



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2025 – 08:52 PM JST

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 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 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

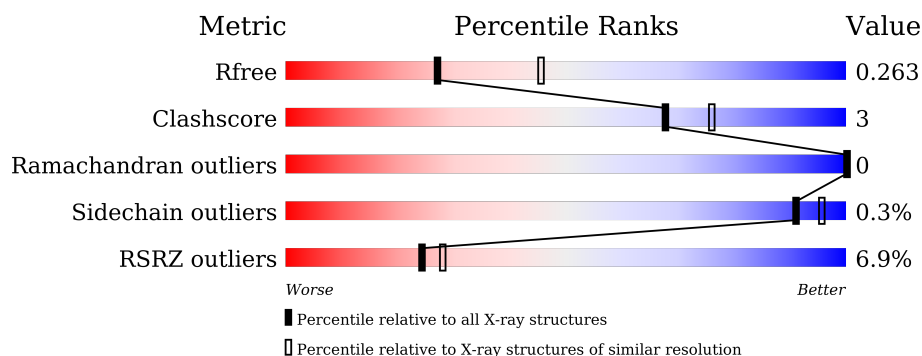
1 Overall quality at a glance

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}	164625	1685 (2.58-2.54)
Clashscore	180529	1779 (2.58-2.54)
Ramachandran outliers	177936	1766 (2.58-2.54)
Sidechain outliers	177891	1766 (2.58-2.54)
RSRZ outliers	164620	1685 (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	<div> <div>4%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	C	450	<div> <div>3%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
2	B	431	<div> <div>6%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
2	D	431	<div> <div>6%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
3	E	143	<div> <div>10%</div> <div>81%</div> <div>.</div> <div>14%</div> </div>
4	F	384	<div> <div>14%</div> <div>82%</div> <div>9%</div> <div>9%</div> </div>

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

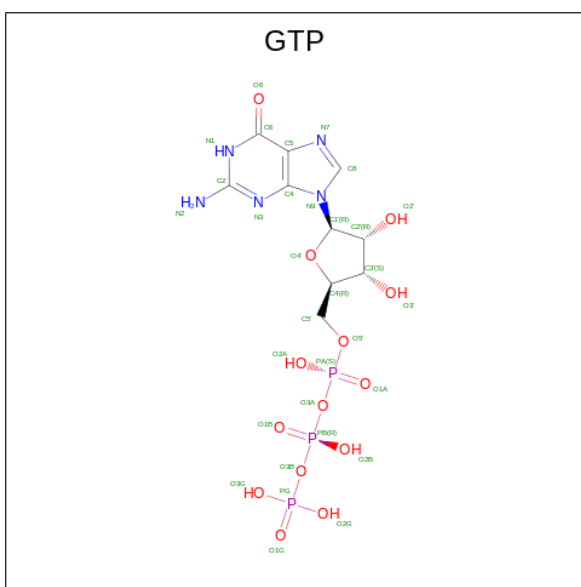
- Molecule 4 is a protein called Tubulin tyrosine ligase.

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 42	C 10	H 10	N 5	O 14	P 3	0	0
5	C	1	Total 42	C 10	H 10	N 5	O 14	P 3	0	0
5	D	1	Total 42	C 10	H 10	N 5	O 14	P 3	0	0

- 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).

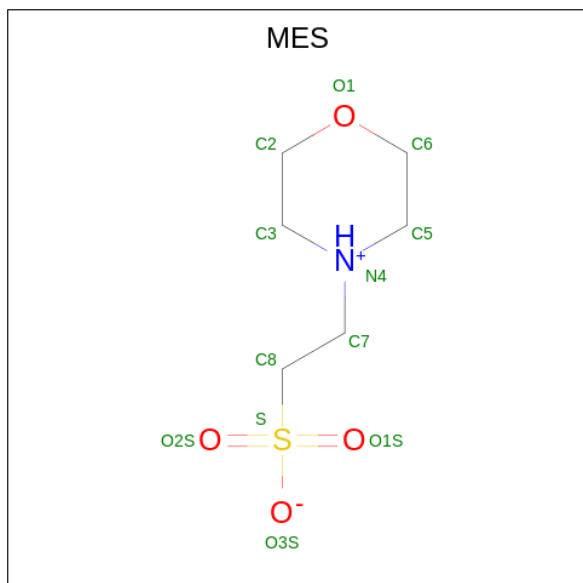
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	2	Total	Ca	0	0
			2	2		

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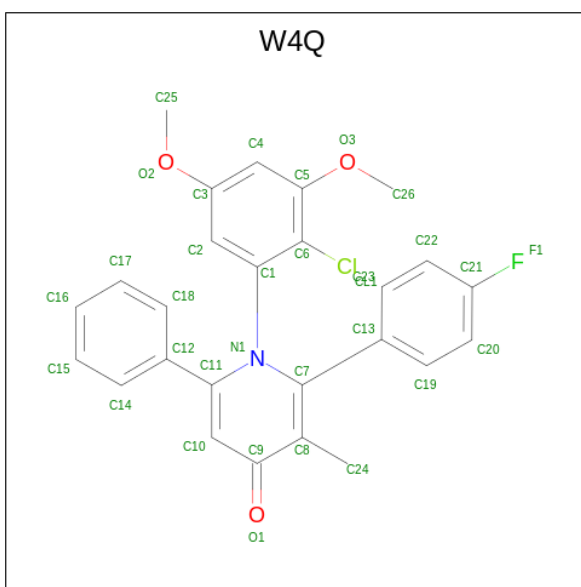
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	2	Total	Ca	0	0
			2	2		
7	D	1	Total	Ca	0	0
			1	1		

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



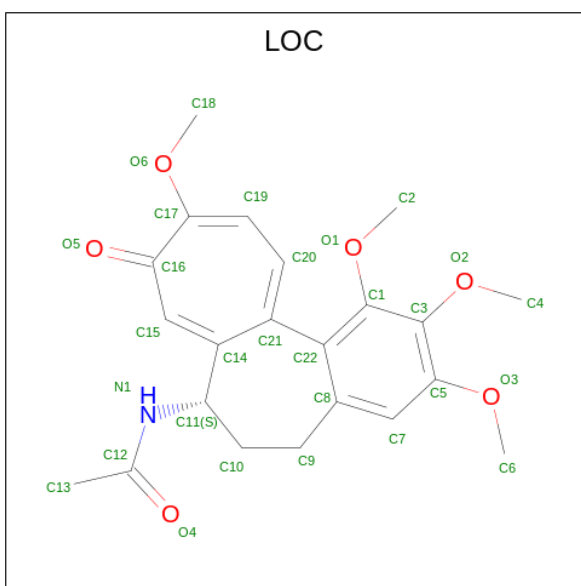
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	S	0	0
			24	6	12	1	4	1		

- 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).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
9	B	1	Total	C	Cl	F	H	N	O	0	0
			53	26	1	1	21	1	3		

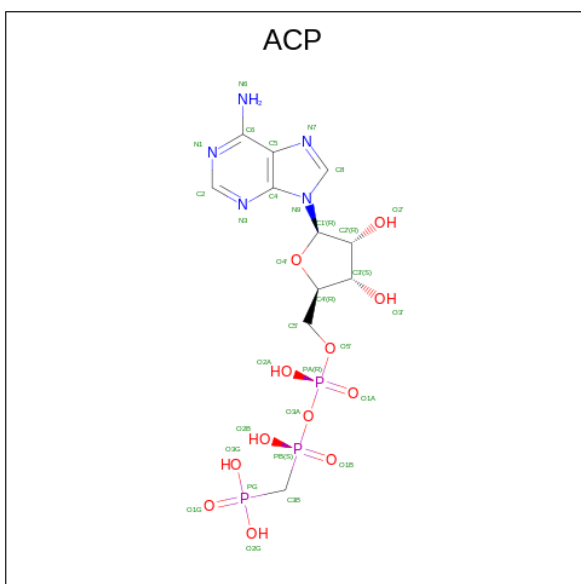
- Molecule 10 is N-[(7S)-1,2,3,10-tetramethoxy-9-oxo-6,7-dihydro-5H-benzo[d]heptalen-7-yl]ethanamide (CCD ID: LOC) (formula: $C_{22}H_{25}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

-
- 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, which is in turn linked to two phosphate groups. The atoms are labeled with their respective element symbols and indices (e.g., N1, C2, O3, P4, O5, P6, 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, O809, O810, O811, O812, O813, O814, O815, O816, O817, O818, O819, O820

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$).



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

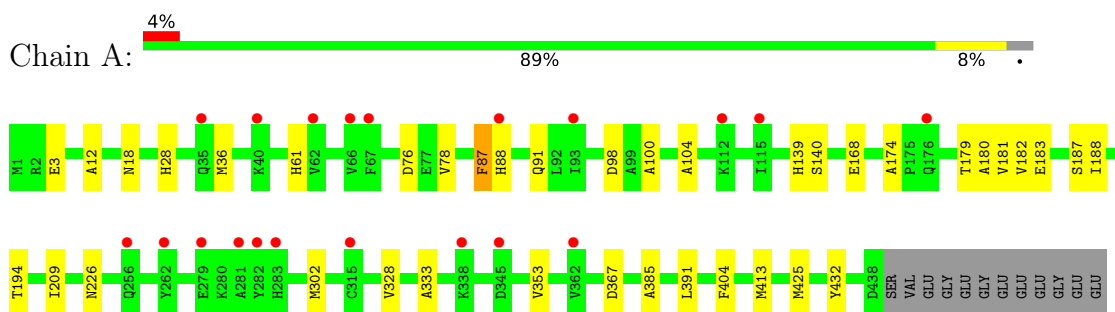
- Molecule 13 is water.

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

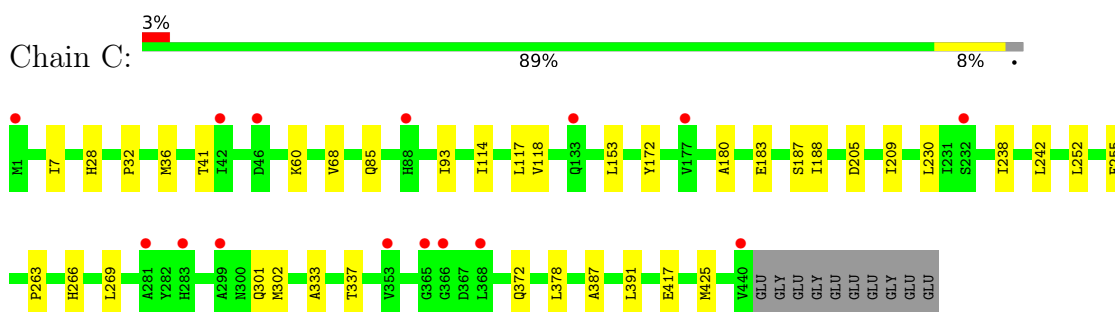
3 Residue-property plots [i](#)

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.

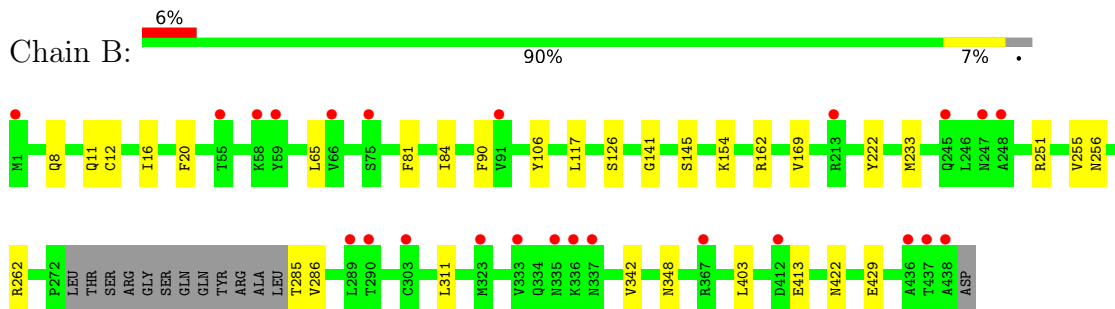
- Molecule 1: Detyrosinated tubulin alpha-1B chain



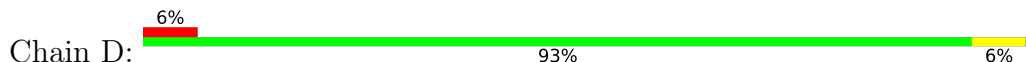
- Molecule 1: Detyrosinated tubulin alpha-1B chain

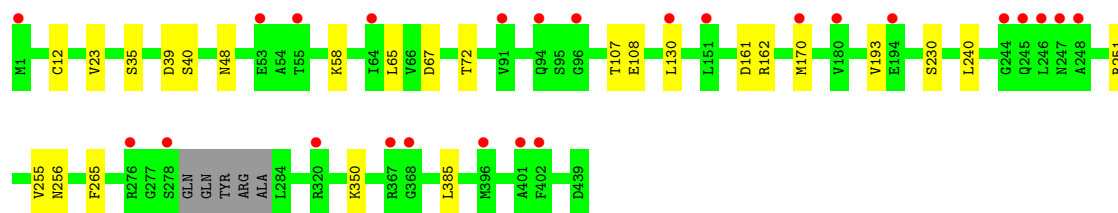


- Molecule 2: Tubulin beta chain

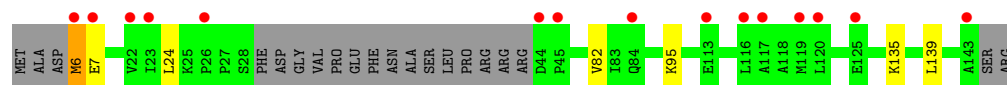
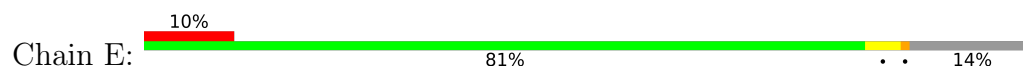


- Molecule 2: Tubulin beta chain

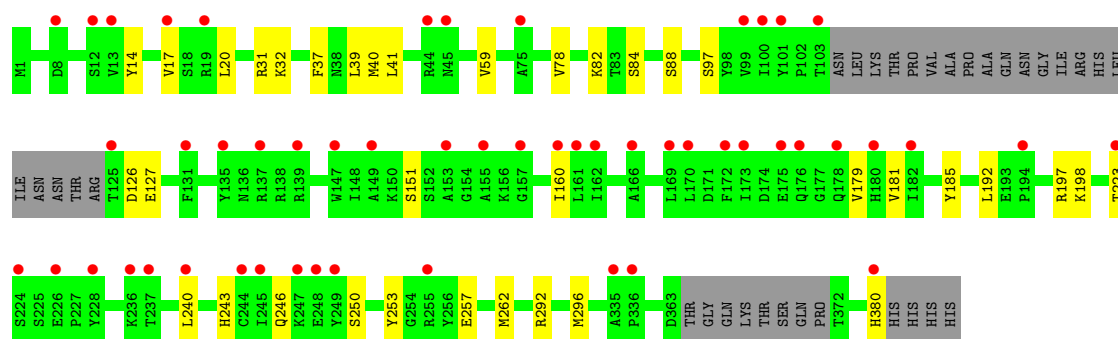
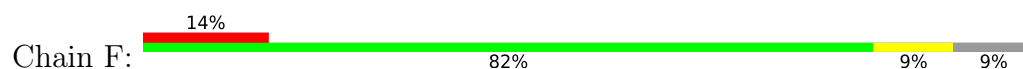




● Molecule 3: Stathmin-4



● 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, MES, CA, W4Q, MG, GDP, LOC, GTP

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

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.

All (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
2:B:262:ARG:NH1	2:B:429:GLU:OE2	2.19	0.75
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.70	0.74
1:A:36:MET:N	13:A:602:HOH:O	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:151:SER:OG	4:F:179:VAL:O	2.07	0.70
2:B:285:THR:N	13:B:602:HOH:O	2.24	0.69
4:F:243:HIS:NE2	4:F:253:TYR:OH	2.25	0.69
2:D:240:LEU:HG	10:D:504:LOC:H6	1.76	0.68
1:A:61:HIS:ND1	13:A:602:HOH:O	2.28	0.66
1:A:104:ALA:HB2	1:A:413:MET:HE3	1.77	0.66
1:A:187:SER:CB	1:A:391:LEU:HD21	2.26	0.65
4:F:14:TYR:HA	4:F:17:VAL:HG12	1.80	0.64
2:B:348:ASN:O	10:B:505:LOC:H18	1.98	0.63
2:D:170:MET:SD	2:D:170:MET:N	2.74	0.61
10:B:505:LOC:H4B	10:B:505:LOC:H6A	1.83	0.60
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.84	0.60
10:D:504:LOC:H4B	10:D:504:LOC:C6	2.32	0.58
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.86	0.57
4:F:82:LYS:NZ	4:F:97:SER:O	2.34	0.57
2:D:35:SER:OG	2:D:58:LYS:NZ	2.21	0.57
2:D:39:ASP:OD1	2:D:40:SER:N	2.37	0.57
1:C:187:SER:CB	1:C:391:LEU:HD21	2.35	0.57
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.88	0.56
4:F:246:GLN:O	4:F:250:SER:OG	2.16	0.55
10:B:505:LOC:H6A	10:B:505:LOC:C4	2.36	0.55
1:A:187:SER:HB2	1:A:391:LEU:HD21	1.89	0.55
4:F:292:ARG:NE	13:F:501:HOH:O	2.41	0.53
1:C:60:LYS:NZ	1:C:85:GLN:O	2.32	0.52
4:F:197:ARG:NH2	4:F:223:THR:HG21	2.24	0.52
2:D:65:LEU:HD12	2:D:65:LEU:N	2.25	0.52
1:C:263:PRO:O	1:C:266:HIS:ND1	2.36	0.51
1:C:255:PHE:HZ	1:C:378:LEU:HD13	1.76	0.51
4:F:160:ILE:HD11	4:F:240:LEU:HD13	1.92	0.51
2:B:8:GLN:NE2	2:B:65:LEU:HD22	2.26	0.50
2:B:262:ARG:NH2	2:B:422:ASN:OD1	2.44	0.50
1:A:139:HIS:NE2	1:A:168:GLU:OE1	2.40	0.50
2:D:251:ARG:O	2:D:255:VAL:HG23	2.12	0.50
4:F:17:VAL:HA	4:F:20:LEU:HD12	1.92	0.50
2:D:130:LEU:O	2:D:162:ARG:NH1	2.40	0.50
2:D:350:LYS:HG3	10:D:504:LOC:C16	2.42	0.50
1:C:117:LEU:HD23	1:C:117:LEU:O	2.12	0.49
1:A:181:VAL:HG11	10:B:505:LOC:H18A	1.95	0.49
1:A:174:ALA:O	1:A:179:THR:HG23	2.13	0.49
1:C:209:ILE:HD11	1:C:302:MET:SD	2.52	0.49
4:F:126:ASP:OD2	4:F:127:GLU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:ASP:OD2	2:D:72:THR:HG21	2.14	0.48
1:A:87:PHE:N	1:A:87:PHE:CD1	2.81	0.48
2:B:81:PHE:O	2:B:84:ILE:HG22	2.13	0.48
1:C:117:LEU:HD23	1:C:117:LEU:C	2.39	0.48
1:A:179:THR:HG22	1:A:183:GLU:OE1	2.13	0.47
1:C:68[A]:VAL:HG11	1:C:118:VAL:HG21	1.95	0.47
1:A:181:VAL:CG1	10:B:505:LOC:H18A	2.44	0.47
2:B:12:CYS:SG	2:B:169:VAL:HG21	2.55	0.47
2:D:385:LEU:C	2:D:385:LEU:HD23	2.40	0.47
1:C:41:THR:O	1:C:41:THR:OG1	2.31	0.47
2:D:107:THR:OG1	2:D:108:GLU:N	2.48	0.47
1:A:180:ALA:HB1	2:B:256:ASN:OD1	2.15	0.47
2:D:23:VAL:HG21	2:D:230:SER:HB2	1.97	0.47
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.51	0.46
4:F:39:LEU:HD21	4:F:41:LEU:HD11	1.96	0.46
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.96	0.46
1:A:98:ASP:OD1	1:A:100:ALA:N	2.48	0.45
1:A:194:THR:HG22	1:A:194:THR:O	2.16	0.45
2:B:65:LEU:HD12	2:B:90:PHE:CE1	2.52	0.45
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.99	0.45
4:F:84:SER:O	4:F:88:SER:N	2.48	0.44
2:B:11:GLN:NE2	13:B:607:HOH:O	2.46	0.44
1:C:172:TYR:OH	1:C:387:ALA:O	2.19	0.44
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.50	0.44
1:C:333:ALA:O	1:C:337:THR:HG23	2.17	0.44
1:A:209:ILE:HD11	1:A:302:MET:SD	2.57	0.44
2:B:403:LEU:HD21	2:B:413:GLU:HG2	1.99	0.44
1:C:238:ILE:HG12	1:C:378:LEU:HD11	1.99	0.44
3:E:135:LYS:O	3:E:139:LEU:HD12	2.18	0.44
1:A:3:GLU:OE1	1:A:3:GLU:N	2.50	0.43
1:C:180:ALA:HB3	1:C:183:GLU:HG3	2.01	0.43
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.54	0.43
2:B:117:LEU:HD11	2:B:154:LYS:HB3	2.00	0.43
1:C:28:HIS:O	1:C:36:MET:HE3	2.19	0.43
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.01	0.43
1:A:88:HIS:N	1:A:91:GLN:OE1	2.52	0.43
1:C:269:LEU:HD11	1:C:301:GLN:HB3	2.01	0.43
2:D:193:VAL:HG22	2:D:265:PHE:HE2	1.84	0.43
1:A:188:ILE:HG23	1:A:425:MET:HG3	2.00	0.43
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.19	0.42
2:B:20:PHE:HB2	2:B:233:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:TYR:CG	3:E:82:VAL:HG11	2.55	0.42
2:B:126:SER:O	2:B:126:SER:OG	2.35	0.42
2:B:222:TYR:N	9:B:504:W4Q:O1	2.52	0.42
1:C:188:ILE:HD12	1:C:425:MET:HG3	2.01	0.42
3:E:6:MET:HE2	3:E:24:LEU:CD2	2.50	0.42
1:A:28:HIS:O	1:A:36:MET:HE3	2.20	0.42
2:B:141:GLY:O	2:B:145:SER:OG	2.32	0.42
1:C:255:PHE:CZ	1:C:378:LEU:HD13	2.55	0.42
2:D:12:CYS:HB2	5:D:503:GTP:C8	2.54	0.42
4:F:192:LEU:HD13	4:F:262:MET:CE	2.49	0.42
2:B:162[B]:ARG:NH1	13:B:606:HOH:O	2.52	0.41
2:B:251:ARG:O	2:B:255:VAL:HG23	2.20	0.41
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.02	0.41
4:F:296:MET:HE1	4:F:380:HIS:CD2	2.55	0.41
1:A:333:ALA:HB2	3:E:6:MET:CE	2.51	0.41
1:A:181:VAL:HG23	1:A:182:VAL:HG13	2.01	0.41
1:A:76:ASP:OD1	13:A:601:HOH:O	2.21	0.41
2:B:16:ILE:HG22	2:B:233:MET:HE1	2.02	0.41
1:A:328:VAL:HG11	1:A:353:VAL:HG11	2.03	0.41
2:D:161:ASP:O	2:D:251:ARG:NH2	2.47	0.41
2:D:256:ASN:HB3	10:D:504:LOC:C16	2.51	0.41
1:C:7:ILE:HG21	1:C:153:LEU:CD2	2.51	0.41
4:F:31:ARG:HD3	4:F:32:LYS:H	1.85	0.40
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.52	0.40
1:A:181:VAL:HG21	1:A:404:PHE:CZ	2.56	0.40
2:B:311:LEU:HD23	2:B:342:VAL:HG11	2.04	0.40

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 ⓘ

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%)	91	96
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%)	91	96
3	E	100/127 (79%)	98 (98%)	2 (2%)	50	67
4	F	286/342 (84%)	285 (100%)	1 (0%)	91	96
All	All	1792/1969 (91%)	1787 (100%)	5 (0%)	91	96

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. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
1	A	342	GLN
1	A	393	HIS
2	B	165	ASN
2	B	404	HIS
2	B	431	GLN
1	C	309	HIS
2	D	11	GLN
2	D	134	GLN
2	D	329	GLN
2	D	434	GLN
3	E	64	GLN

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
5	GTP	D	503	6	26,34,34	1.09	2 (7%)	32,54,54	1.51	7 (21%)
8	MES	B	501	-	12,12,12	2.20	1 (8%)	14,16,16	1.69	3 (21%)
9	W4Q	B	504	-	35,35,35	4.78	25 (71%)	42,50,50	1.11	3 (7%)
10	LOC	D	504	-	31,31,31	3.75	12 (38%)	44,44,44	3.16	15 (34%)
5	GTP	C	502	6	26,34,34	1.13	2 (7%)	32,54,54	1.44	7 (21%)
10	LOC	B	505	-	31,31,31	3.76	13 (41%)	44,44,44	3.30	18 (40%)
12	ACP	F	402	6	27,33,33	1.37	5 (18%)	32,52,52	1.43	4 (12%)
11	GDP	B	506	-	24,30,30	0.97	1 (4%)	30,47,47	1.28	4 (13%)
5	GTP	A	501	6	26,34,34	1.14	2 (7%)	32,54,54	1.53	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	D	503	6	-	4/18/38/38	0/3/3/3
8	MES	B	501	-	-	1/6/14/14	0/1/1/1
9	W4Q	B	504	-	-	2/16/16/16	0/4/4/4
10	LOC	D	504	-	-	3/12/25/25	0/3/3/3
5	GTP	C	502	6	-	7/18/38/38	0/3/3/3
10	LOC	B	505	-	-	4/12/25/25	0/3/3/3
12	ACP	F	402	6	-	5/15/38/38	0/3/3/3
11	GDP	B	506	-	-	0/12/32/32	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	504	LOC	C20-C21	11.71	1.54	1.37
10	B	505	LOC	C20-C21	11.57	1.54	1.37
10	B	505	LOC	C15-C14	10.21	1.54	1.36
10	D	504	LOC	C15-C14	10.06	1.54	1.36
9	B	504	W4Q	C1-C6	-9.58	1.31	1.40
9	B	504	W4Q	C4-C3	8.30	1.53	1.38
9	B	504	W4Q	C20-C21	8.01	1.52	1.37
9	B	504	W4Q	C19-C13	7.94	1.52	1.39
9	B	504	W4Q	C18-C12	7.93	1.52	1.39
10	B	505	LOC	C21-C14	7.90	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	W4Q	C2-C1	7.85	1.52	1.39
9	B	504	W4Q	C23-C22	7.70	1.52	1.38
8	B	501	MES	C8-S	-7.36	1.67	1.77
10	D	504	LOC	C21-C14	7.34	1.53	1.44
9	B	504	W4Q	C5-C6	7.20	1.52	1.40
9	B	504	W4Q	C15-C14	6.70	1.53	1.38
9	B	504	W4Q	O1-C9	5.77	1.39	1.24
9	B	504	W4Q	C16-C17	5.66	1.53	1.38
10	D	504	LOC	C22-C21	5.47	1.56	1.50
10	B	505	LOC	C22-C21	5.34	1.56	1.50
10	D	504	LOC	C19-C17	5.30	1.53	1.39
10	B	505	LOC	C19-C17	5.07	1.52	1.39
9	B	504	W4Q	C23-C13	-4.36	1.31	1.39
10	D	504	LOC	C19-C20	4.19	1.53	1.41
10	B	505	LOC	C19-C20	4.15	1.52	1.41
9	B	504	W4Q	C14-C12	-4.12	1.32	1.39
10	D	504	LOC	C17-C16	4.10	1.53	1.47
9	B	504	W4Q	C11-N1	4.07	1.48	1.40
5	C	502	GTP	C5-C6	-4.03	1.39	1.47
5	A	501	GTP	C5-C6	-3.99	1.39	1.47
9	B	504	W4Q	C2-C3	-3.96	1.32	1.38
10	B	505	LOC	C17-C16	3.93	1.53	1.47
9	B	504	W4Q	C19-C20	-3.83	1.31	1.38
5	D	503	GTP	C5-C6	-3.81	1.39	1.47
9	B	504	W4Q	C12-C11	3.29	1.53	1.48
9	B	504	W4Q	C17-C18	-3.24	1.32	1.38
9	B	504	W4Q	C4-C5	-3.24	1.32	1.38
10	D	504	LOC	C12-N1	3.20	1.45	1.34
10	B	505	LOC	C12-N1	3.20	1.45	1.34
12	F	402	ACP	PG-O3G	3.00	1.61	1.54
12	F	402	ACP	PG-O2G	2.90	1.61	1.54
11	B	506	GDP	C6-N1	-2.78	1.33	1.37
9	B	504	W4Q	C6-CL1	2.74	1.78	1.72
9	B	504	W4Q	C13-C7	2.74	1.52	1.48
9	B	504	W4Q	C7-N1	2.73	1.48	1.40
10	B	505	LOC	C15-C16	2.60	1.53	1.44
10	D	504	LOC	C15-C16	2.58	1.53	1.44
10	D	504	LOC	O6-C17	2.51	1.40	1.35
10	B	505	LOC	O6-C17	2.46	1.40	1.35
12	F	402	ACP	C5-C4	2.45	1.47	1.40
9	B	504	W4Q	C22-C21	-2.44	1.32	1.37
9	B	504	W4Q	O3-C5	2.41	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	402	ACP	PB-O3A	2.36	1.61	1.58
10	D	504	LOC	O5-C16	-2.23	1.18	1.24
9	B	504	W4Q	C16-C15	-2.23	1.32	1.38
5	A	501	GTP	C2-N3	2.19	1.38	1.33
10	B	505	LOC	O5-C16	-2.19	1.18	1.24
10	B	505	LOC	O3-C5	2.16	1.40	1.37
12	F	402	ACP	PB-O2B	2.16	1.61	1.56
5	D	503	GTP	C2-N3	2.14	1.38	1.33
10	D	504	LOC	O6-C18	-2.12	1.40	1.45
10	B	505	LOC	O6-C18	-2.11	1.40	1.45
5	C	502	GTP	C2-N3	2.04	1.38	1.33

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	504	LOC	C15-C14-C21	-12.02	115.78	127.62
10	B	505	LOC	O6-C17-C16	10.54	119.84	109.56
10	B	505	LOC	C15-C14-C21	-10.53	117.25	127.62
10	D	504	LOC	O6-C17-C16	7.71	117.08	109.56
10	D	504	LOC	C14-C15-C16	-6.46	120.94	133.89
10	B	505	LOC	C14-C11-N1	-6.25	109.42	114.34
10	D	504	LOC	C14-C11-N1	-6.12	109.52	114.34
10	B	505	LOC	C14-C15-C16	-6.04	121.80	133.89
10	B	505	LOC	C19-C17-C16	-5.79	119.07	128.62
10	B	505	LOC	C19-C20-C21	-5.03	119.98	130.56
10	B	505	LOC	C20-C19-C17	-4.92	119.43	130.07
10	D	504	LOC	C19-C17-C16	-4.92	120.51	128.62
10	D	504	LOC	C20-C21-C14	-4.85	119.24	124.83
10	D	504	LOC	C19-C20-C21	-4.83	120.39	130.56
10	D	504	LOC	C20-C19-C17	-4.21	120.96	130.07
12	F	402	ACP	PB-O3A-PA	-3.78	120.57	132.56
8	B	501	MES	C5-N4-C3	3.63	116.99	108.83
10	B	505	LOC	C1-C22-C21	3.54	124.78	121.09
12	F	402	ACP	N3-C2-N1	-3.49	123.22	128.68
11	B	506	GDP	C3'-C2'-C1'	3.41	106.11	100.98
9	B	504	W4Q	C11-C10-C9	-3.38	119.84	123.45
10	B	505	LOC	C8-C22-C21	-3.38	116.29	120.25
5	D	503	GTP	PA-O3A-PB	-3.34	121.37	132.83
10	B	505	LOC	C20-C21-C14	-3.30	121.03	124.83
12	F	402	ACP	C3'-C2'-C1'	3.28	105.91	100.98
5	A	501	GTP	PB-O3B-PG	-3.21	121.81	132.83
5	A	501	GTP	C5-C6-N1	3.19	119.59	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	503	GTP	C8-N7-C5	3.15	108.98	102.99
10	D	504	LOC	O3-C5-C3	3.08	120.57	115.16
10	B	505	LOC	O3-C5-C3	3.05	120.53	115.16
5	A	501	GTP	C8-N7-C5	3.05	108.81	102.99
5	D	503	GTP	C5-C6-N1	3.04	119.32	113.95
10	D	504	LOC	C6-O3-C5	-3.01	112.98	117.53
5	C	502	GTP	C5-C6-N1	2.91	119.09	113.95
5	A	501	GTP	PA-O3A-PB	-2.89	122.89	132.83
5	C	502	GTP	C8-N7-C5	2.88	108.47	102.99
5	A	501	GTP	C2-N1-C6	-2.81	119.93	125.10
5	D	503	GTP	PB-O3B-PG	-2.74	123.44	132.83
8	B	501	MES	O2S-S-C8	2.73	110.20	106.92
11	B	506	GDP	PA-O3A-PB	-2.69	123.60	132.83
9	B	504	W4Q	C24-C8-C9	2.64	120.38	114.99
5	C	502	GTP	PA-O3A-PB	-2.62	123.82	132.83
5	D	503	GTP	C2-N1-C6	-2.62	120.27	125.10
12	F	402	ACP	C4-C5-N7	-2.62	106.67	109.40
10	D	504	LOC	C1-C22-C21	2.58	123.78	121.09
10	D	504	LOC	O3-C5-C7	-2.56	119.71	124.12
5	C	502	GTP	C2-N1-C6	-2.56	120.38	125.10
10	B	505	LOC	C9-C8-C22	-2.52	116.04	119.97
11	B	506	GDP	C8-N7-C5	2.50	107.76	102.99
8	B	501	MES	O3S-S-C8	2.50	109.81	105.77
10	D	504	LOC	C8-C22-C21	-2.48	117.34	120.25
10	B	505	LOC	C10-C9-C8	-2.39	108.46	113.68
5	C	502	GTP	C3'-C2'-C1'	2.39	104.57	100.98
10	B	505	LOC	O3-C5-C7	-2.37	120.04	124.12
10	D	504	LOC	O6-C17-C19	-2.33	118.62	122.30
10	B	505	LOC	C9-C8-C7	2.32	124.53	119.42
5	D	503	GTP	O2G-PG-O3B	2.31	112.37	104.64
11	B	506	GDP	C5-C6-N1	2.30	118.02	113.95
9	B	504	W4Q	O3-C5-C6	2.27	118.22	115.53
5	C	502	GTP	C2'-C3'-C4'	2.22	106.95	102.64
5	C	502	GTP	PB-O3B-PG	-2.17	125.38	132.83
10	B	505	LOC	C13-C12-N1	2.17	119.77	116.10
10	D	504	LOC	C10-C9-C8	-2.11	109.07	113.68
5	A	501	GTP	O6-C6-C5	-2.07	120.33	124.37
10	B	505	LOC	C6-O3-C5	-2.07	114.41	117.53
5	A	501	GTP	C3'-C2'-C1'	2.06	104.08	100.98
10	B	505	LOC	C11-C14-C15	-2.04	115.19	117.12
5	D	503	GTP	C3'-C2'-C1'	2.00	103.99	100.98

There are no chirality outliers.

All (32) torsion outliers are listed below:

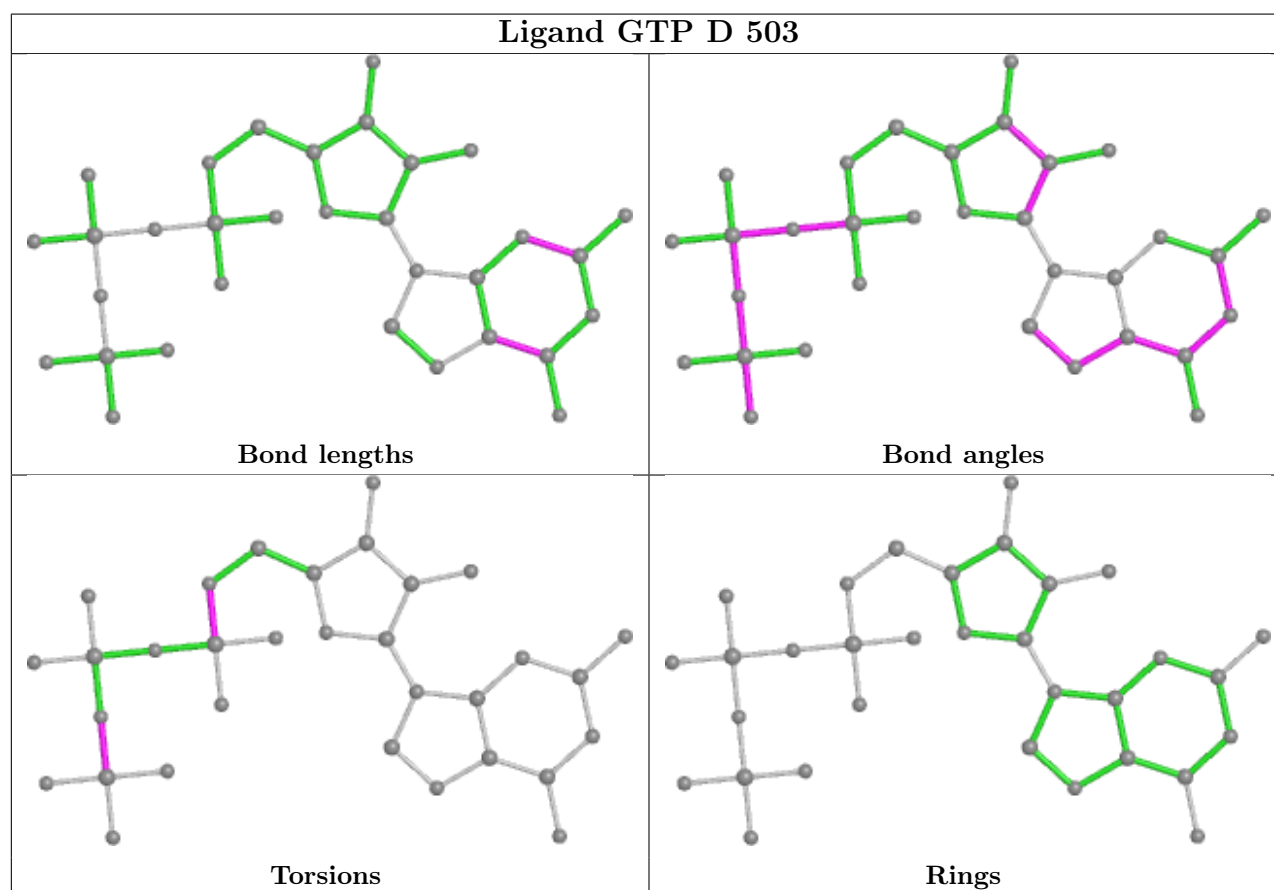
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	502	GTP	C5'-O5'-PA-O1A
5	C	502	GTP	C5'-O5'-PA-O2A
5	D	503	GTP	C5'-O5'-PA-O1A
5	D	503	GTP	C5'-O5'-PA-O2A
10	B	505	LOC	C19-C17-O6-C18
10	B	505	LOC	C16-C17-O6-C18
10	D	504	LOC	C19-C17-O6-C18
12	F	402	ACP	C5'-O5'-PA-O1A
12	F	402	ACP	C5'-O5'-PA-O3A
12	F	402	ACP	O4'-C4'-C5'-O5'
12	F	402	ACP	C3'-C4'-C5'-O5'
10	D	504	LOC	C3-C5-O3-C6
10	D	504	LOC	C7-C5-O3-C6
10	B	505	LOC	C7-C5-O3-C6
10	B	505	LOC	C3-C5-O3-C6
5	D	503	GTP	PB-O3B-PG-O1G
9	B	504	W4Q	C2-C3-O2-C25
9	B	504	W4Q	C4-C3-O2-C25
5	A	501	GTP	C4'-C5'-O5'-PA
12	F	402	ACP	C5'-O5'-PA-O2A
5	C	502	GTP	C4'-C5'-O5'-PA
8	B	501	MES	C8-C7-N4-C3
5	A	501	GTP	PB-O3B-PG-O1G
5	C	502	GTP	PB-O3B-PG-O2G
5	C	502	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	C5'-O5'-PA-O3A
5	D	503	GTP	C5'-O5'-PA-O3A
5	C	502	GTP	PB-O3B-PG-O1G

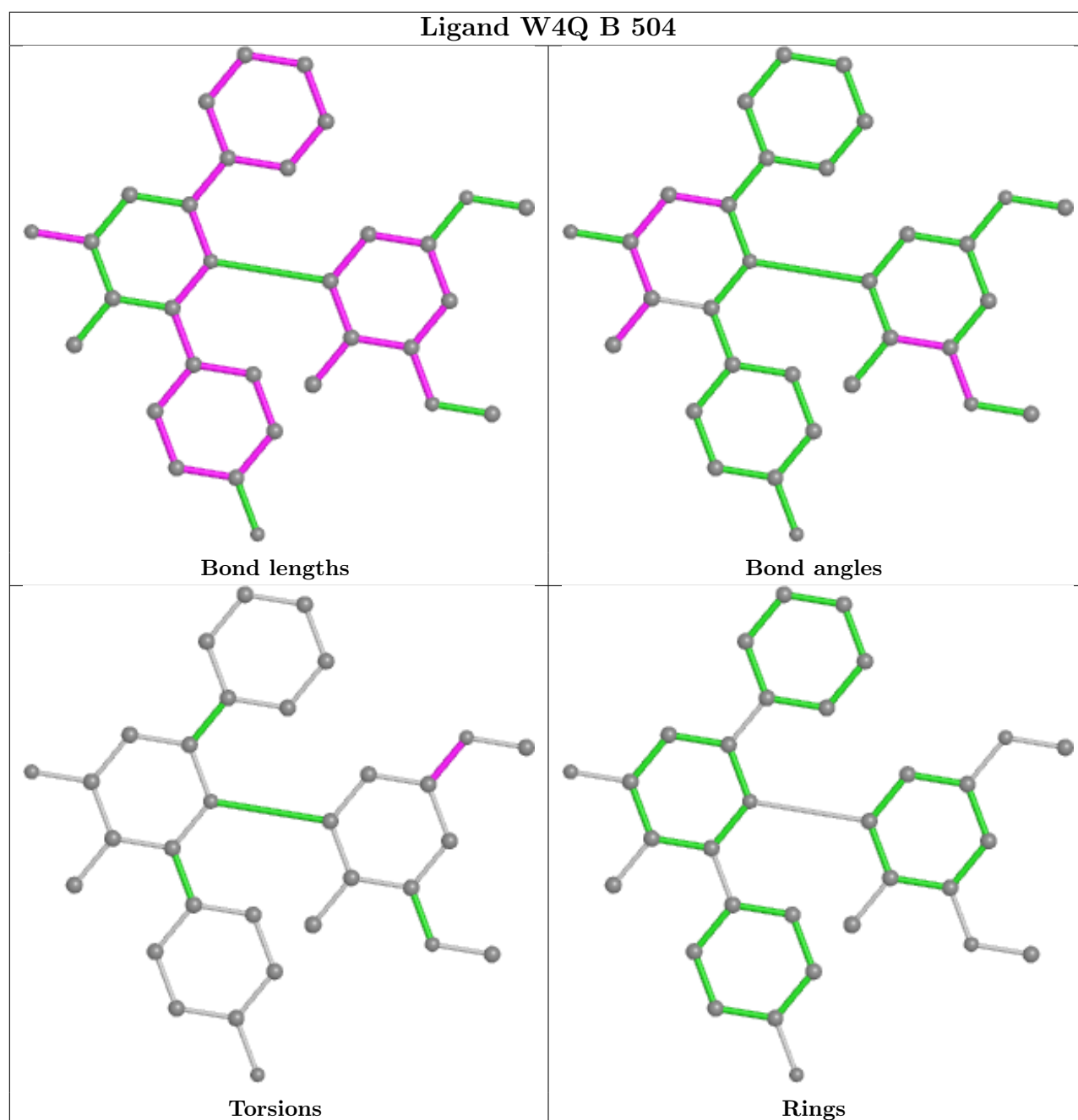
There are no ring outliers.

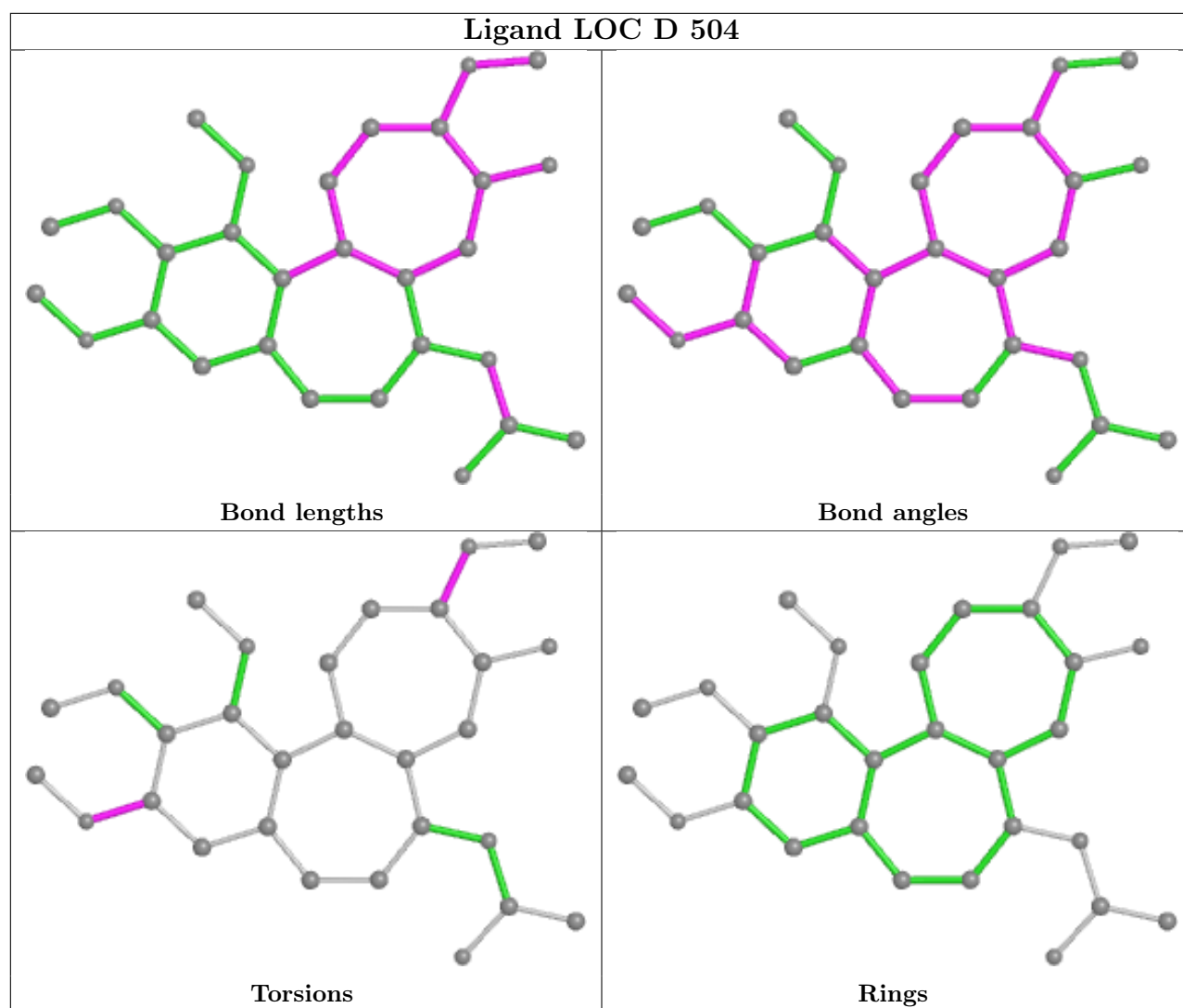
4 monomers are involved in 12 short contacts:

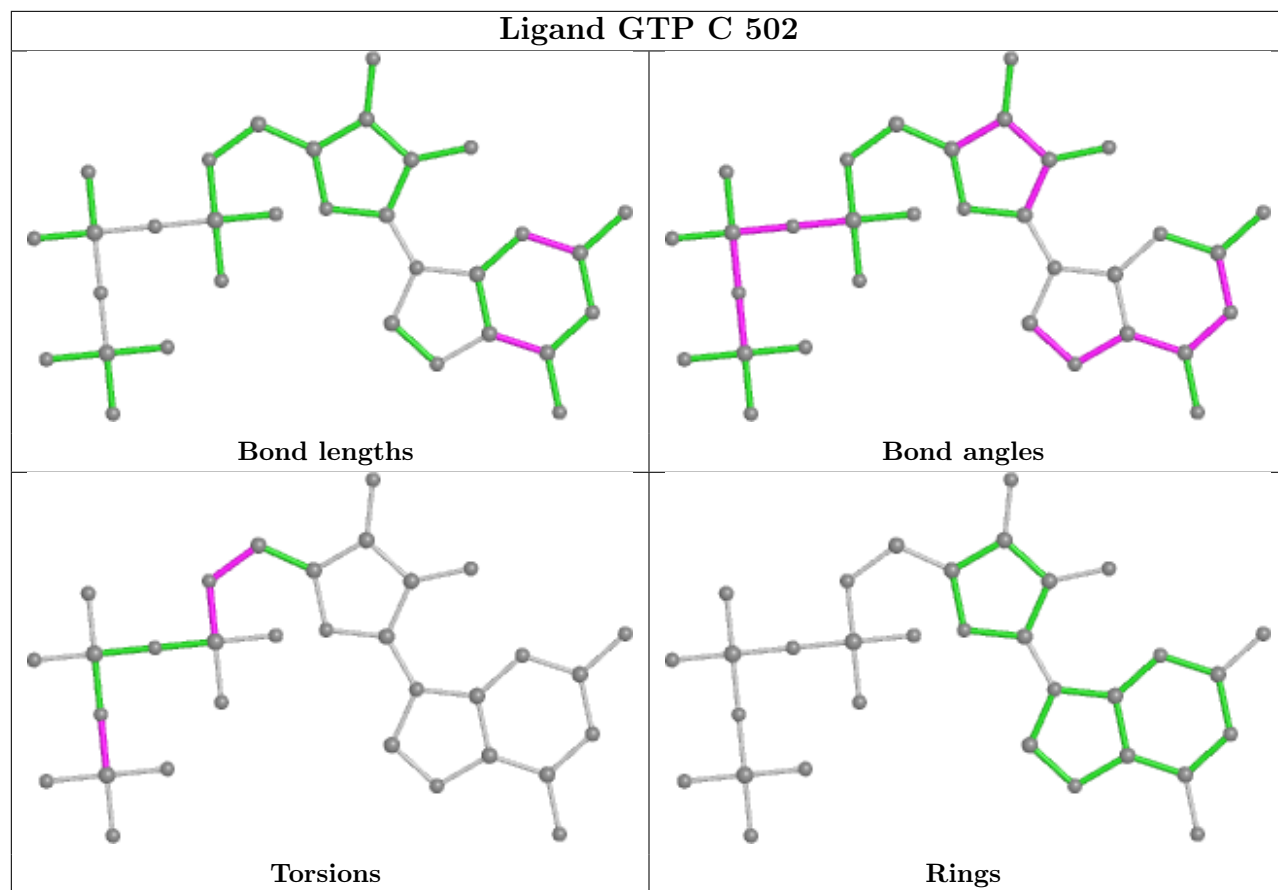
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	503	GTP	1	0
9	B	504	W4Q	1	0
10	D	504	LOC	5	0
10	B	505	LOC	5	0

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.

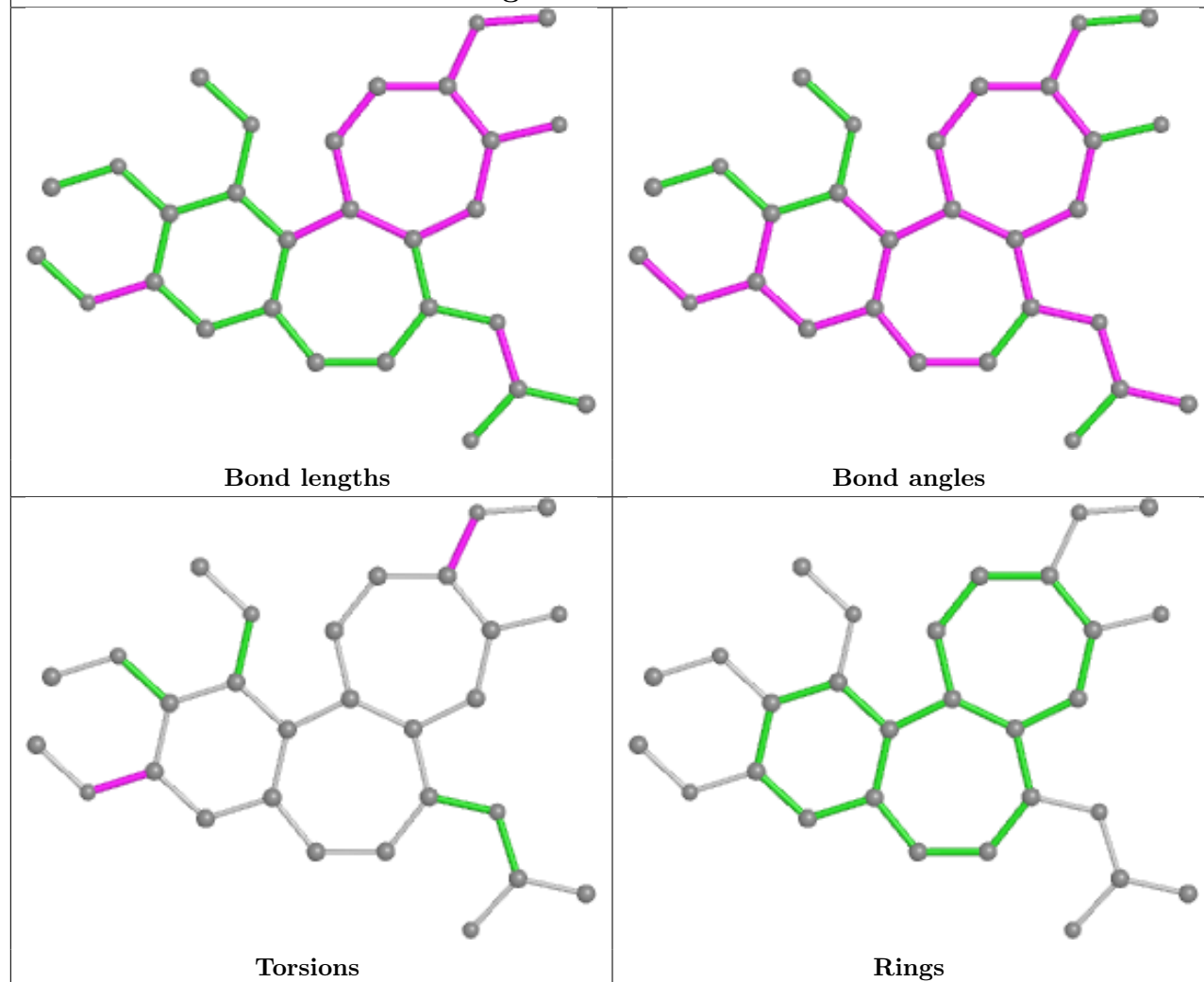




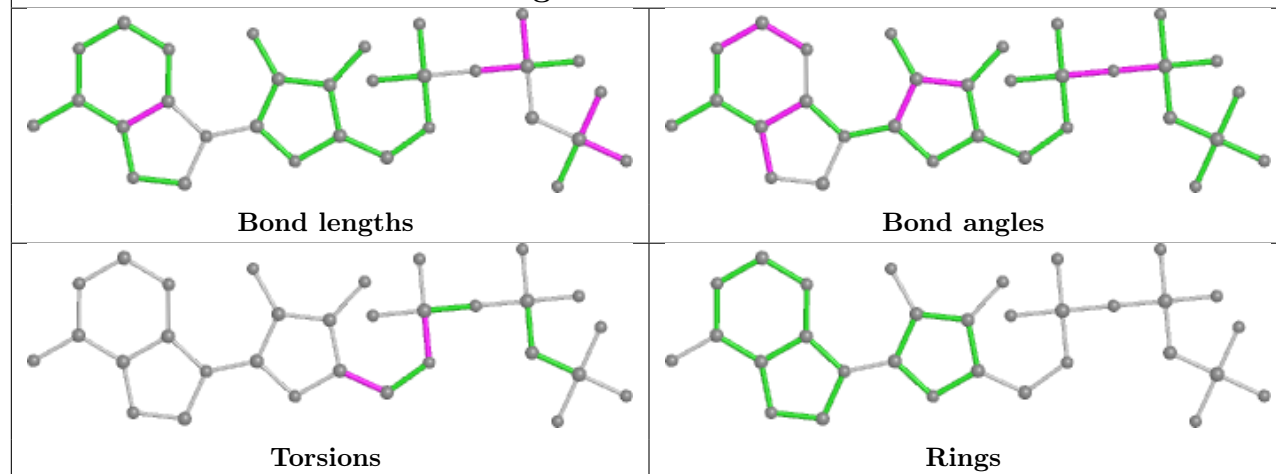


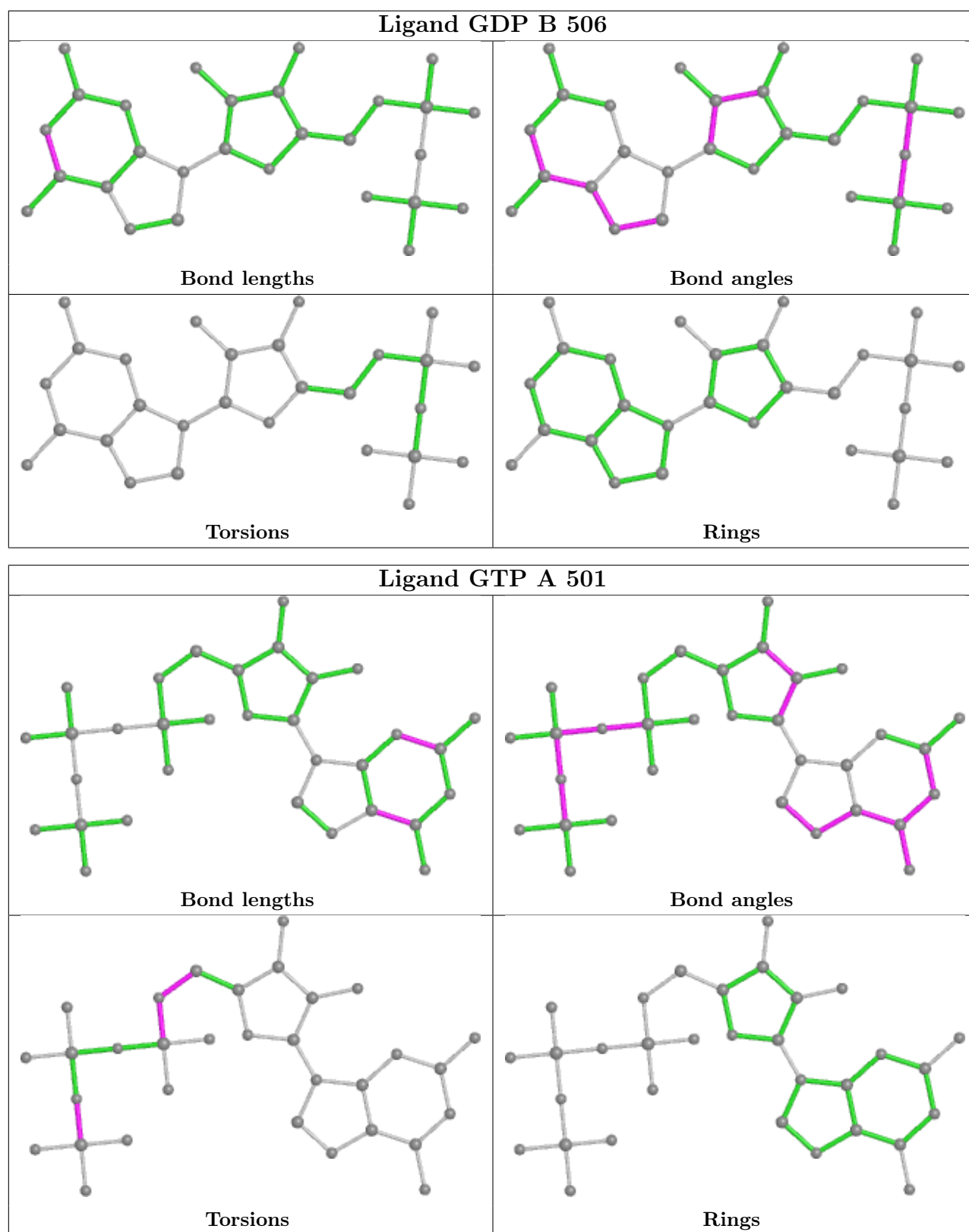


Ligand LOC B 505



Ligand ACP F 402





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

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	438/450 (97%)	0.57	20 (4%)	38	43	34, 70, 91, 108	2 (0%)
1	C	440/450 (97%)	0.19	15 (3%)	48	53	30, 59, 78, 90	3 (0%)
2	B	418/431 (96%)	0.49	24 (5%)	30	34	38, 68, 92, 115	1 (0%)
2	D	426/431 (98%)	0.62	25 (5%)	29	33	51, 74, 96, 109	0
3	E	123/143 (86%)	0.79	15 (12%)	10	12	61, 79, 101, 116	0
4	F	351/384 (91%)	1.04	52 (14%)	7	8	61, 85, 121, 129	0
All	All	2196/2289 (95%)	0.58	151 (6%)	24	28	30, 71, 101, 129	6 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	173	ILE	5.6
4	F	100	ILE	5.3
1	C	366	GLY	4.9
3	E	7	GLU	4.7
2	D	245	GLN	4.4
4	F	103	THR	4.4
2	B	337	ASN	4.3
2	D	247	ASN	4.3
1	A	282	TYR	4.3
3	E	143	ALA	4.3
4	F	249	TYR	4.2
4	F	135	TYR	4.2
1	C	365	GLY	4.2
4	F	172	PHE	4.1
2	D	1	MET	3.9
2	B	55	THR	3.8
4	F	155	ALA	3.8
1	C	46	ASP	3.6
4	F	380	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	194	GLU	3.6
2	D	368	GLY	3.6
4	F	170	LEU	3.5
2	B	245	GLN	3.5
3	E	120	LEU	3.4
2	D	96	GLY	3.4
4	F	245	ILE	3.4
1	A	281	ALA	3.3
1	A	62	VAL	3.3
4	F	161	LEU	3.3
2	B	1	MET	3.3
2	D	55	THR	3.3
4	F	166	ALA	3.3
1	C	1	MET	3.2
1	A	93	ILE	3.2
4	F	125	THR	3.2
1	A	256	GLN	3.2
2	B	438	ALA	3.2
4	F	131	PHE	3.2
3	E	125	GLU	3.1
4	F	180	HIS	3.1
4	F	17	VAL	3.0
2	D	278	SER	3.0
1	C	177	VAL	3.0
2	D	53	GLU	3.0
2	B	213	ARG	3.0
4	F	44	ARG	3.0
2	D	248	ALA	3.0
4	F	45	ASN	3.0
3	E	44	ASP	3.0
1	C	88[A]	HIS	3.0
1	C	283	HIS	3.0
4	F	19	ARG	2.9
1	C	368	LEU	2.9
4	F	255	ARG	2.9
4	F	336	PRO	2.9
4	F	75	ALA	2.9
1	A	283	HIS	2.8
2	B	303	CYS	2.8
4	F	137	ARG	2.8
4	F	176	GLN	2.8
2	D	151	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	170	MET	2.7
4	F	237	THR	2.7
4	F	162	ILE	2.6
2	B	247	ASN	2.6
2	B	335	ASN	2.6
4	F	147	TRP	2.6
2	D	246	LEU	2.6
4	F	149	ALA	2.6
4	F	101	TYR	2.6
4	F	153	ALA	2.6
3	E	45	PRO	2.6
3	E	84	GLN	2.6
2	D	396	MET	2.5
4	F	247	LYS	2.5
4	F	12	SER	2.5
1	A	66	VAL	2.5
2	B	91	VAL	2.5
3	E	119	MET	2.5
2	B	58	LYS	2.5
2	B	59	TYR	2.5
2	B	66	VAL	2.4
4	F	13	VAL	2.4
2	D	276	ARG	2.4
1	C	299	ALA	2.4
4	F	226	GLU	2.4
1	A	35	GLN	2.4
2	D	94	GLN	2.4
2	D	401	ALA	2.4
1	A	112	LYS	2.3
3	E	26	PRO	2.3
2	D	320	ARG	2.3
3	E	113	GLU	2.3
1	C	133	GLN	2.3
1	A	338	LYS	2.3
3	E	6	MET	2.3
2	D	64	ILE	2.3
3	E	116	LEU	2.3
4	F	169	LEU	2.3
1	A	362	VAL	2.3
1	A	315	CYS	2.3
2	B	75	SER	2.3
4	F	157	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	367	ARG	2.3
2	D	180	VAL	2.3
3	E	23	ILE	2.3
2	B	248	ALA	2.3
2	B	436	ALA	2.3
1	C	42	ILE	2.2
4	F	160	ILE	2.2
1	A	40	LYS	2.2
4	F	244	CYS	2.2
2	B	323	MET	2.2
2	D	402	PHE	2.2
4	F	175	GLU	2.2
1	C	440	VAL	2.2
4	F	228	TYR	2.2
2	D	244	GLY	2.2
1	C	232	SER	2.2
4	F	223	THR	2.2
4	F	8	ASP	2.2
4	F	182	ILE	2.2
2	D	367	ARG	2.2
1	A	176	GLN	2.2
2	D	91	VAL	2.2
4	F	335	ALA	2.2
1	A	262	TYR	2.1
2	B	289	LEU	2.1
4	F	139	ARG	2.1
1	A	67	PHE	2.1
4	F	224	SER	2.1
1	A	279	GLU	2.1
4	F	178	GLN	2.1
2	B	333	VAL	2.1
3	E	117	ALA	2.1
4	F	194	PRO	2.1
2	B	412	ASP	2.1
1	C	281	ALA	2.1
2	D	130	LEU	2.1
1	C	353	VAL	2.1
4	F	99	VAL	2.1
2	B	336	LYS	2.1
4	F	248	GLU	2.1
1	A	88	HIS	2.1
1	A	115	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	345	ASP	2.1
4	F	240	LEU	2.0
2	B	290	THR	2.0
3	E	22	VAL	2.0
4	F	236	LYS	2.0
2	B	437	THR	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 oligosaccharides 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
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

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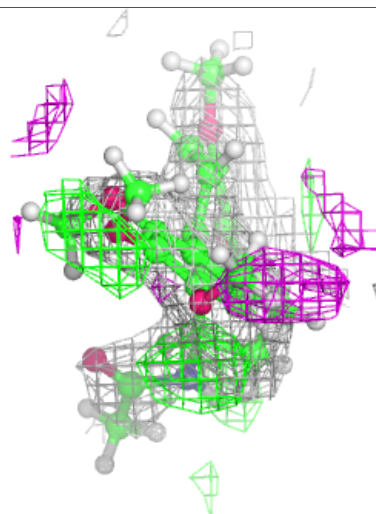
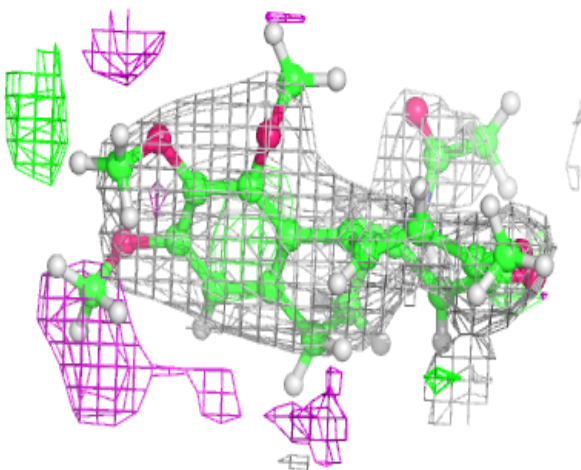
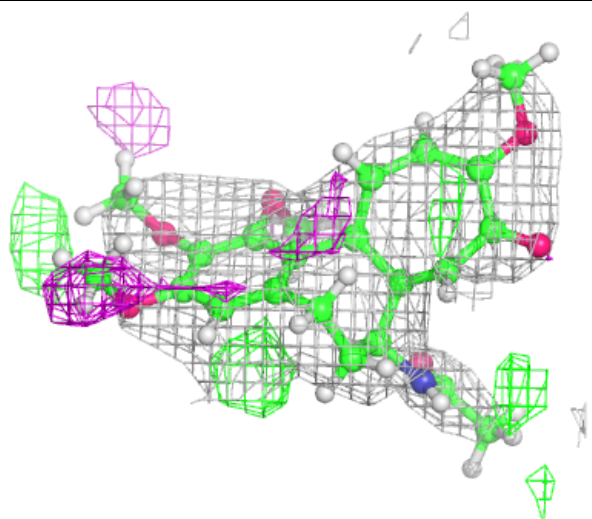
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GTP	C	502	32/32	0.95	0.09	41,48,58,70	0
5	GTP	A	501	32/32	0.96	0.08	50,57,71,74	0
6	MG	C	503	1/1	0.98	0.05	49,49,49,49	0
6	MG	D	501	1/1	0.98	0.12	67,67,67,67	0

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.

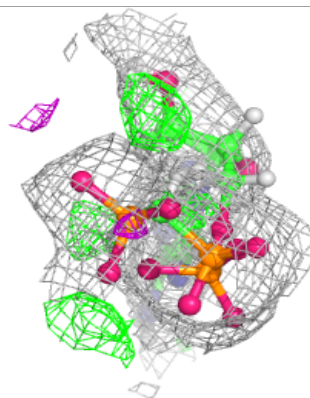
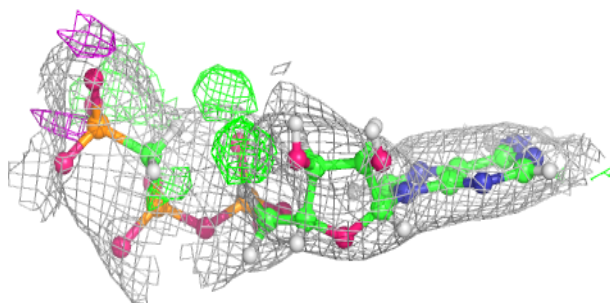
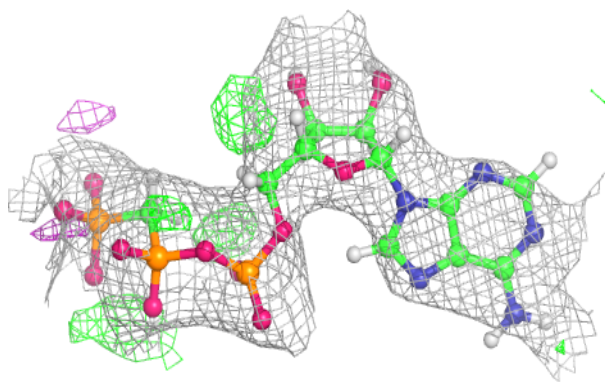
Electron density around LOC D 504:

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



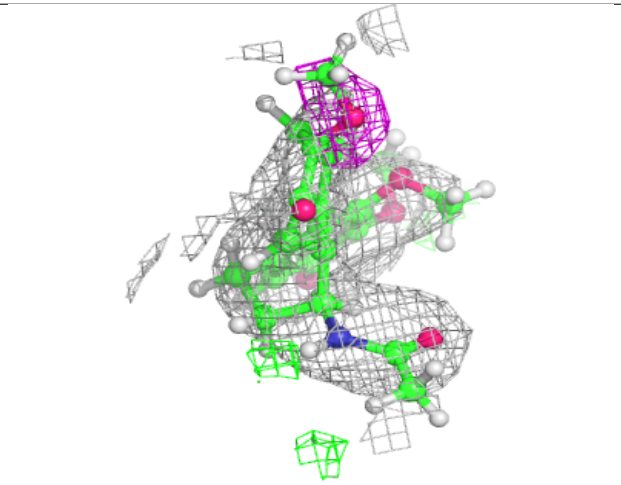
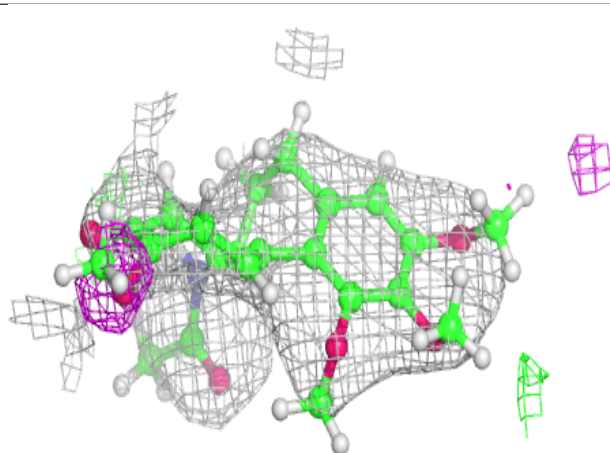
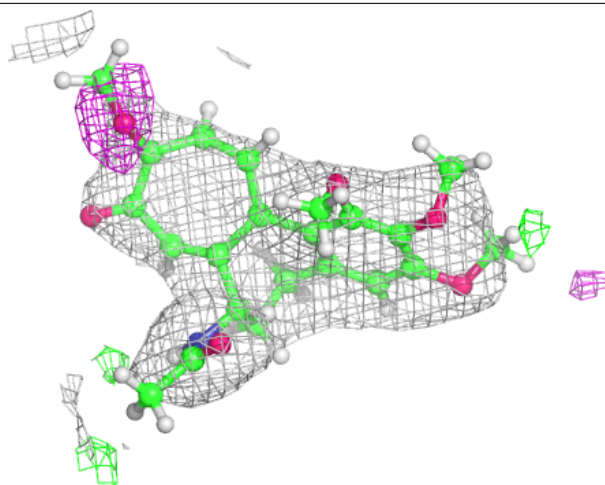
Electron density around ACP F 402:

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



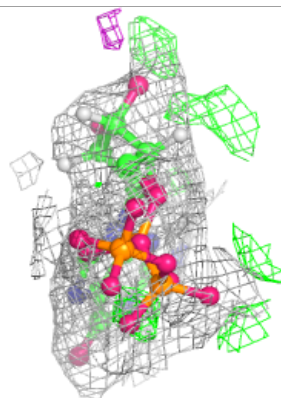
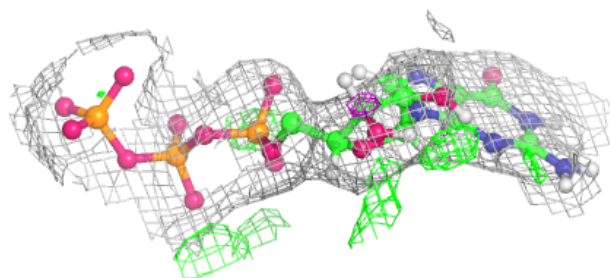
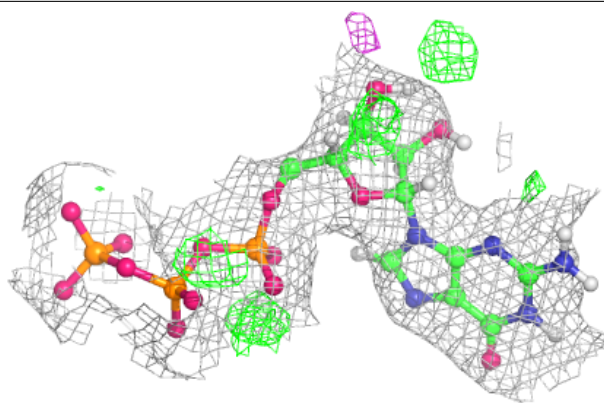
Electron density around LOC B 505:

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



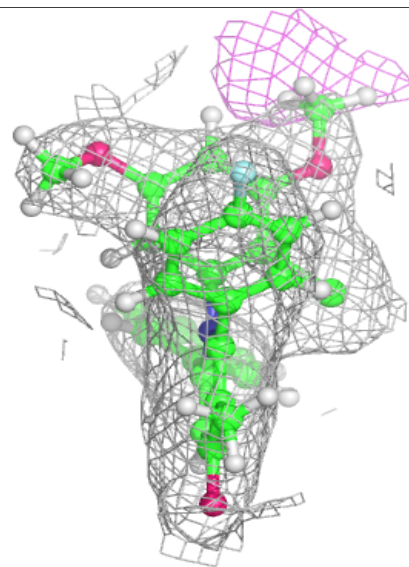
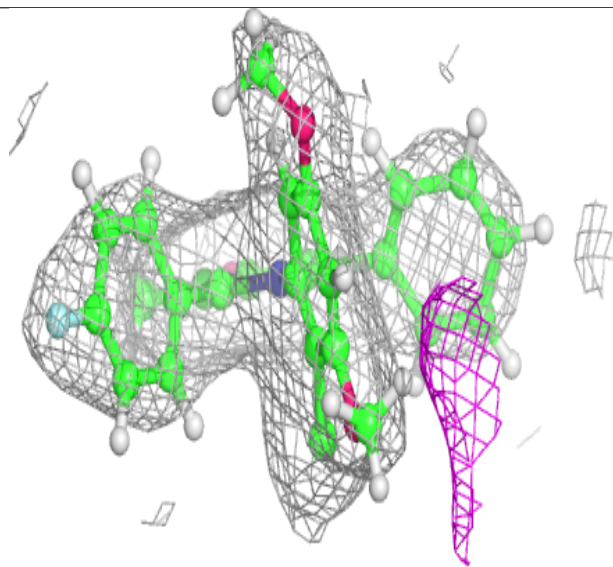
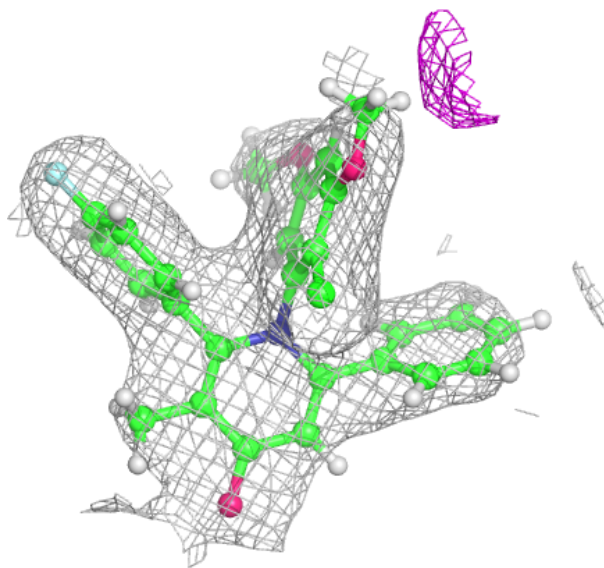
Electron density around GTP D 503:

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



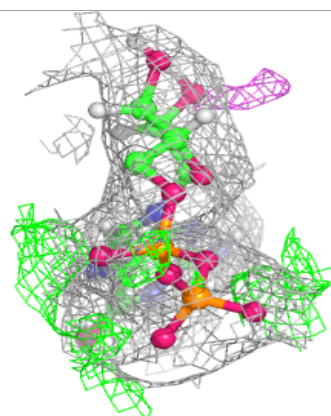
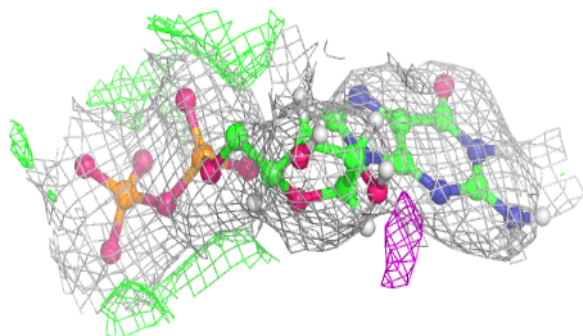
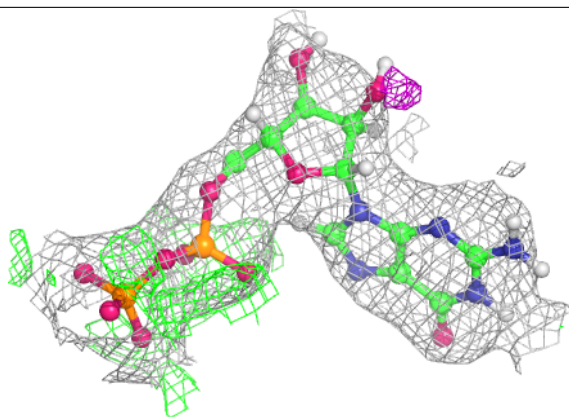
Electron density around W4Q B 504:

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

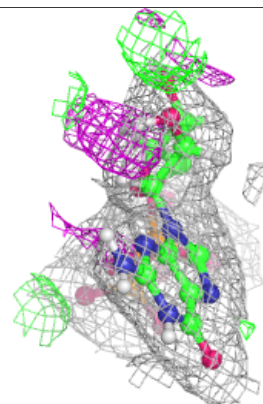
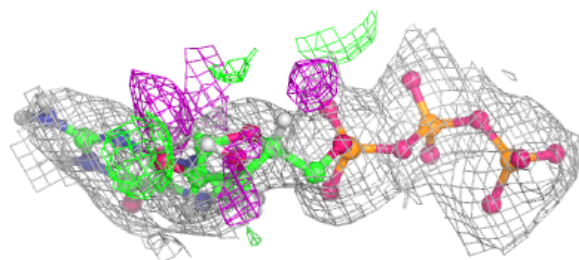
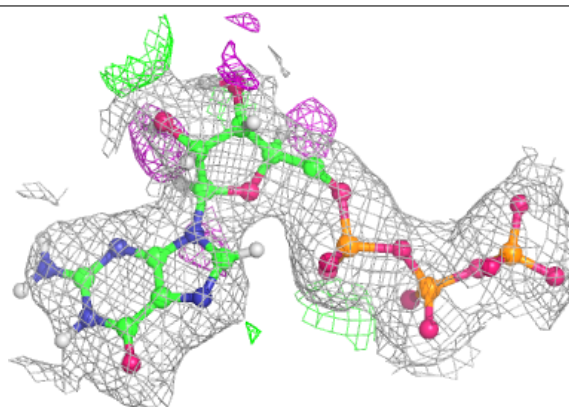


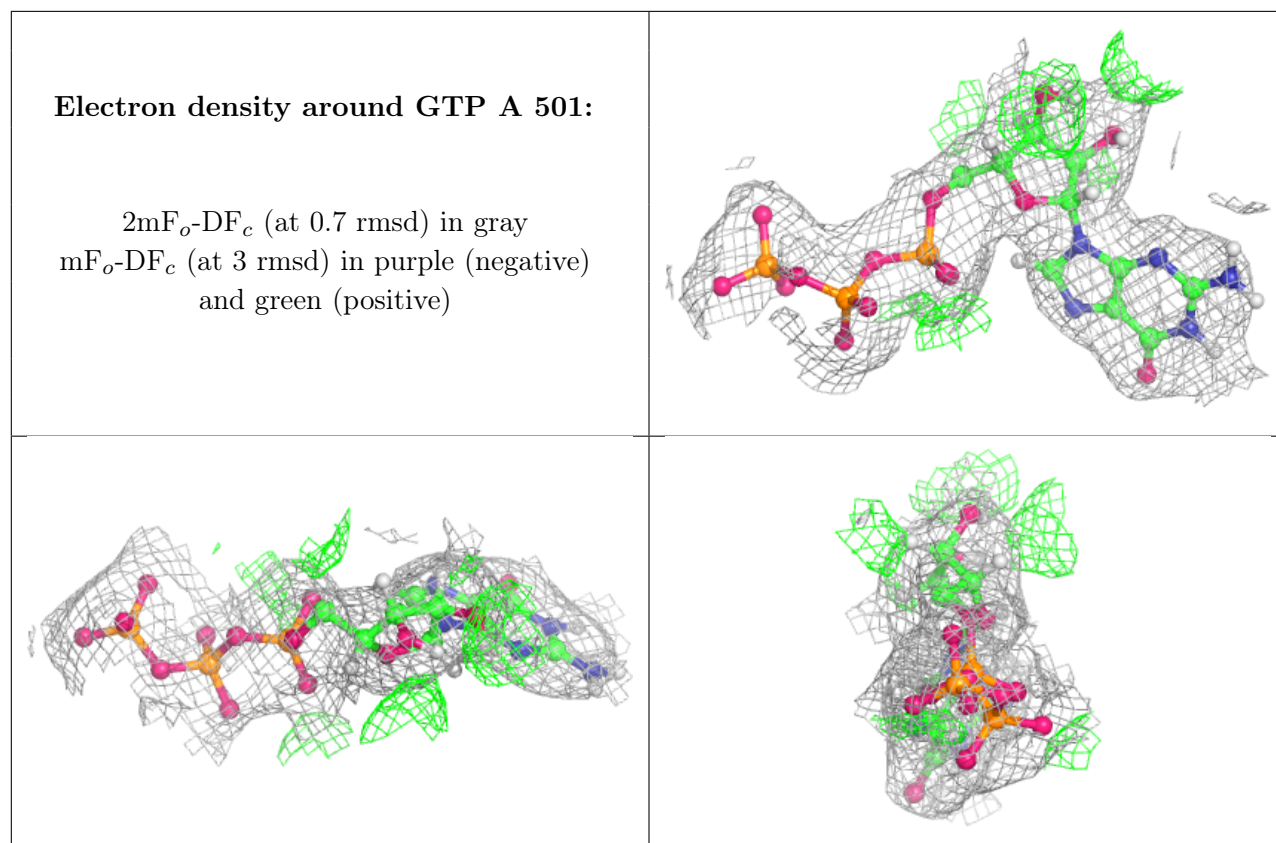
Electron density around GDP B 506:

$2mF_o-DF_c$ (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.