



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:59 AM UTC

PDB ID : 7E4Z / pdb_00007e4z
Title : Crystal structure of tubulin in complex with Maytansinol
Authors : Wang, Y.; Li, W.
Deposited on : 2021-02-16
Resolution : 2.69 Å(reported)

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

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A user guide is available at

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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

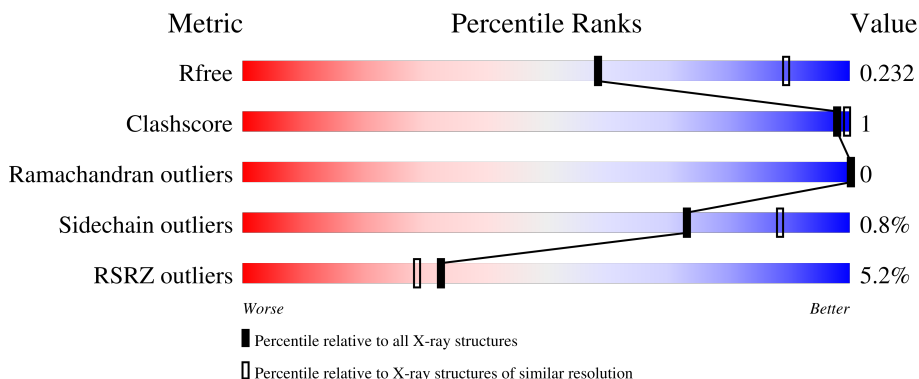
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	440	0% 98% .
1	C	440	2% 97% .
2	B	431	2% 97% ..
2	D	431	6% 96% ..
3	E	138	4% 86% 11%

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Mol	Chain	Length	Quality of chain
4	F	384	17% 87% • 9%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 35521 atoms, of which 17355 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	H	N	O	S	0	6	0
			6869	2194	3402	589	660	24			
1	C	440	Total	C	H	N	O	S	0	10	0
			6890	2201	3414	586	664	25			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	425	Total	C	H	N	O	S	0	6	0
			6668	2126	3286	579	650	27			
2	D	421	Total	C	H	N	O	S	0	4	0
			6513	2085	3196	562	644	26			

- 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	2	0
			2072	632	1048	184	202	6			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	348	Total	C	H	N	O	S	0	5	0
			5765	1855	2879	494	521	16			

There are 6 discrepancies between the modelled and reference sequences:

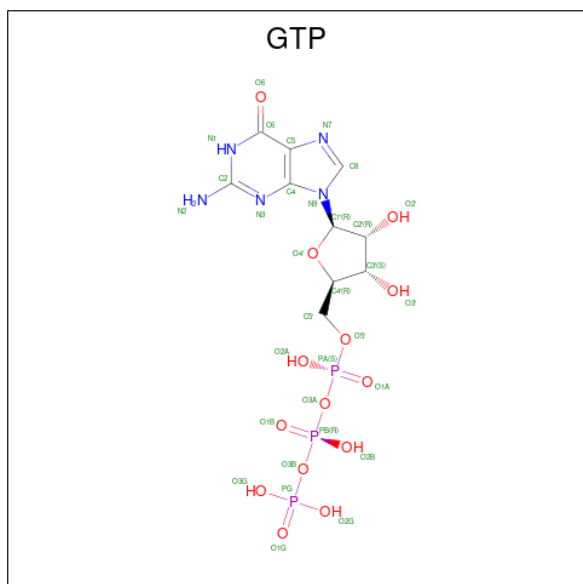
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43

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

- 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	B	2	Total	Mg	0	0
			2	2		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

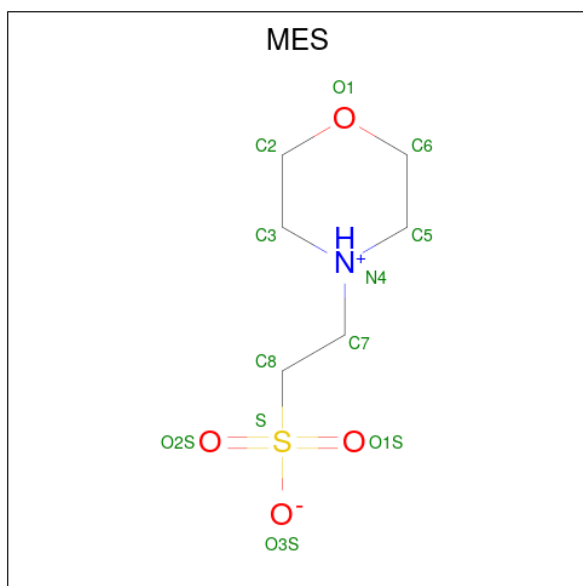
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

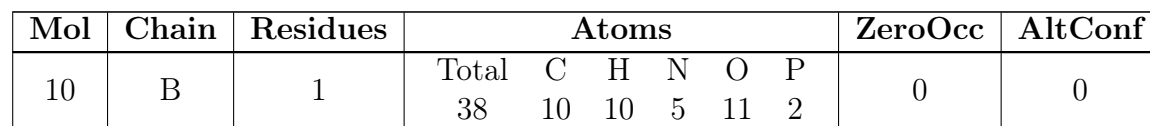
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



-
- The chemical structure of BKL (Brevibactin L) is a 14-membered lactam ring. The ring atoms are labeled C1 through C14, with the carbonyl oxygen at C1 labeled O19. The ring is substituted with several groups: a hydroxyl group (OH) at C2 (O32), a chlorine atom (Cl) at C3 (Cl3), a methyl group (CH3) at C4 (C30), a hydroxyl group (OH) at C5 (O35), a methyl group (CH3) at C6 (C38), a chlorine atom (Cl) at C7 (Cl3), a methyl group (CH3) at C8 (C37), a hydroxyl group (OH) at C9 (O36), a methyl group (CH3) at C10 (C39), a chlorine atom (Cl) at C11 (Cl3), a methyl group (CH3) at C12 (C38), a hydroxyl group (OH) at C13 (O35), and a methyl group (CH3) at C14 (C37). The structure is shown in a 2D representation with stereochemistry indicated by wedges and dashes.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	D	1	Total	C	Cl	H	N	O	0	0
			76	28	1	37	2	8		

- # ACP
-
- The chemical structure of Adenosine 3'-phosphate (ACP) is shown. It consists of an adenosine moiety (adenine base and ribose sugar) linked to a triphosphate chain. The adenosine moiety is represented by a blue-colored structure, while the triphosphate chain is shown in red and black. The triphosphate chain is composed of three phosphate groups (P1, P2, P3) connected by phosphodiester bonds. The 3' carbon of the ribose sugar is linked to the gamma phosphate (P3) via a phosphodiester bond. The structure is labeled with atom names (N1, N3, N7, N9, 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

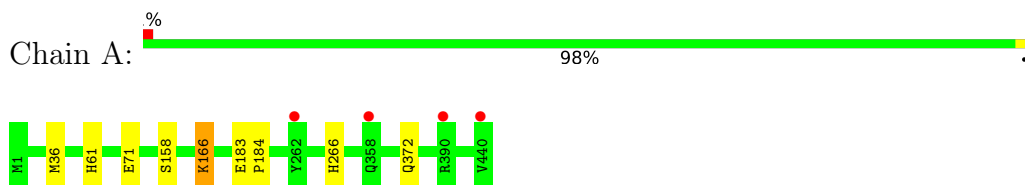
- Molecule 13 is water.



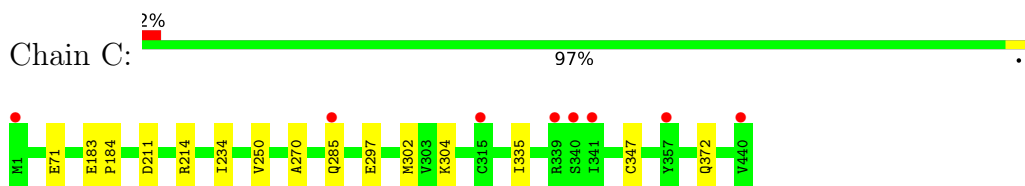
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

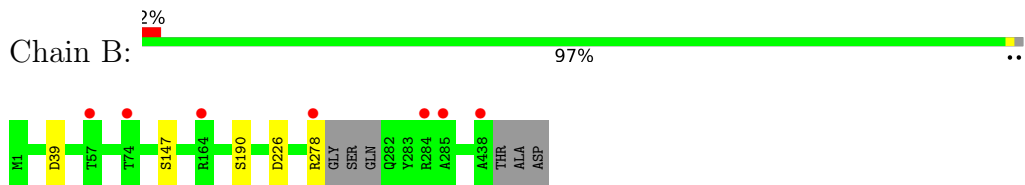
- Molecule 1: Tubulin alpha-1B chain



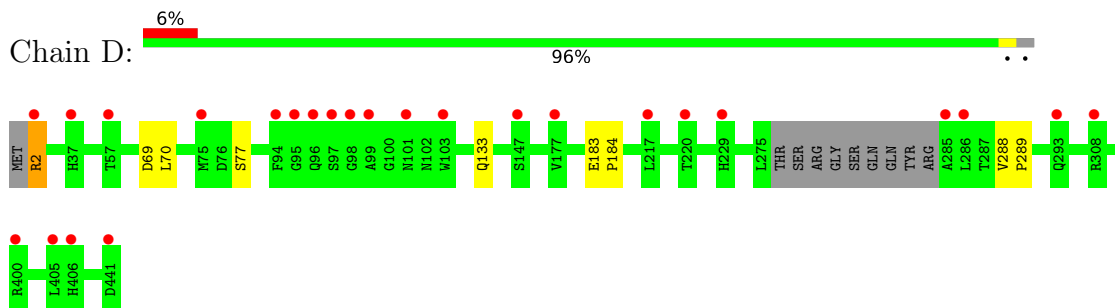
- Molecule 1: Tubulin alpha-1B chain



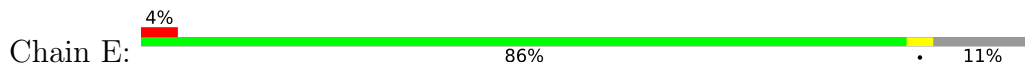
- Molecule 2: Tubulin beta-2B chain

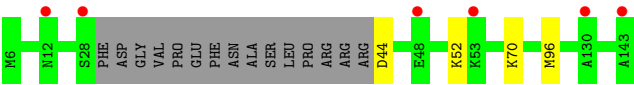


- Molecule 2: Tubulin beta-2B chain

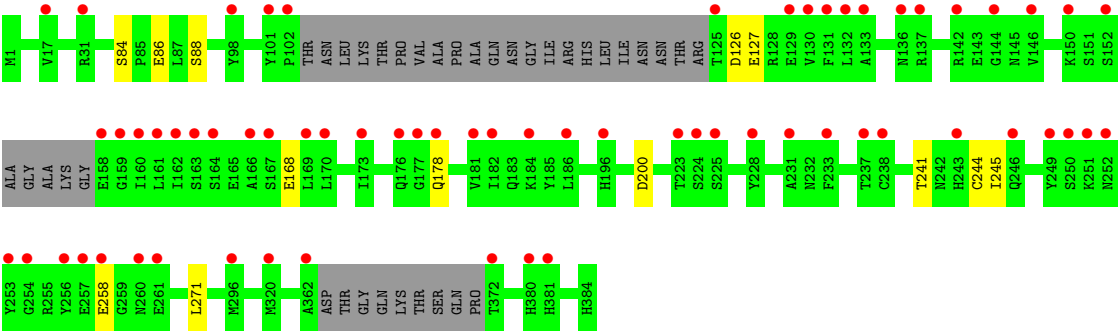
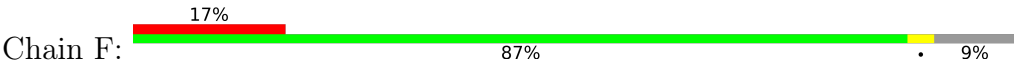


- Molecule 3: Stathmin-4





● Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.43Å 156.63Å 182.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.28 – 2.69 38.28 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.28-2.69) 99.5 (38.28-2.69)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.61 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.192 , 0.228 0.196 , 0.232	Depositor DCC
R_{free} test set	4061 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.3	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	0.94	EDS
Total number of atoms	35521	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: GTP, MG, ACP, CA, CL, GDP, MES, BKL

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	0.30	0/3563	0.63	0/4836
1	C	0.29	0/3581	0.62	0/4861
2	B	0.29	0/3481	0.60	0/4713
2	D	0.29	0/3401	0.61	0/4608
3	E	0.27	0/1038	0.58	0/1377
4	F	0.26	0/2969	0.62	2/4010 (0.0%)
All	All	0.29	0/18033	0.62	2/24405 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	258	GLU	CA-C-N	9.99	139.54	120.66
4	F	258	GLU	C-N-CA	9.99	139.54	120.66

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	3467	3402	3390	4	0
1	C	3476	3414	3400	6	0
2	B	3382	3286	3266	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3317	3196	3196	5	0
3	E	1024	1048	1044	2	0
4	F	2886	2879	2863	6	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	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	A	1	0	0	0	0
9	A	12	13	13	0	0
9	B	24	26	25	0	0
10	B	28	10	12	0	0
11	D	39	37	0	0	0
12	F	31	14	14	1	0
13	A	92	0	0	0	0
13	B	72	0	0	0	0
13	C	142	0	0	1	0
13	D	31	0	0	0	0
13	E	11	0	0	2	0
13	F	26	0	0	1	0
All	All	18166	17355	17259	26	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 26 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)
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.12	0.67
3:E:44:ASP:N	13:E:301:HOH:O	2.32	0.63
1:C:214:ARG:NH2	13:C:603:HOH:O	2.33	0.61
4:F:168:GLU:O	13:F:501:HOH:O	2.17	0.59
2:B:226:ASP:OD1	2:B:278:ARG:NH1	2.37	0.58

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	444/440 (101%)	430 (97%)	14 (3%)	0	100	100
1	C	447/440 (102%)	435 (97%)	12 (3%)	0	100	100
2	B	427/431 (99%)	417 (98%)	10 (2%)	0	100	100
2	D	420/431 (97%)	407 (97%)	13 (3%)	0	100	100
3	E	121/138 (88%)	119 (98%)	2 (2%)	0	100	100
4	F	345/384 (90%)	326 (94%)	19 (6%)	0	100	100
All	All	2204/2264 (97%)	2134 (97%)	70 (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	377/371 (102%)	373 (99%)	4 (1%)	65	85
1	C	380/371 (102%)	375 (99%)	5 (1%)	61	83
2	B	374/372 (100%)	374 (100%)	0	100	100
2	D	366/372 (98%)	364 (100%)	2 (0%)	81	92
3	E	112/123 (91%)	110 (98%)	2 (2%)	51	78
4	F	319/342 (93%)	315 (99%)	4 (1%)	61	83
All	All	1928/1951 (99%)	1911 (99%)	17 (1%)	73	87

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	178	GLN
4	F	271[B]	LEU
1	C	335	ILE
1	C	347	CYS
2	D	2	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	18	GLN
3	E	103	GLN
4	F	242	ASN
4	F	232	ASN
1	C	393	HIS

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 19 ligands modelled in this entry, 10 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
9	MES	B	505	-	12,12,12	2.32	1 (8%)	15,16,16	1.69	2 (13%)
10	GDP	B	501	6	29,30,30	1.17	3 (10%)	45,47,47	1.73	5 (11%)
11	BKL	D	603	-	40,42,42	1.65	6 (15%)	44,64,64	2.08	8 (18%)
9	MES	B	504	-	12,12,12	2.30	1 (8%)	15,16,16	1.66	4 (26%)
5	GTP	C	501	6	33,34,34	1.01	3 (9%)	50,54,54	1.57	8 (16%)
5	GTP	D	602	6	33,34,34	0.88	1 (3%)	50,54,54	1.59	8 (16%)
5	GTP	A	501	6	33,34,34	0.99	2 (6%)	50,54,54	1.57	9 (18%)
9	MES	A	505	-	12,12,12	2.33	1 (8%)	15,16,16	1.32	2 (13%)
12	ACP	F	401	-	31,33,33	4.14	10 (32%)	47,52,52	1.67	10 (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
9	MES	B	505	-	-	2/6/14/14	0/1/1/1
10	GDP	B	501	6	-	5/16/32/32	0/3/3/3
11	BKL	D	603	-	-	16/42/68/68	0/2/4/4
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
5	GTP	D	602	6	-	0/22/38/38	0/3/3/3
5	GTP	A	501	6	-	7/22/38/38	0/3/3/3
9	MES	A	505	-	-	3/6/14/14	0/1/1/1
12	ACP	F	401	-	-	5/19/38/38	0/3/3/3

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	PB-O3A	19.59	1.80	1.58
9	A	505	MES	C8-S	-7.82	1.66	1.77
9	B	505	MES	C8-S	-7.77	1.66	1.77
9	B	504	MES	C8-S	-7.72	1.66	1.77
12	F	401	ACP	PA-O5'	7.50	1.88	1.59

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	603	BKL	C12-O34-C14	7.74	65.20	60.81
10	B	501	GDP	C5-C4-N3	-5.94	118.94	128.39
11	D	603	BKL	O37-C02-C01	5.47	121.43	115.44
5	A	501	GTP	C5-C4-N3	-5.03	120.39	128.39
5	C	501	GTP	C5-C4-N3	-5.00	120.44	128.39

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

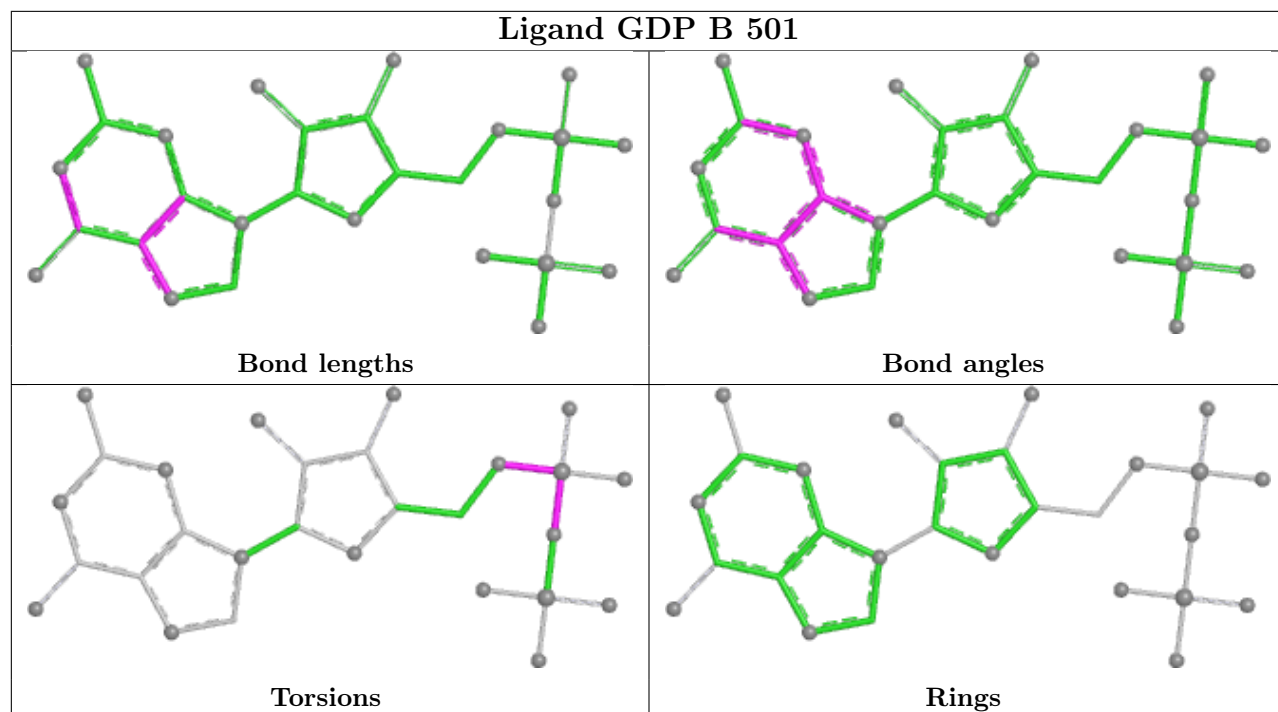
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

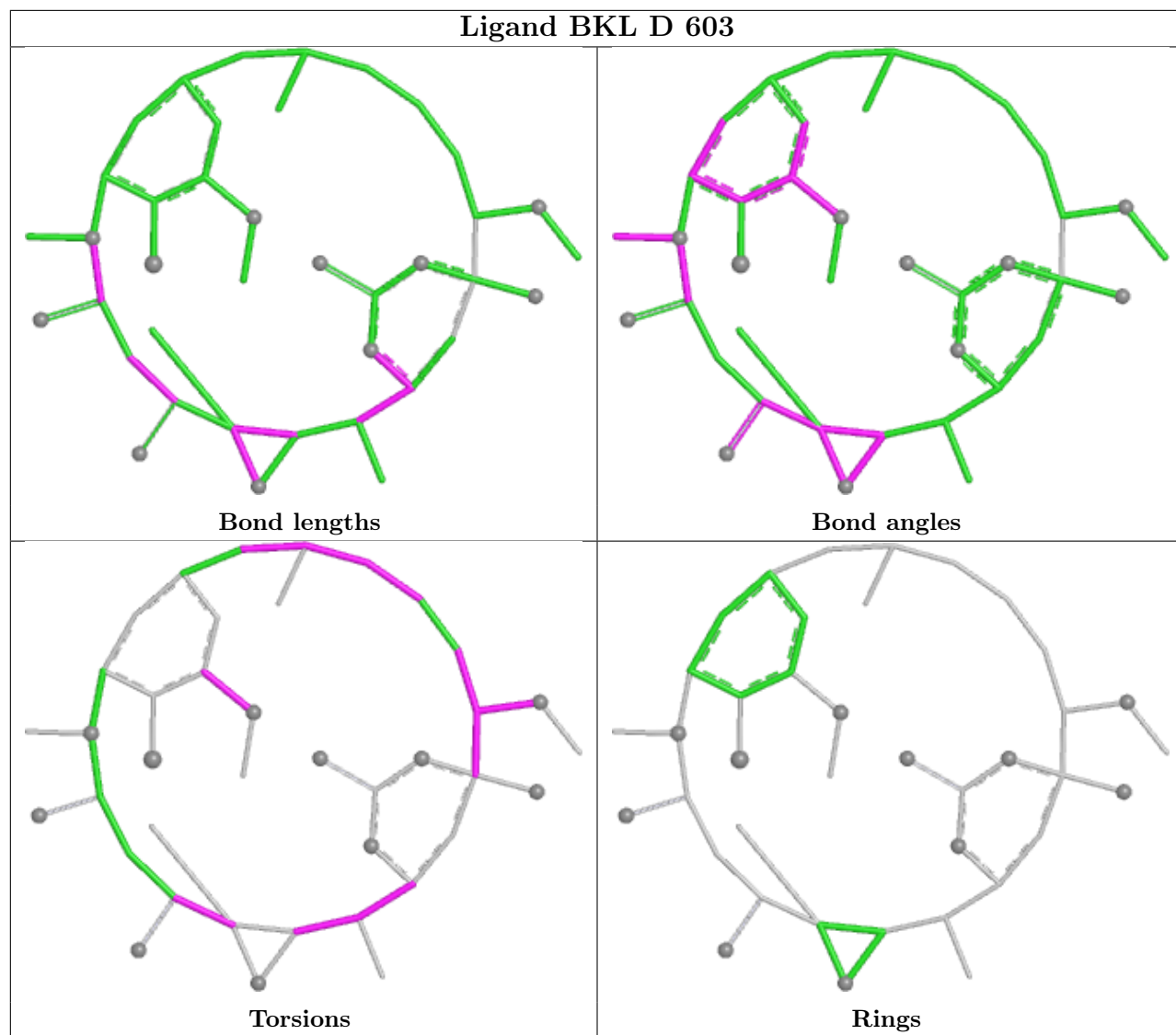
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	602	GTP	1	0
12	F	401	ACP	1	0

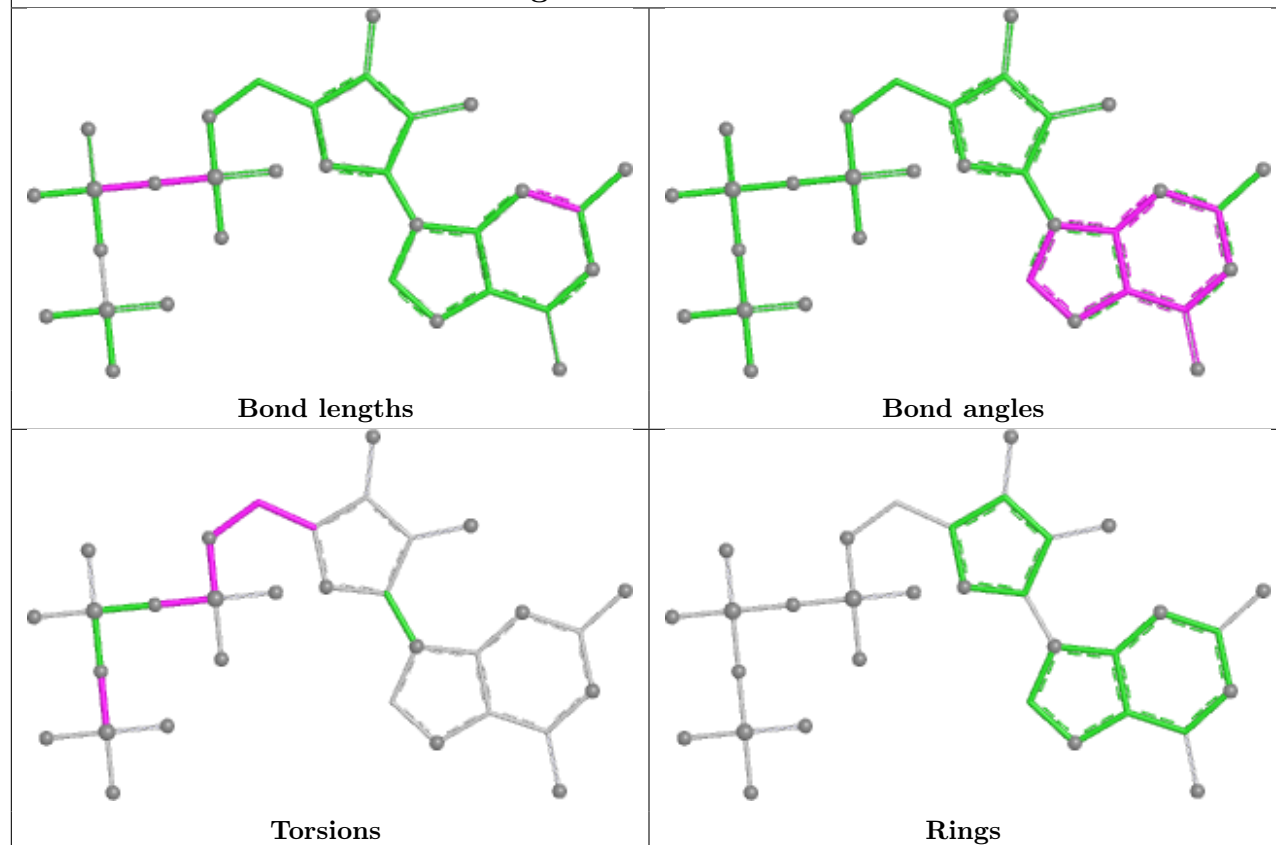
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



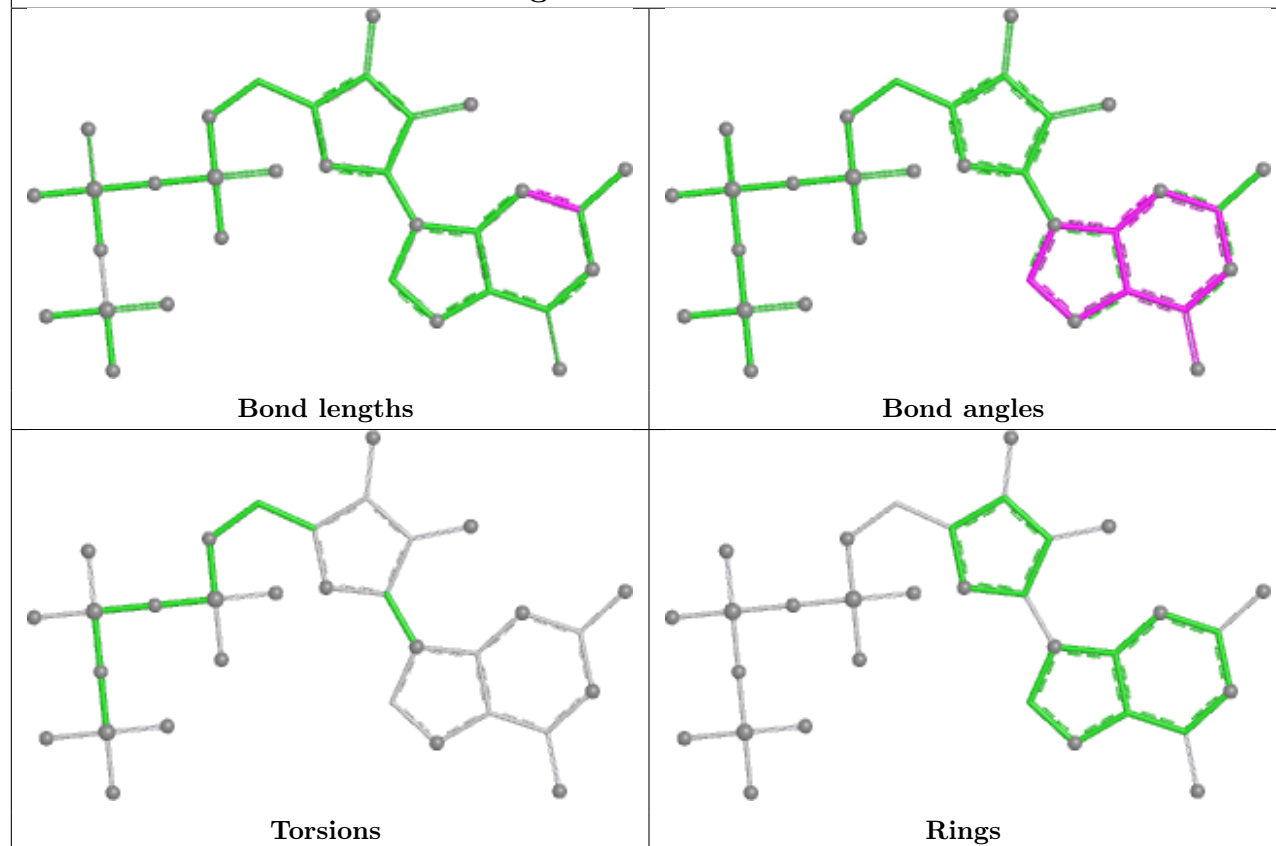
Ligand BKL D 603

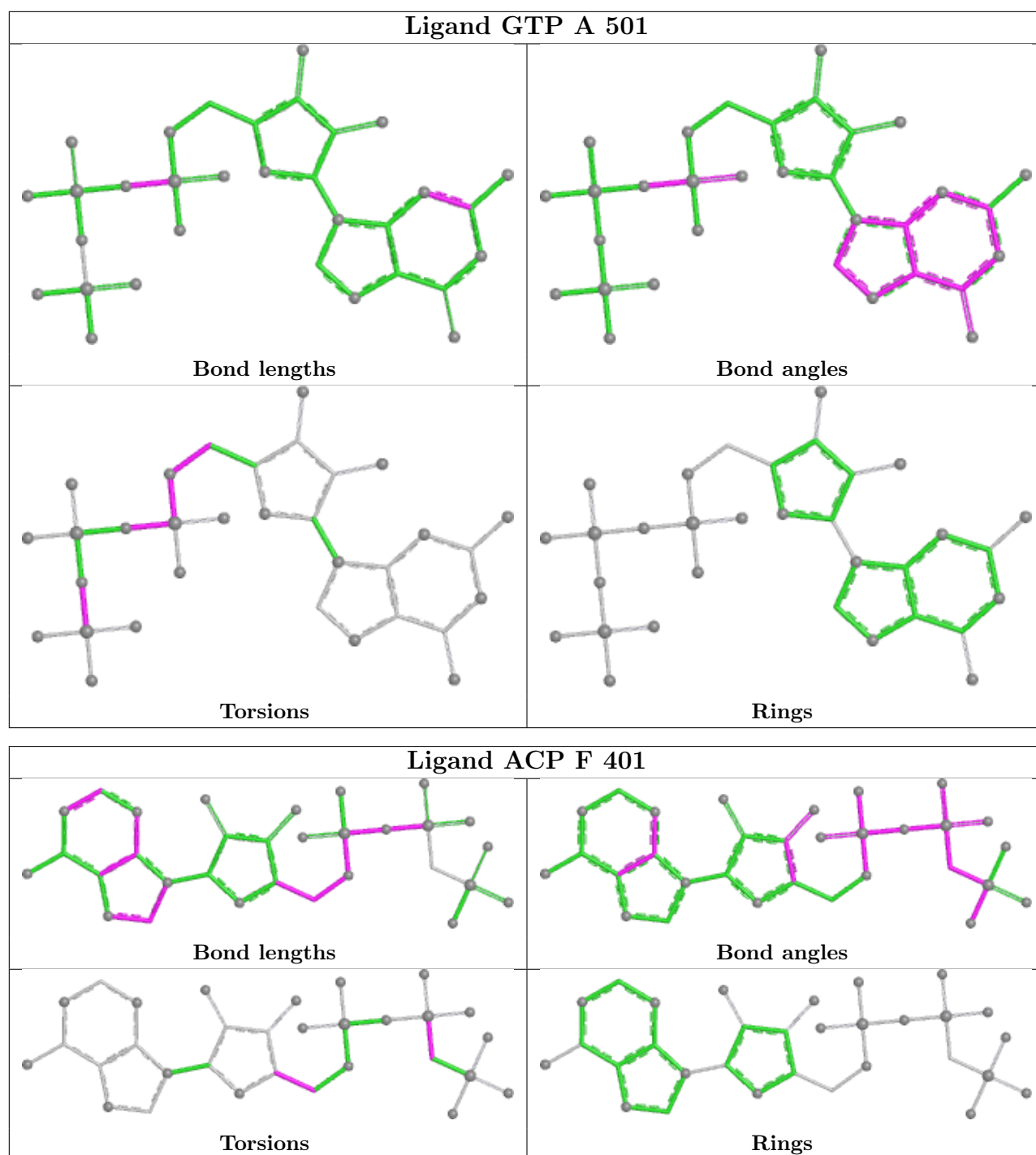


Ligand GTP C 501



Ligand GTP D 602





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	440/440 (100%)	-0.14	4 (0%) 81 80	22, 39, 75, 152	6 (1%)
1	C	440/440 (100%)	-0.35	8 (1%) 67 65	19, 33, 62, 98	9 (2%)
2	B	425/431 (98%)	-0.08	7 (1%) 70 68	18, 40, 76, 142	5 (1%)
2	D	421/431 (97%)	0.49	25 (5%) 28 25	28, 59, 102, 147	6 (1%)
3	E	123/138 (89%)	0.53	6 (4%) 35 31	28, 59, 106, 139	2 (1%)
4	F	348/384 (90%)	0.94	65 (18%) 3 3	32, 75, 151, 181	5 (1%)
All	All	2197/2264 (97%)	0.16	115 (5%) 33 29	18, 47, 107, 181	33 (1%)

The worst 5 of 115 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	143	ALA	7.5
4	F	169	LEU	5.6
2	D	285	ALA	4.6
3	E	28	SER	4.2
1	A	440	VAL	4.2

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 ⓘ

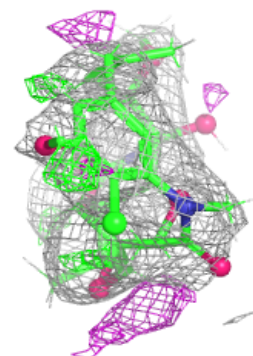
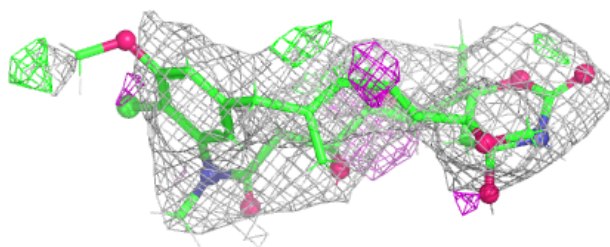
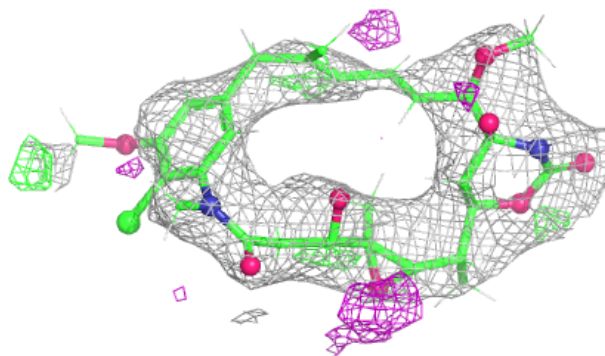
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	506	1/1	0.64	0.33	66,66,66,66	0
9	MES	A	505	12/12	0.73	0.22	63,93,113,165	0
11	BKL	D	603	39/39	0.77	0.18	57,87,107,152	0
12	ACP	F	401	31/31	0.79	0.17	71,101,140,191	0
5	GTP	D	602	32/32	0.90	0.12	46,58,72,114	0
9	MES	B	504	12/12	0.94	0.10	31,46,59,63	0
9	MES	B	505	12/12	0.94	0.10	46,57,77,83	0
8	CL	A	504	1/1	0.94	0.07	54,54,54,54	0
7	CA	B	503	1/1	0.94	0.07	70,70,70,70	0
10	GDP	B	501	28/28	0.95	0.09	18,28,39,43	0
6	MG	D	601	1/1	0.95	0.06	78,78,78,78	0
7	CA	E	201	1/1	0.95	0.13	69,69,69,69	0
7	CA	A	503	1/1	0.96	0.04	49,49,49,49	0
5	GTP	A	501	32/32	0.96	0.08	18,26,39,46	0
6	MG	C	502	1/1	0.97	0.05	28,28,28,28	0
5	GTP	C	501	32/32	0.97	0.07	16,23,35,44	0
6	MG	B	502	1/1	0.98	0.03	21,21,21,21	0
6	MG	A	502	1/1	0.99	0.04	27,27,27,27	0
7	CA	C	503	1/1	0.99	0.02	39,39,39,39	0

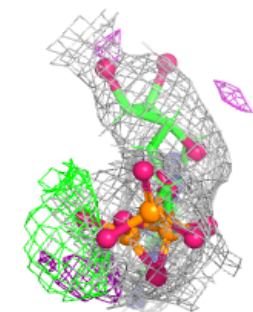
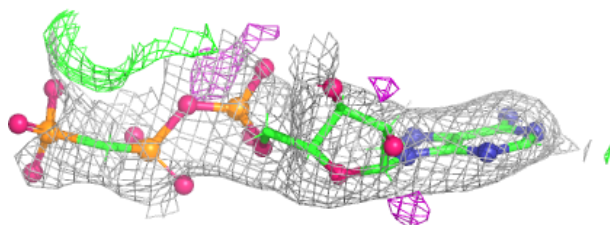
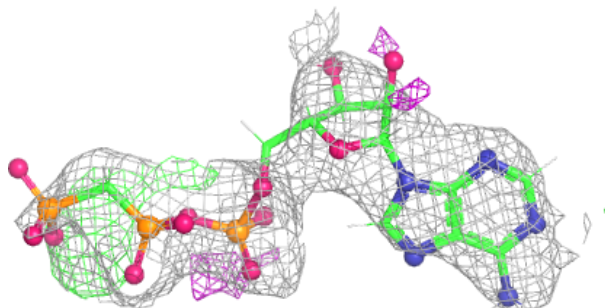
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BKL D 603:

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

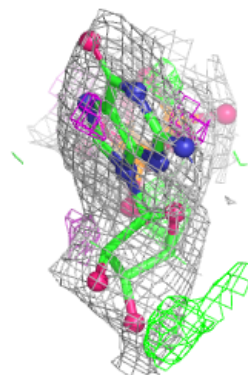
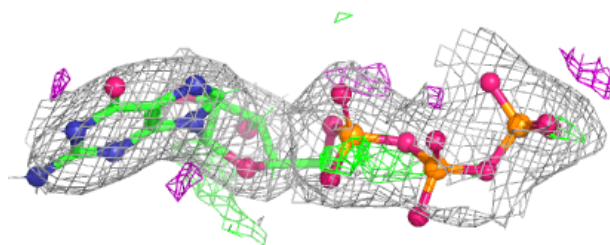
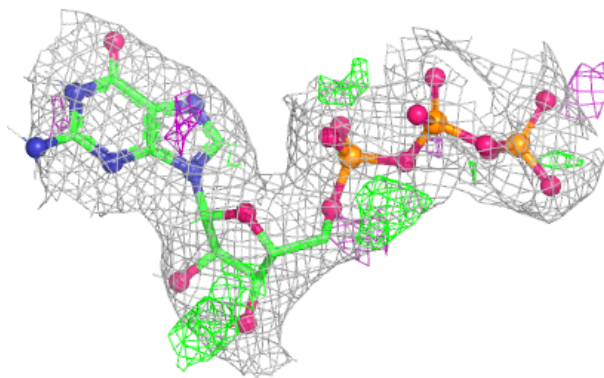
**Electron density around ACP F 401:**

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



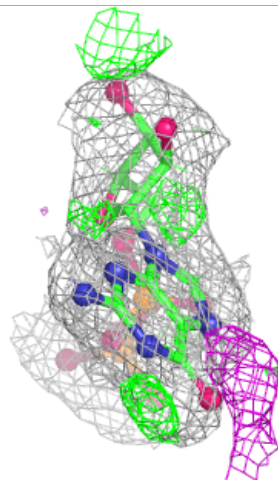
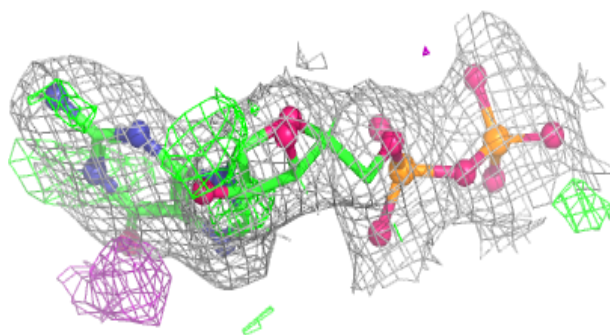
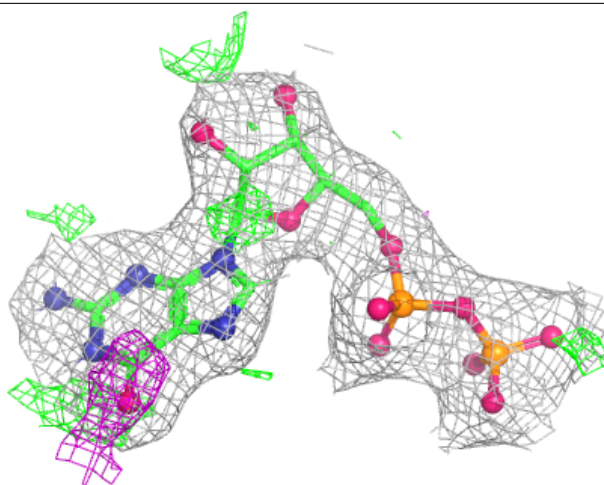
Electron density around GTP D 602:

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



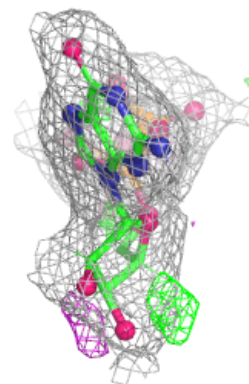
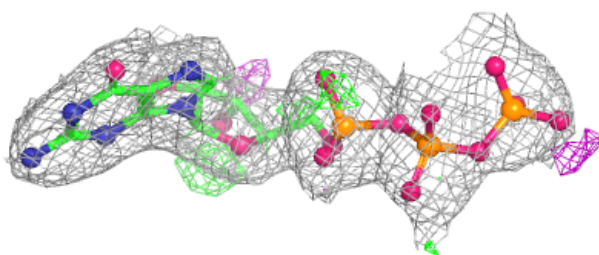
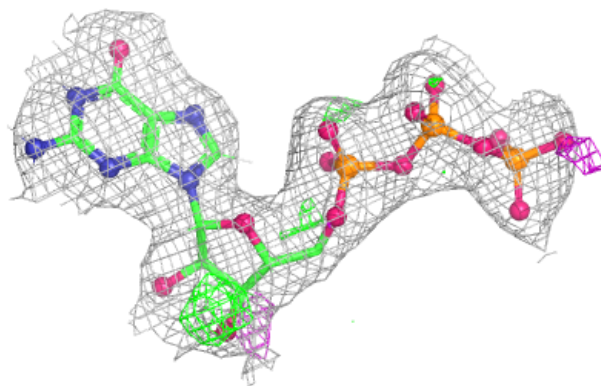
Electron density around GDP B 501:

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

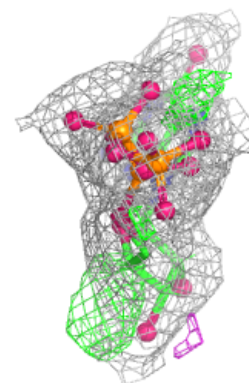
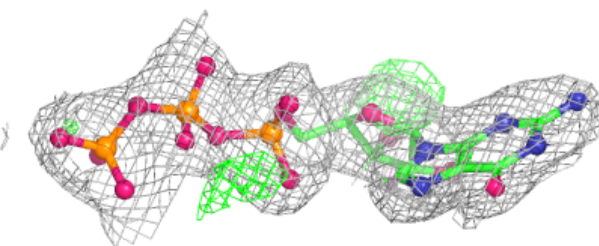
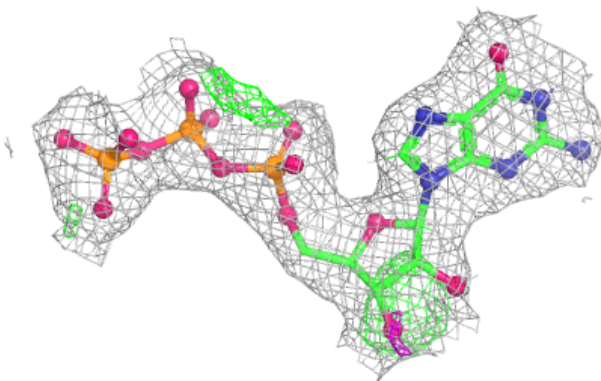


Electron density around GTP A 501:

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

**Electron density around GTP C 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.