O744, O745, O746, O747, O748, O749, O750, O751, O752, O753, O754, O755, O756, O757, O758, O759, O760, O761, O762, O763, O764, O765, O766, O767, O768, O769, O770, O771, O772, O773, O774, O775, O776, O777, O778, O779, O780, O781, O782, O783, O784, O785, O786, O787, O788, O789, O790, O791, O792, O793, O794, O795, O796, O797, O798, O799, O800, O801, O802, O803, O804, O805, O806, O807, O808, O

ACP

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

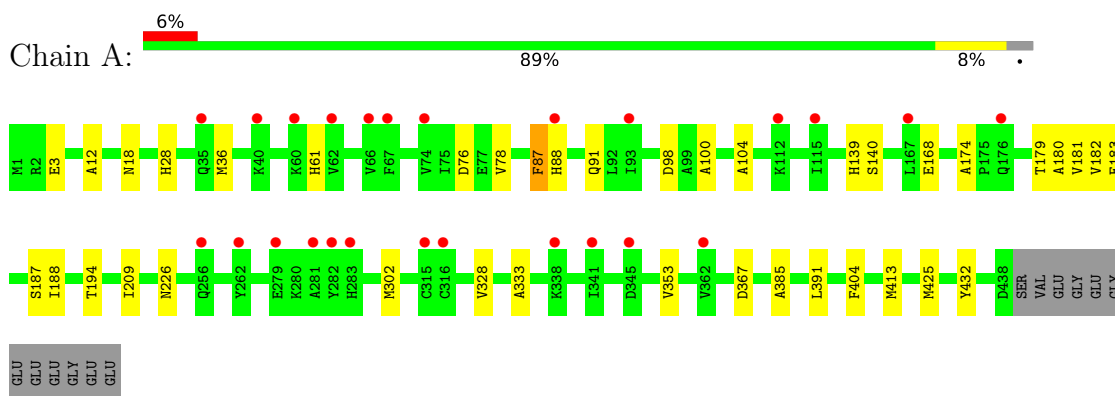
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	14	Total 14	O 14	0	0
13	B	18	Total 18	O 18	0	0
13	C	50	Total 50	O 50	0	0
13	D	16	Total 16	O 16	0	0
13	E	3	Total 3	O 3	0	0
13	F	7	Total 7	O 7	0	0

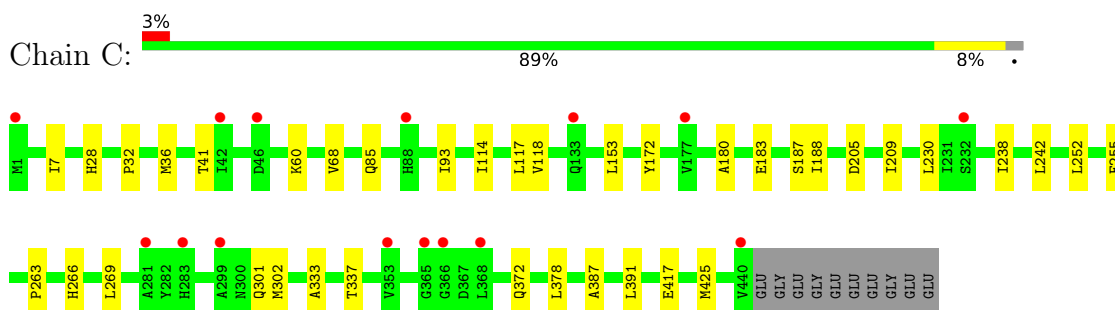
3 Residue-property plots

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.

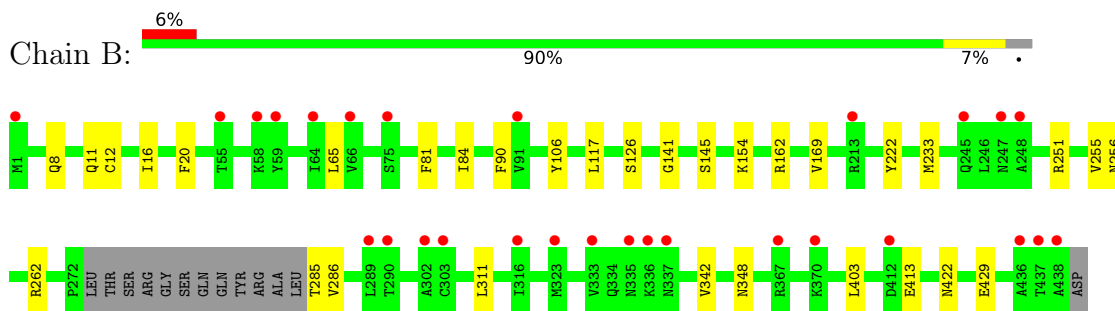
- Molecule 1: Detyrosinated tubulin alpha-1B chain



- Molecule 1: Detyrosinated tubulin alpha-1B chain

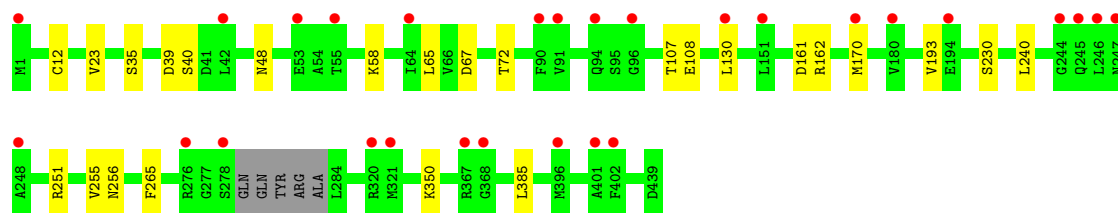


- Molecule 2: Tubulin beta chain

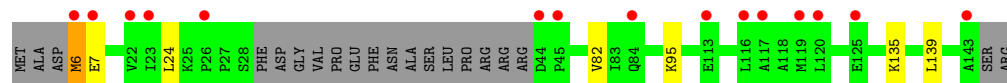
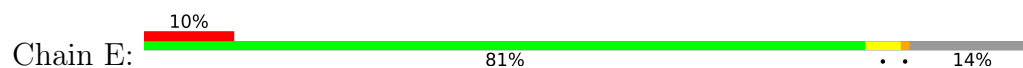


- Molecule 2: Tubulin beta chain

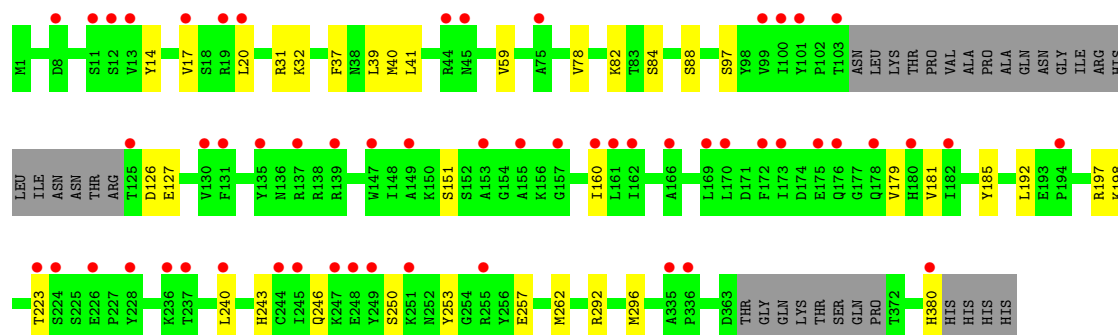
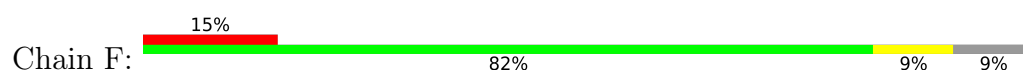




● Molecule 3: Stathmin-4



● 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	159.81Å 174.68Å 104.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.30 – 2.56 39.30 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.7 (39.30-2.56) 98.6 (39.30-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.228 , 0.262 0.229 , 0.263	Depositor DCC
R_{free} test set	2000 reflections (2.11%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.3	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	0.93	EDS
Total number of atoms	33462	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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: W4Q, MG, GTP, MES, LOC, GDP, CA, ACP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.14	0/3408	0.28	0/4646
1	C	0.15	0/3502	0.31	0/4767
2	B	0.17	1/3304 (0.0%)	0.28	0/4488
2	D	0.13	0/3338	0.28	0/4534
3	E	0.16	0/985	0.28	0/1313
4	F	0.12	0/2805	0.28	0/3807
All	All	0.15	1/17342 (0.0%)	0.29	0/23555

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	286	VAL	CA-CB	5.62	1.56	1.54

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	3329	3122	3145	29	0
1	C	3406	3245	3265	26	1
2	B	3228	3037	3050	21	0
2	D	3267	3069	3090	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	977	942	946	4	1
4	F	2743	2583	2594	19	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	12	1	0
6	A	1	0	0	0	0
6	C	2	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	2	0	0	0	0
7	D	1	0	0	0	0
8	B	12	12	12	0	0
9	B	32	21	0	1	0
10	B	29	25	25	5	0
10	D	29	25	25	5	0
11	B	28	10	12	0	0
12	F	31	14	14	0	0
13	A	14	0	0	3	0
13	B	18	0	0	3	0
13	C	50	0	0	2	0
13	D	16	0	0	0	0
13	E	3	0	0	0	0
13	F	7	0	0	1	0
All	All	17327	16135	16214	116	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 116 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:226:ASN:ND2	1:A:367:ASP:OD2	2.15	0.80
1:C:32:PRO:O	13:C:601:HOH:O	1.99	0.79
10:D:504:LOC:H6A	10:D:504:LOC:H4B	1.65	0.78
1:C:417:GLU:OE1	13:C:602:HOH:O	2.02	0.78
1:C:242:LEU:HD21	1:C:252:LEU:HG	1.66	0.77

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:GLN:OE1	3:E:95:LYS:NZ[2_554]	1.97	0.23

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/450 (97%)	426 (97%)	12 (3%)	0	100	100
1	C	442/450 (98%)	431 (98%)	11 (2%)	0	100	100
2	B	415/431 (96%)	405 (98%)	10 (2%)	0	100	100
2	D	422/431 (98%)	409 (97%)	13 (3%)	0	100	100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	345/384 (90%)	330 (96%)	15 (4%)	0	100	100
All	All	2181/2289 (95%)	2119 (97%)	62 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/378 (92%)	345 (100%)	1 (0%)	86	91
1	C	364/378 (96%)	364 (100%)	0	100	100
2	B	346/372 (93%)	346 (100%)	0	100	100
2	D	350/372 (94%)	349 (100%)	1 (0%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	100/127 (79%)	98 (98%)	2 (2%)	48	64
4	F	286/342 (84%)	285 (100%)	1 (0%)	86	91
All	All	1792/1969 (91%)	1787 (100%)	5 (0%)	86	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	PHE
2	D	48	ASN
3	E	6	MET
3	E	7	GLU
4	F	59	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	11	GLN
2	D	134	GLN
3	E	64	GLN
2	D	329	GLN
2	B	165	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 21 ligands modelled in this entry, 12 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	$\# Z > 2$
12	ACP	F	402	6	31,33,33	1.64	8 (25%)	47,52,52	1.88	10 (21%)
9	W4Q	B	504	-	35,35,35	5.18	25 (71%)	44,50,50	1.03	2 (4%)
5	GTP	D	503	6	33,34,34	0.97	2 (6%)	50,54,54	1.57	9 (18%)
10	LOC	B	505	-	31,31,31	3.56	13 (41%)	44,44,44	3.55	19 (43%)
8	MES	B	501	-	12,12,12	2.25	1 (8%)	15,16,16	1.56	2 (13%)
5	GTP	C	502	6	33,34,34	1.01	3 (9%)	50,54,54	1.56	10 (20%)
10	LOC	D	504	-	31,31,31	3.55	12 (38%)	44,44,44	3.44	17 (38%)
11	GDP	B	506	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	6 (13%)
5	GTP	A	501	6	33,34,34	0.94	1 (3%)	50,54,54	1.60	8 (16%)

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
12	ACP	F	402	6	-	5/19/38/38	0/3/3/3
9	W4Q	B	504	-	-	2/16/16/16	0/4/4/4
5	GTP	D	503	6	-	4/22/38/38	0/3/3/3
10	LOC	B	505	-	-	4/12/25/25	0/3/3/3
8	MES	B	501	-	-	1/6/14/14	0/1/1/1
5	GTP	C	502	6	-	7/22/38/38	0/3/3/3
10	LOC	D	504	-	-	3/12/25/25	0/3/3/3
11	GDP	B	506	-	-	0/16/32/32	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	504	LOC	C20-C21	9.93	1.54	1.37
10	B	505	LOC	C15-C14	9.82	1.54	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	505	LOC	C20-C21	9.81	1.54	1.37
10	D	504	LOC	C15-C14	9.67	1.54	1.36
9	B	504	W4Q	C1-C6	-9.50	1.31	1.40

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	504	LOC	C15-C14-C21	-13.82	115.78	127.56
10	B	505	LOC	C15-C14-C21	-12.09	117.25	127.56
10	B	505	LOC	O6-C17-C16	11.15	119.85	109.60
10	D	504	LOC	O6-C17-C16	8.14	117.08	109.60
10	D	504	LOC	C14-C15-C16	-7.44	120.94	134.20

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
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	502	GTP	C5'-O5'-PA-O3A

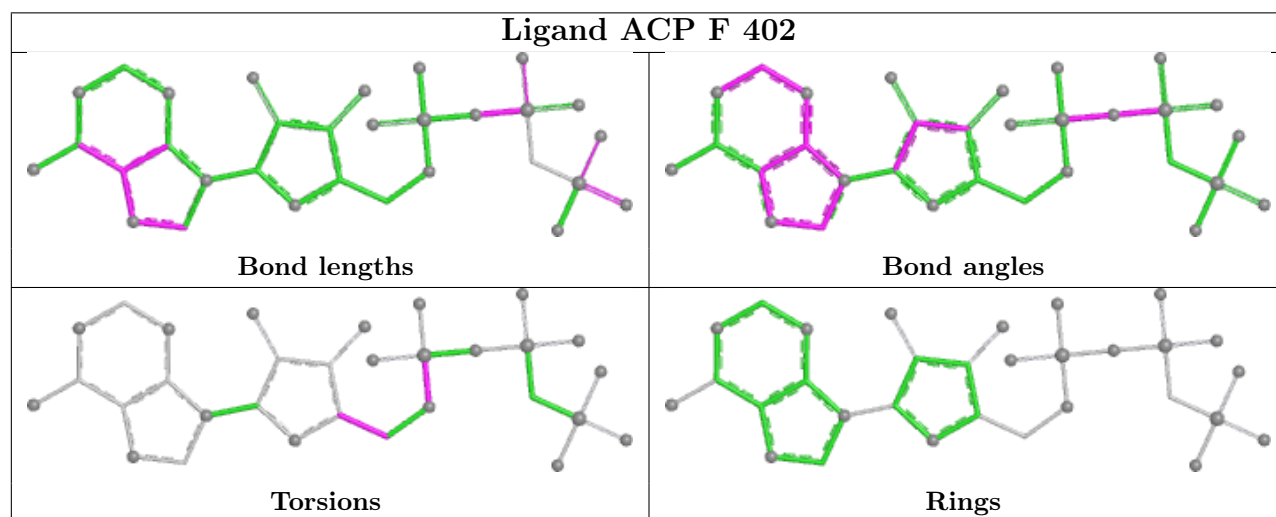
There are no ring outliers.

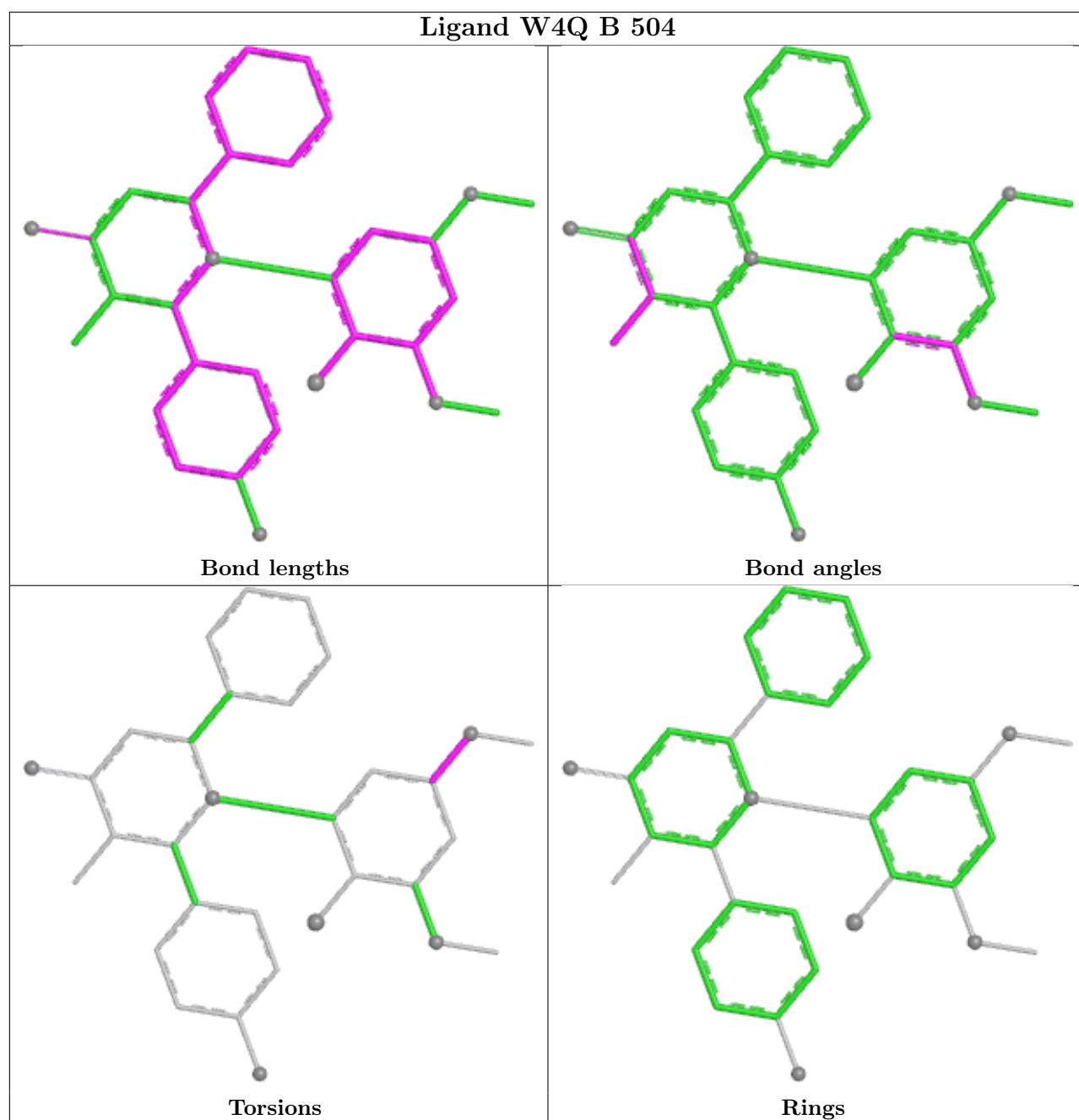
4 monomers are involved in 12 short contacts:

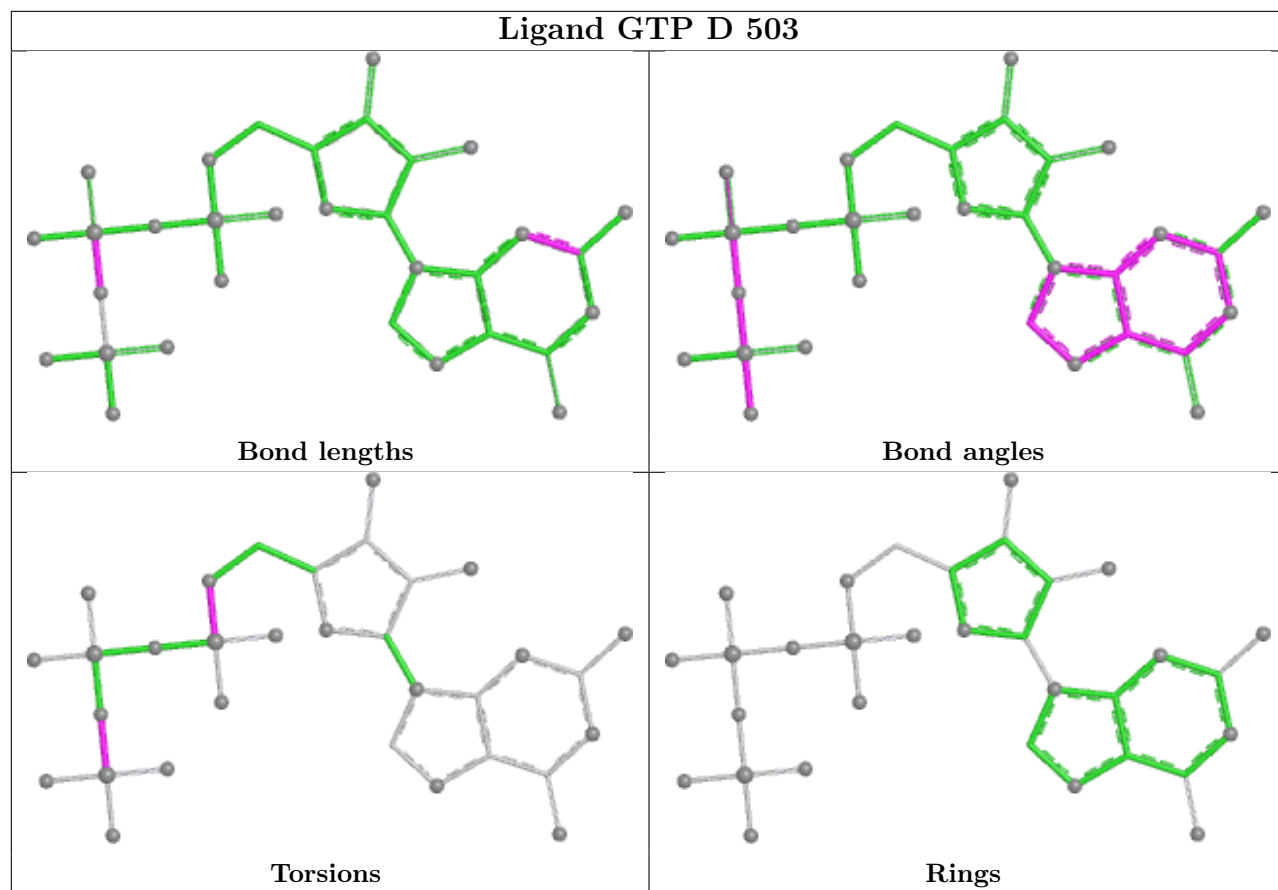
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	504	W4Q	1	0
5	D	503	GTP	1	0
10	B	505	LOC	5	0
10	D	504	LOC	5	0

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.

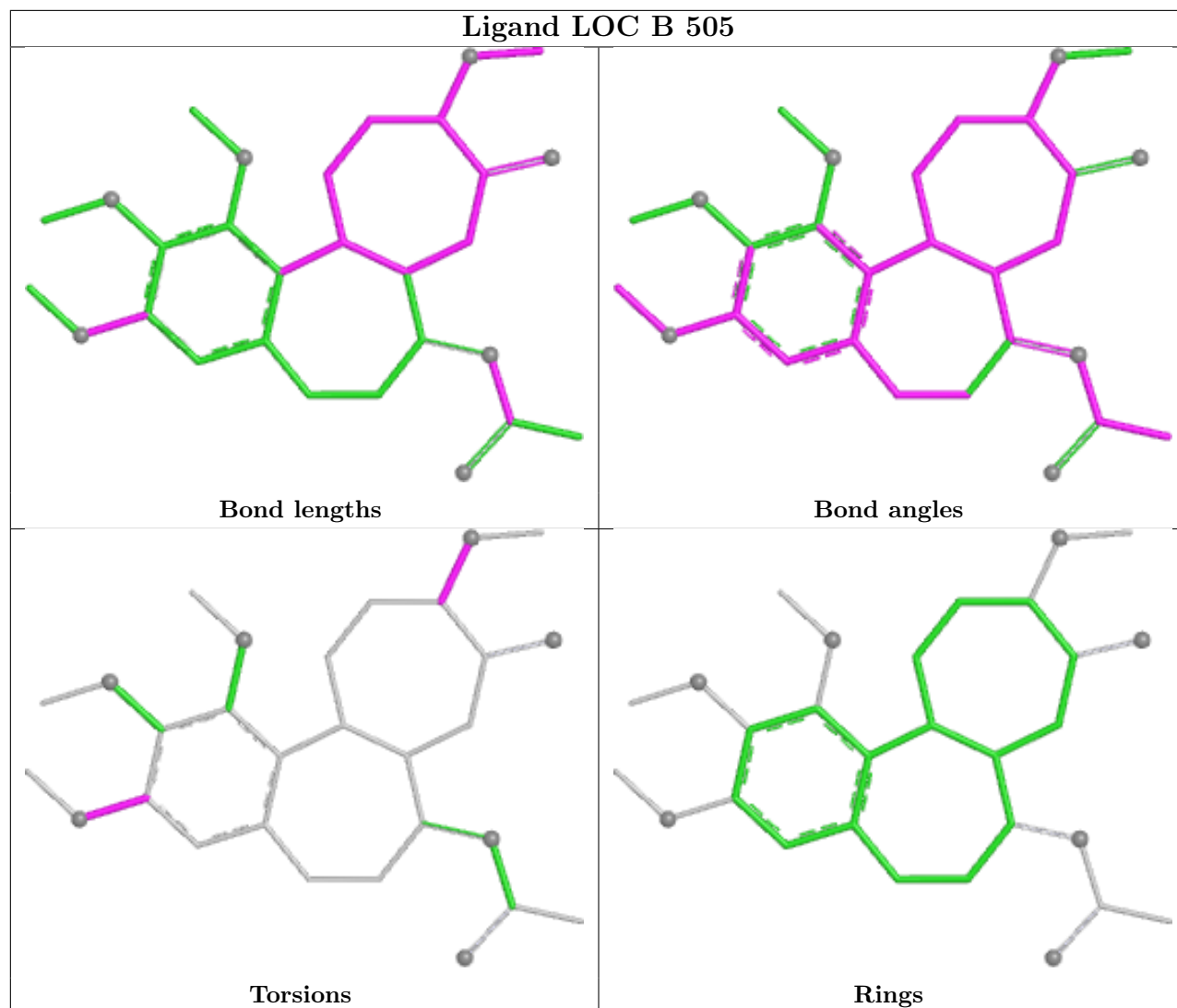
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

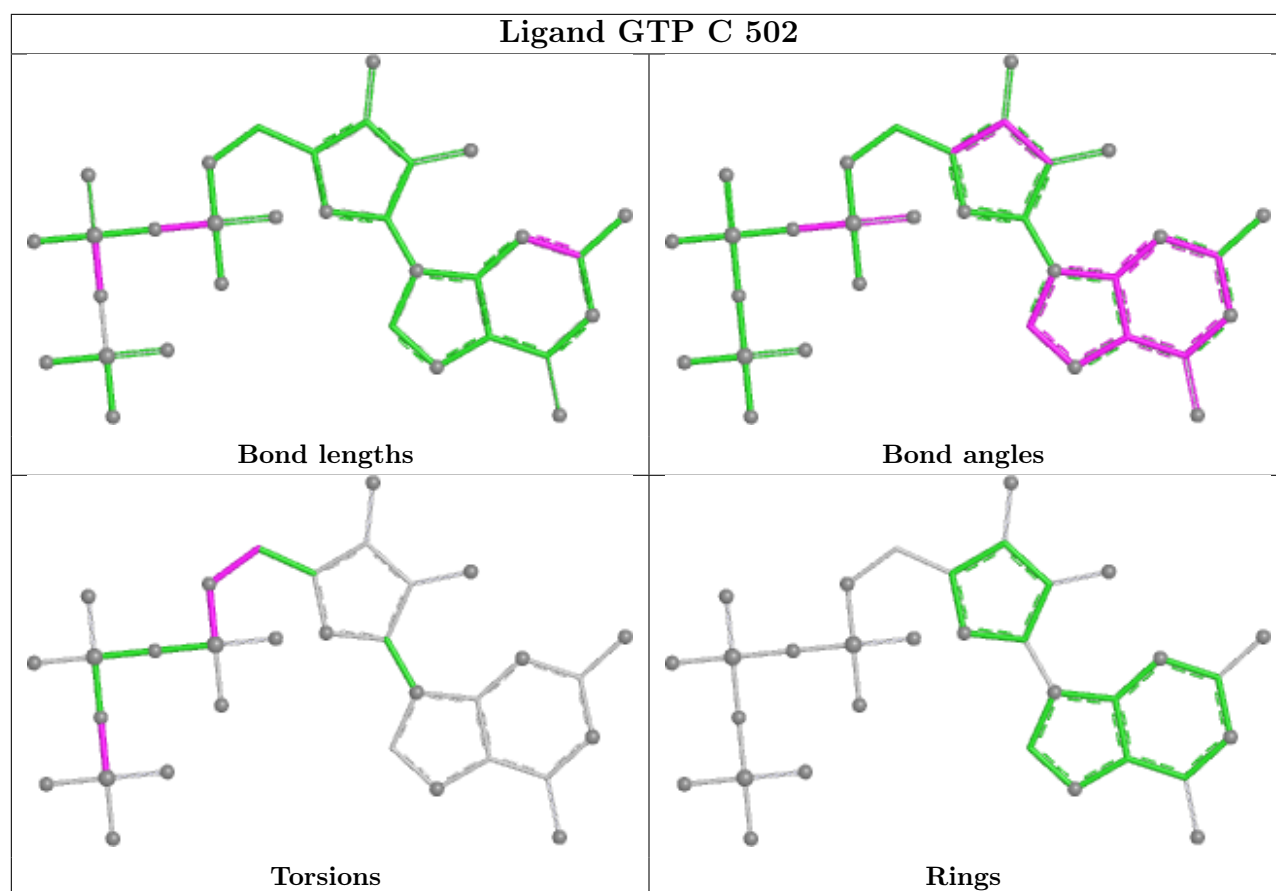


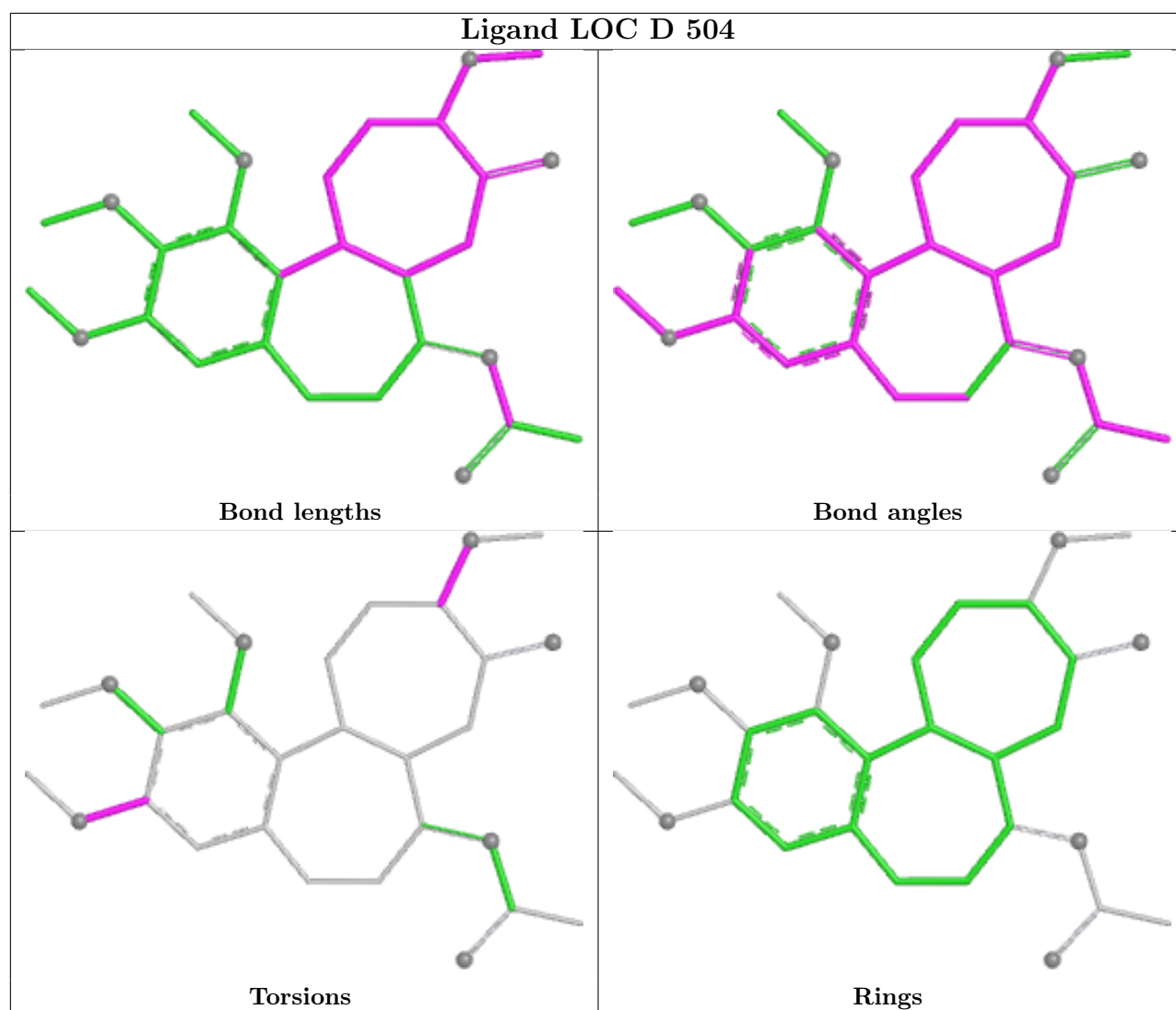


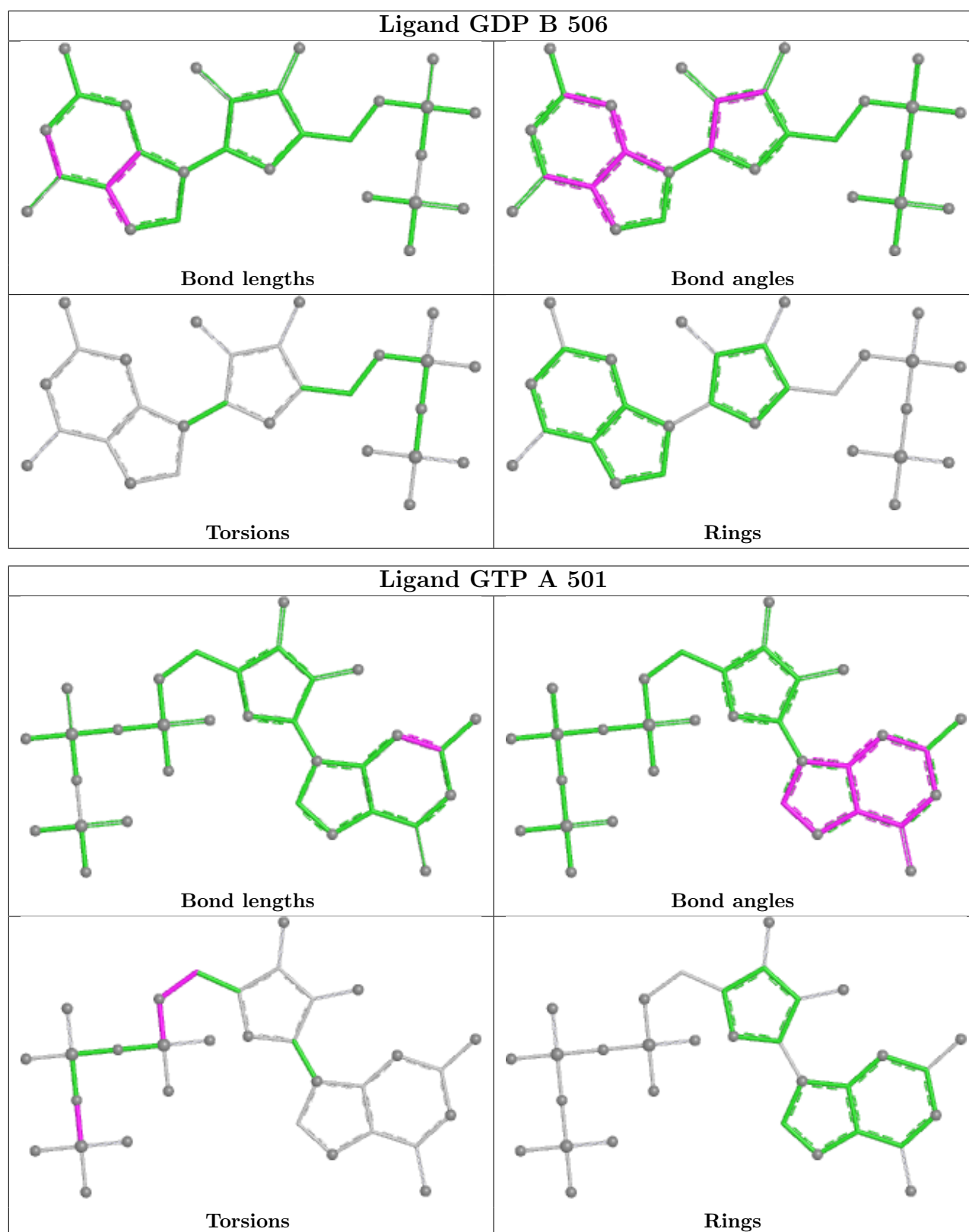


Ligand LOC B 505









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	438/450 (97%)	0.67	25 (5%)	29	29	34, 70, 91, 108	2 (0%)
1	C	440/450 (97%)	0.29	15 (3%)	48	49	30, 59, 78, 90	3 (0%)
2	B	418/431 (96%)	0.59	28 (6%)	24	23	38, 68, 92, 115	1 (0%)
2	D	426/431 (98%)	0.71	28 (6%)	24	24	51, 74, 96, 109	0
3	E	123/143 (86%)	0.87	15 (12%)	8	8	61, 79, 101, 116	0
4	F	351/384 (91%)	1.13	56 (15%)	5	4	61, 85, 121, 129	0
All	All	2196/2289 (95%)	0.67	167 (7%)	20	19	30, 71, 101, 129	6 (0%)

The worst 5 of 167 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	5.7
4	F	100	ILE	5.4
1	C	366	GLY	4.9
3	E	7	GLU	4.6
4	F	103	THR	4.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

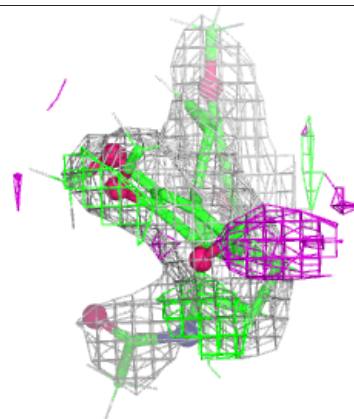
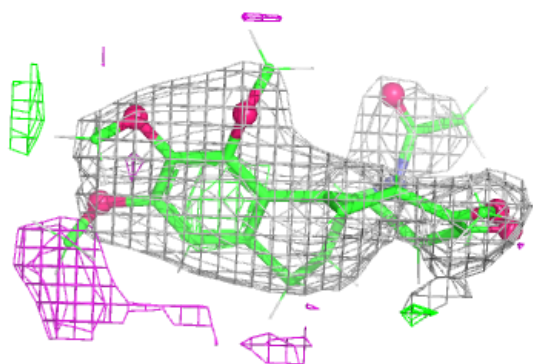
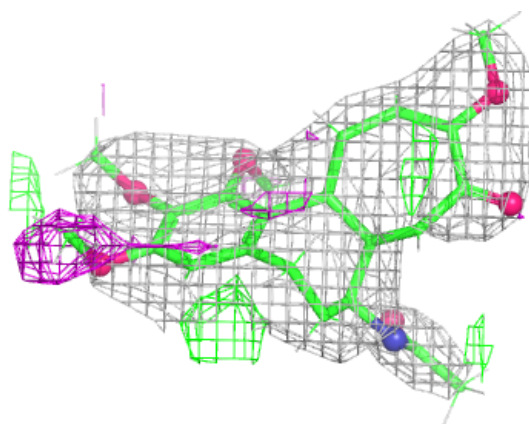
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	F	401	1/1	0.72	0.24	90,90,90,90	0
7	CA	C	505	1/1	0.74	0.15	96,96,96,96	0
7	CA	B	503	1/1	0.84	0.15	87,87,87,87	0
10	LOC	D	504	29/29	0.84	0.16	55,68,82,83	0
12	ACP	F	402	31/31	0.84	0.13	81,96,115,117	0
7	CA	D	502	1/1	0.86	0.11	86,86,86,86	0
7	CA	C	504	1/1	0.87	0.21	81,81,81,81	0
6	MG	C	501	1/1	0.88	0.15	54,54,54,54	0
10	LOC	B	505	29/29	0.88	0.15	57,66,80,80	0
7	CA	B	502	1/1	0.89	0.10	92,92,92,92	0
7	CA	A	504	1/1	0.89	0.17	94,94,94,94	0
8	MES	B	501	12/12	0.90	0.13	58,70,78,80	0
5	GTP	D	503	32/32	0.92	0.11	61,66,80,83	0
9	W4Q	B	504	32/32	0.94	0.11	49,54,64,66	0
11	GDP	B	506	28/28	0.94	0.10	48,54,67,69	0
7	CA	A	503	1/1	0.94	0.07	91,91,91,91	0
6	MG	A	502	1/1	0.95	0.13	56,56,56,56	0
5	GTP	C	502	32/32	0.95	0.09	41,48,58,70	0
5	GTP	A	501	32/32	0.96	0.08	50,57,71,74	0
6	MG	C	503	1/1	0.98	0.05	49,49,49,49	0
6	MG	D	501	1/1	0.98	0.12	67,67,67,67	0

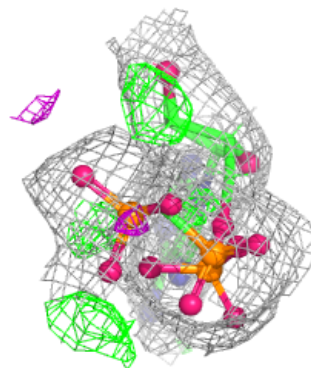
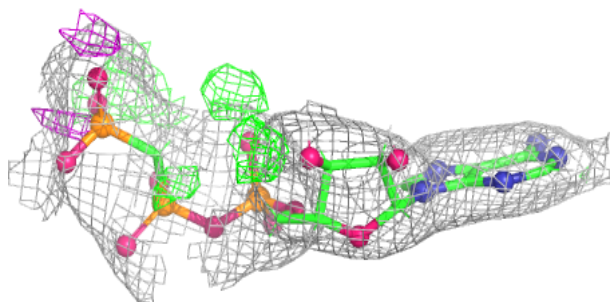
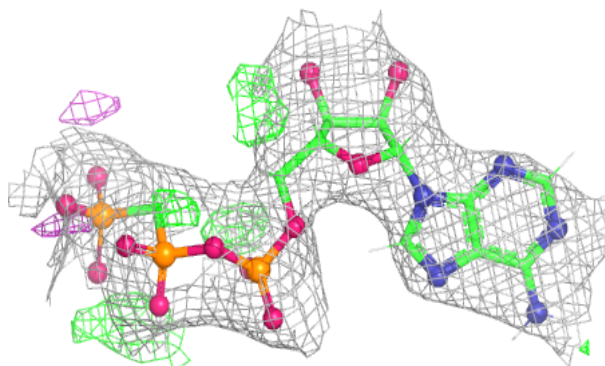
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LOC D 504:

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

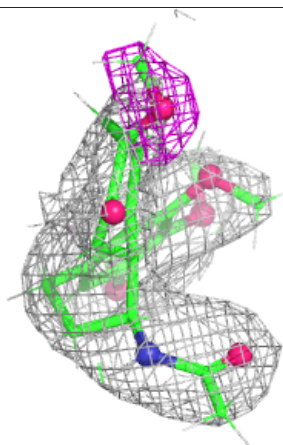
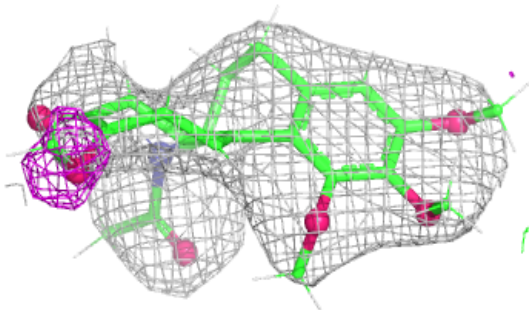
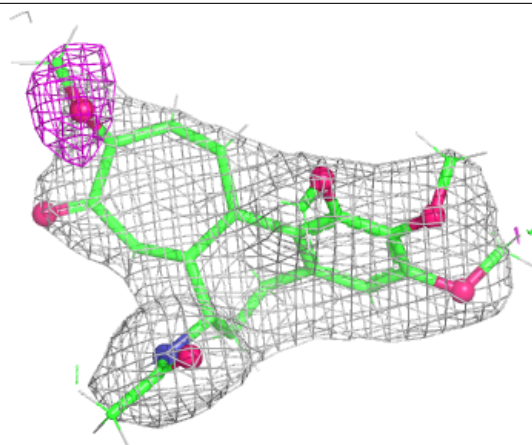
**Electron density around ACP F 402:**

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

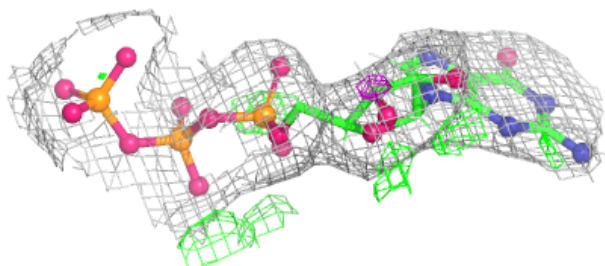
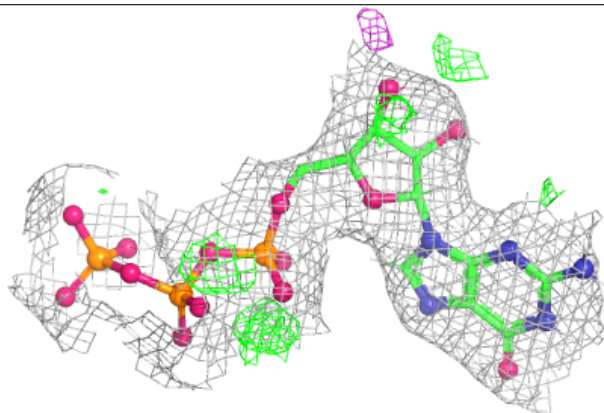


Electron density around LOC B 505:

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

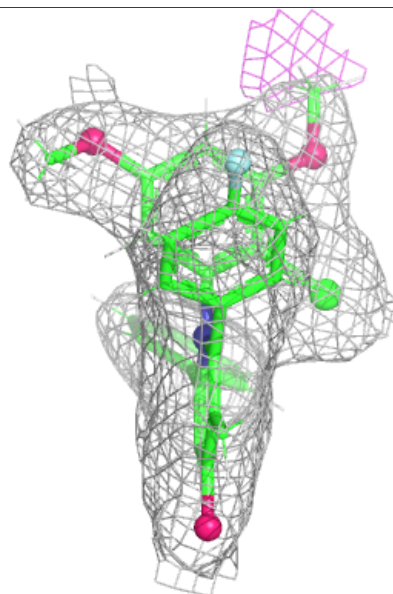
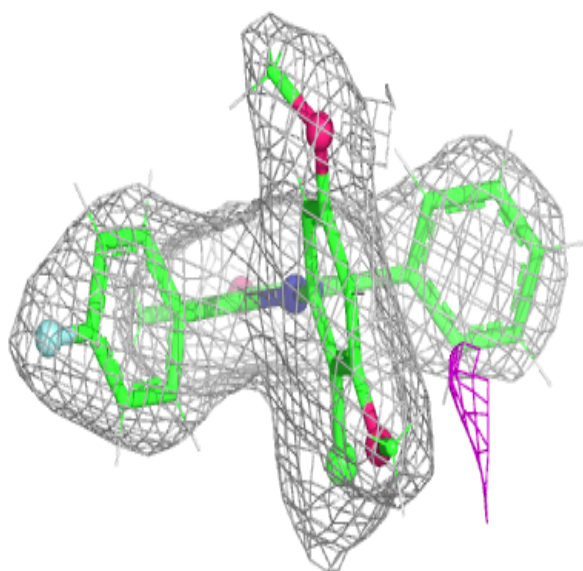
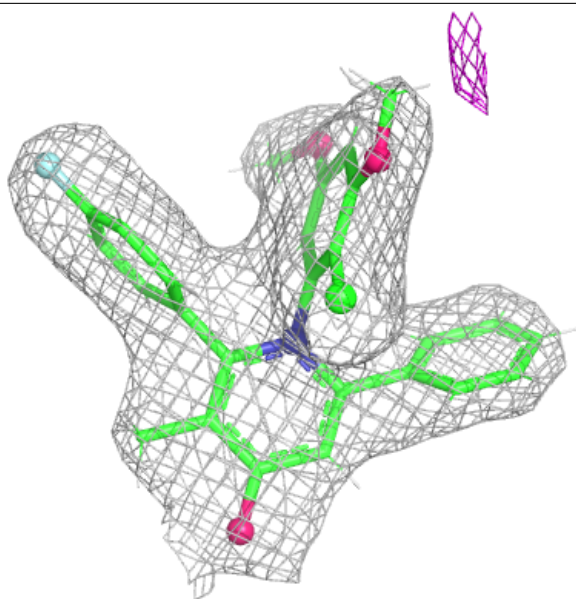
**Electron density around GTP D 503:**

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



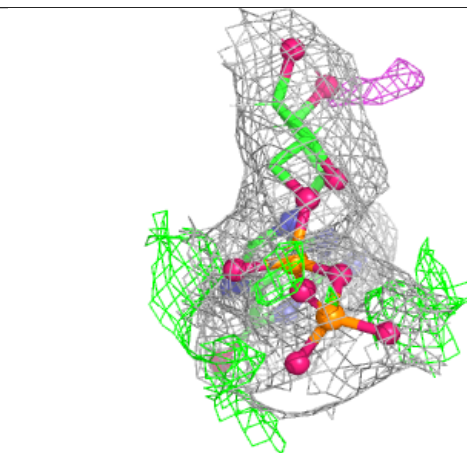
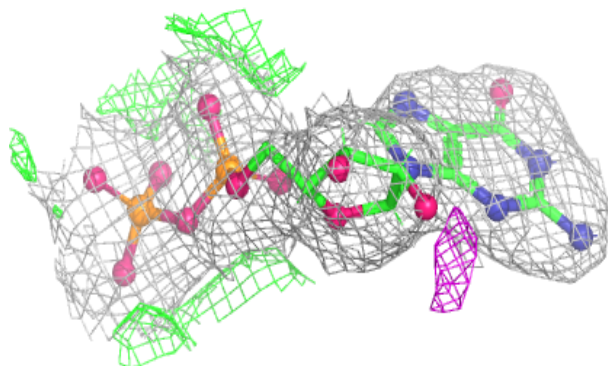
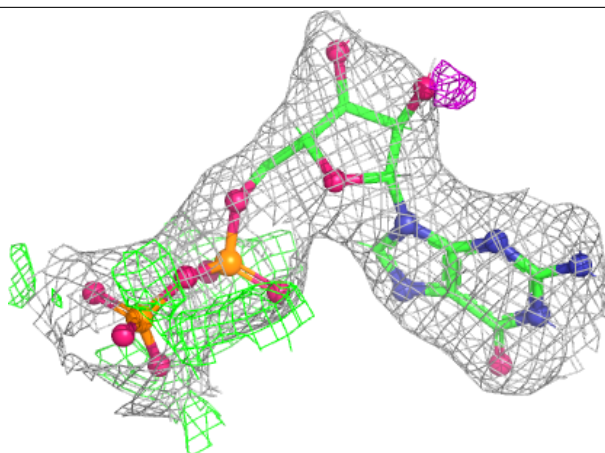
Electron density around W4Q B 504:

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

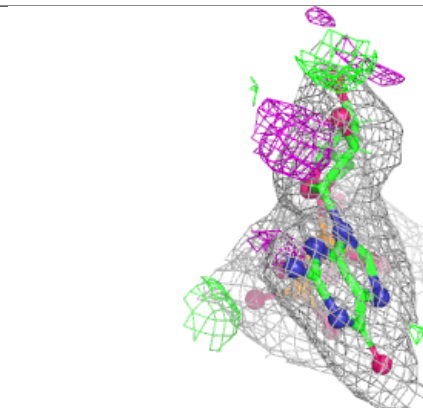
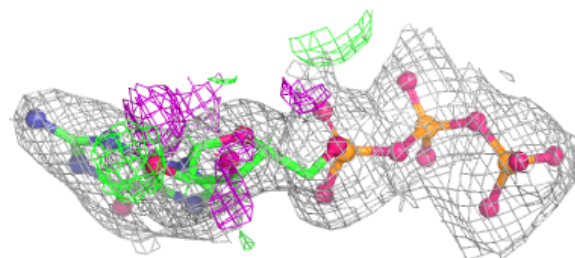
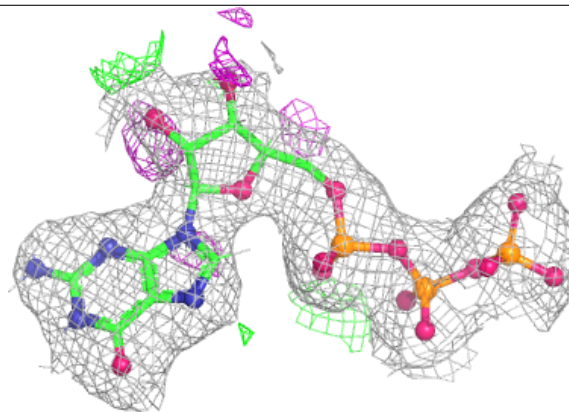


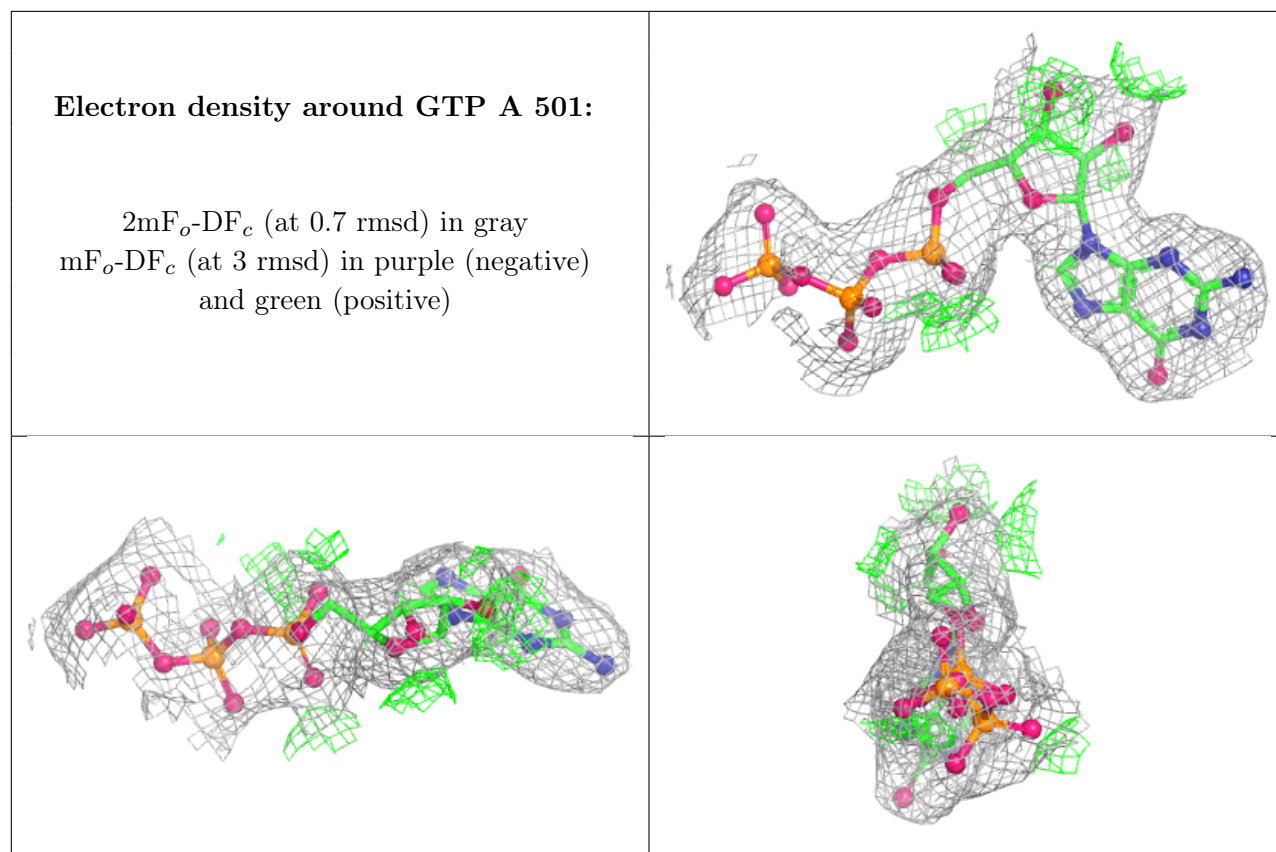
Electron density around GDP B 506:

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

**Electron density around GTP C 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.