



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 15, 2020 – 08:00 PM BST

PDB ID : 7JFR  
Title : Auristatin bound to tubulin  
Authors : Moquist, P.N.; Waight, A.  
Deposited on : 2020-07-17  
Resolution : 2.35 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4

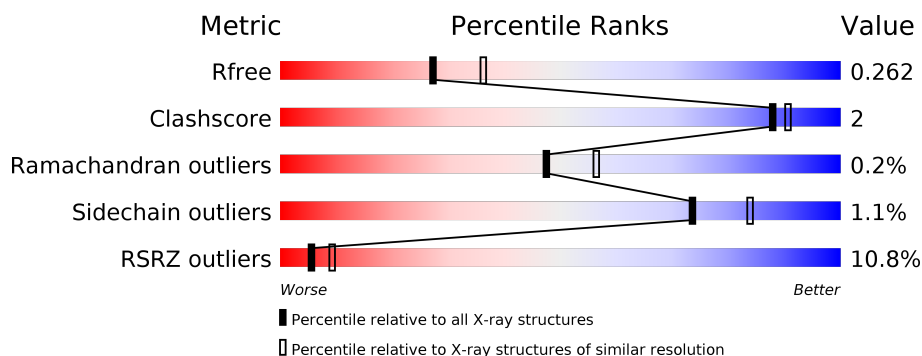
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>5%</div> <div>96%</div> <div>.</div> </div>
1	C	440	<div> <div>3%</div> <div>95%</div> <div>5%</div> </div>
2	B	445	<div> <div>2%</div> <div>91%</div> <div>5%</div> <div>.</div> </div>
2	D	445	<div> <div>10%</div> <div>91%</div> <div>5%</div> <div>5%</div> </div>
3	E	138	<div> <div>12%</div> <div>84%</div> <div>5%</div> <div>11%</div> </div>
4	F	378	<div> <div>35%</div> <div>79%</div> <div>12%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
5	L	5	 A horizontal bar chart showing the quality of chain L. The bar is divided into three segments: a green segment representing 60%, a yellow segment representing 20%, and an orange segment representing 20%. The percentages are labeled below the bar.

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 35292 atoms, of which 17339 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	439	Total	C	H	N	O	S	14	8	0
			6864	2203	3397	584	657	23			
1	C	440	Total	C	H	N	O	S	0	12	0
			6898	2212	3411	585	666	24			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	428	Total	C	H	N	O	S	39	14	0
			6762	2158	3336	580	659	29			
2	D	422	Total	C	H	N	O	S	0	4	0
			6533	2093	3205	563	645	27			

- 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	6	0
			2108	644	1066	186	206	6			

- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	344	Total	C	H	N	O	S	0	2	0
			5605	1808	2787	479	517	14			

- Molecule 5 is a protein called Auristatin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	5	Total	C	H	N	O	0	0	0
			147	49	85	5	8			

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:

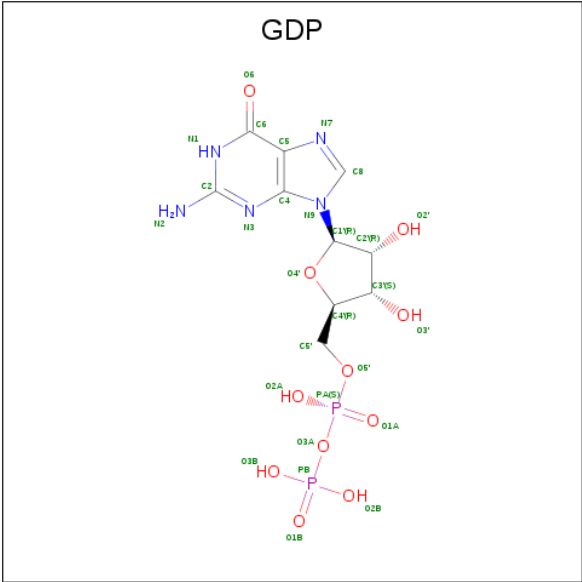
The chemical structure of GTP (Guanosine Triphosphate) is shown. It consists of a guanine base (a purine ring system with an amino group at position 2) linked to a ribose sugar (a five-membered ring with hydroxyl groups at positions 2' and 3'). The ribose sugar is linked to a chain of three phosphate groups (labeled G3P, G2P, and G1P) via a triphosphate bridge. The structure is labeled with atom names (N1, N2, N3, N4, N5, N6, N7, N8, 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, O804, O805, O806, O

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total 41	C 10	H 9	N 5	O 14	P 3	0	0
6	C	1	Total 41	C 10	H 9	N 5	O 14	P 3	0	0

- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 7   | B     | 2        | Total Mg<br>2 2 | 0       | 0       |
| 7   | A     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 7   | C     | 2        | Total Mg<br>2 2 | 0       | 0       |

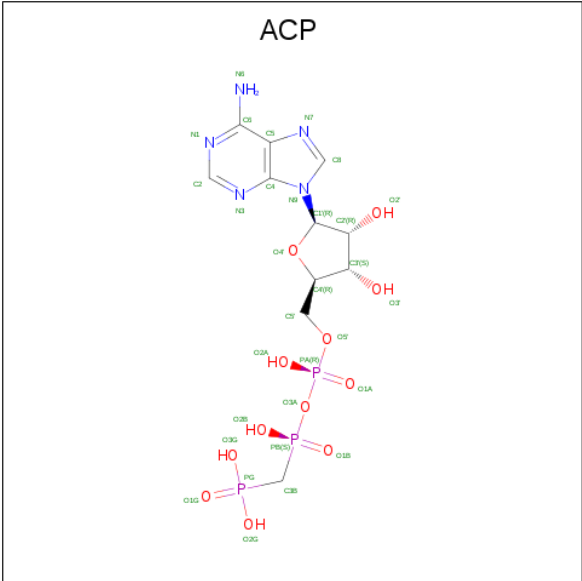
- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 8   | A     | 1        | Total Ca<br>1 1 | 0       | 0       |

- 



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	B	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		
9	D	1	Total	C	H	N	O	P	0	0
			38	10	10	5	11	2		

- Molecule 10 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



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

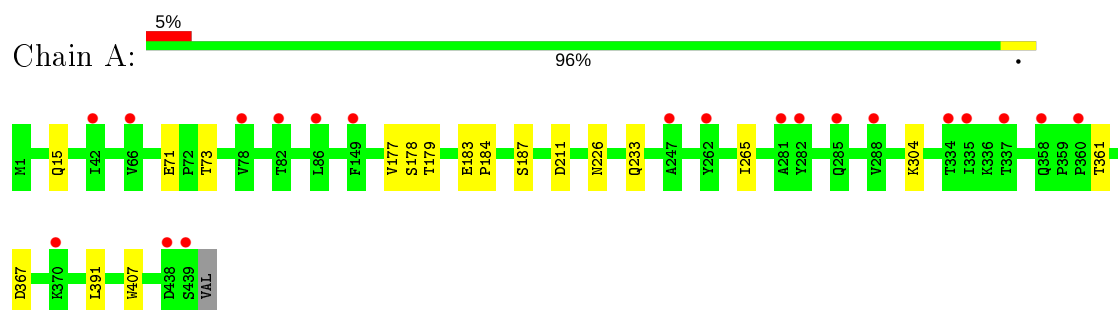
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	17	Total 17	O 17	0	0
11	B	53	Total 53	O 53	0	0
11	C	46	Total 46	O 46	0	0
11	D	20	Total 20	O 20	0	0
11	E	13	Total 13	O 13	0	0
11	F	17	Total 17	O 17	0	0

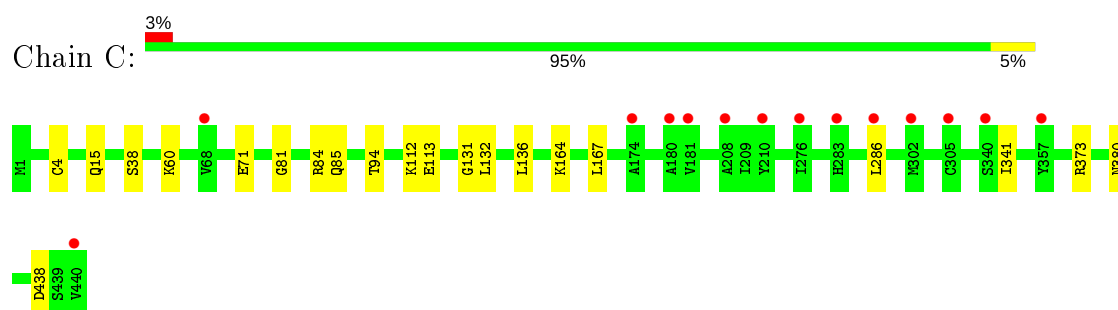
### 3 Residue-property plots [i](#)

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

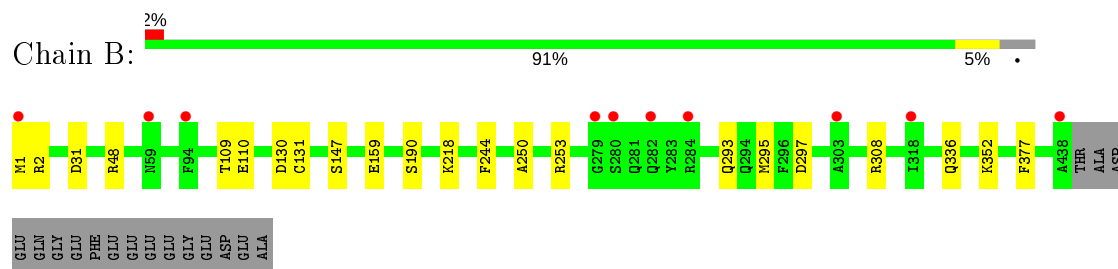
- Molecule 1: Tubulin alpha-1B chain



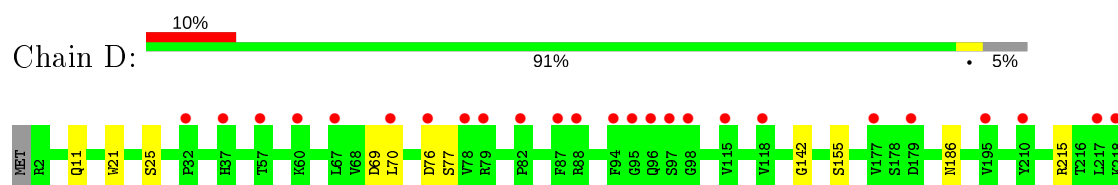
- Molecule 1: Tubulin alpha-1B chain

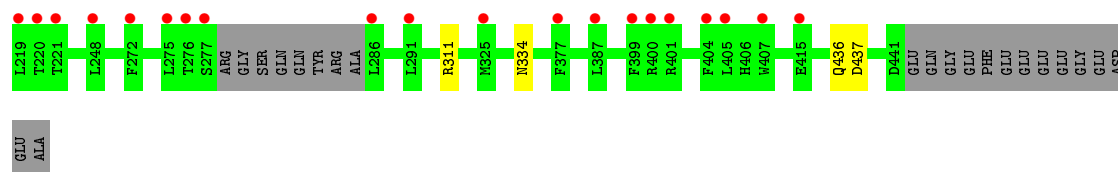


- Molecule 2: Tubulin beta-2B chain

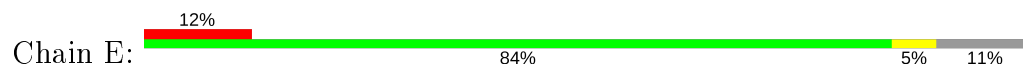


- Molecule 2: Tubulin beta-2B chain

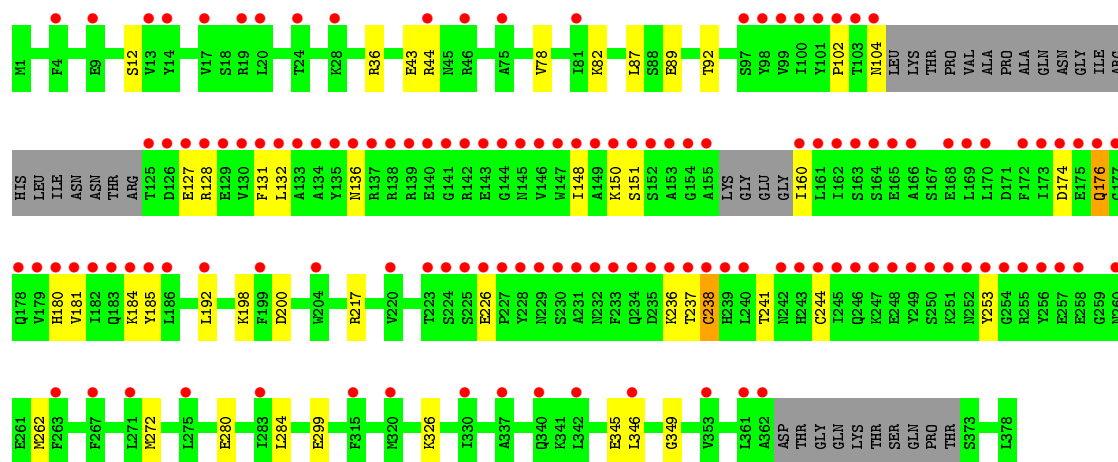
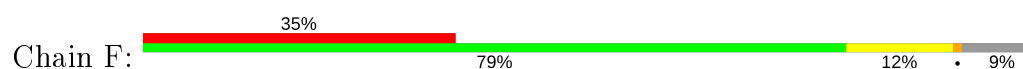




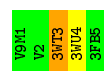
- Molecule 3: Stathmin-4



- Molecule 4: Uncharacterized protein



- Molecule 5: Auristatin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.49Å 155.15Å 181.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.74 – 2.35 62.74 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.9 (62.74-2.35) 96.9 (62.74-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.91 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.226 , 0.256 0.233 , 0.262	Depositor DCC
$R_{free}$ test set	1954 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.7	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	35292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, 3FB, CA, GTP, ACP, 3WU, 3WT, V9M

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	0.23	0/3570	0.41	0/4847
1	C	0.25	0/3601	0.41	0/4892
2	B	0.25	0/3550	0.40	0/4807
2	D	0.24	0/3413	0.39	0/4624
3	E	0.23	0/1068	0.35	0/1418
4	F	0.24	0/2886	0.42	0/3899
5	L	1.55	0/6	1.53	0/7
All	All	0.24	0/18094	0.40	0/24494

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	3397	3410	9	0
1	C	3487	3411	3424	12	0
2	B	3426	3336	3336	14	0
2	D	3328	3205	3215	11	0
3	E	1042	1066	1070	4	0
4	F	2818	2787	2796	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	62	85	54	2	0
6	A	32	9	12	1	0
6	C	32	9	12	1	0
7	A	1	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
8	A	1	0	0	0	0
9	B	28	10	12	0	0
9	D	28	10	12	1	0
10	F	31	14	14	2	0
11	A	17	0	0	1	0
11	B	53	0	0	5	0
11	C	46	0	0	4	0
11	D	20	0	0	5	0
11	E	13	0	0	1	0
11	F	17	0	0	4	0
All	All	17953	17339	17367	71	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 2.

The worst 5 of 71 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:437:ASP:OD1	11:D:601:HOH:O	1.83	0.96
2:B:1:MET:N	2:B:131:CYS:SG	2.49	0.86
2:B:308:ARG:NE	11:B:602:HOH:O	2.09	0.83
2:B:159:GLU:OE1	11:B:601:HOH:O	1.97	0.80
1:C:94:THR:OG1	11:C:601:HOH:O	1.91	0.80

There are no symmetry-related clashes.

## 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	445/440 (101%)	428 (96%)	16 (4%)	1 (0%)	47	56
1	C	450/440 (102%)	436 (97%)	12 (3%)	2 (0%)	34	38
2	B	440/445 (99%)	428 (97%)	12 (3%)	0	100	100
2	D	422/445 (95%)	407 (96%)	15 (4%)	0	100	100
3	E	125/138 (91%)	125 (100%)	0	0	100	100
4	F	338/378 (89%)	319 (94%)	18 (5%)	1 (0%)	41	47
All	All	2220/2286 (97%)	2143 (96%)	73 (3%)	4 (0%)	47	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	237	THR
1	C	341	ILE
1	A	177	VAL
1	C	131	GLY

### 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	378/371 (102%)	376 (100%)	2 (0%)	88	94
1	C	383/371 (103%)	382 (100%)	1 (0%)	92	96
2	B	384/383 (100%)	382 (100%)	2 (0%)	88	94
2	D	369/383 (96%)	369 (100%)	0	100	100
3	E	116/123 (94%)	113 (97%)	3 (3%)	46	56
4	F	310/336 (92%)	297 (96%)	13 (4%)	30	36
5	L	1/1 (100%)	1 (100%)	0	100	100
All	All	1941/1968 (99%)	1920 (99%)	21 (1%)	73	84

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	F	89	GLU
4	F	132	LEU
4	F	244	CYS
4	F	87	LEU
4	F	253	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	139	HIS
2	B	192	HIS
4	F	104	ASN
4	F	243	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	3WT	L	3	5	11,12,13	0.92	1 (9%)	8,14,16	2.53	1 (12%)
5	3WU	L	4	5	12,12,13	1.30	1 (8%)	9,15,17	1.37	1 (11%)

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	3WT	L	3	5	-	3/17/17/18	-
5	3WU	L	4	5	-	0/11/19/21	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	4	3WU	C3-C2	-2.42	1.49	1.53
5	L	3	3WT	C26-C27	2.22	1.55	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	3	3WT	C25-N3-C19	6.80	124.29	114.38
5	L	4	3WU	C3-C2-N1	2.61	107.96	103.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	3	3WT	C20-C19-N3-C25
5	L	3	3WT	O5-C20-C26-C27
5	L	3	3WT	C19-C20-C26-C27

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	3	3WT	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	GDP	B	501	-	24,30,30	1.05	2 (8%)	31,47,47	1.89	7 (22%)
6	GTP	A	501	7	26,34,34	0.97	1 (3%)	33,54,54	1.64	6 (18%)
10	ACP	F	401	-	27,33,33	1.44	6 (22%)	32,52,52	1.32	5 (15%)
6	GTP	C	501	7	26,34,34	0.96	1 (3%)	33,54,54	1.70	7 (21%)
9	GDP	D	501	-	24,30,30	1.14	2 (8%)	31,47,47	1.89	9 (29%)

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	GDP	B	501	-	-	4/12/32/32	0/3/3/3
6	GTP	A	501	7	-	8/18/38/38	0/3/3/3
10	ACP	F	401	-	-	8/15/38/38	0/3/3/3
6	GTP	C	501	7	-	9/18/38/38	0/3/3/3
9	GDP	D	501	-	-	4/12/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	501	GDP	C6-C5	3.94	1.48	1.41
10	F	401	ACP	PB-O3A	3.57	1.62	1.58
9	B	501	GDP	C6-C5	3.43	1.47	1.41
6	A	501	GTP	C6-N1	2.99	1.38	1.33
6	C	501	GTP	C6-N1	2.96	1.38	1.33

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	501	GTP	N3-C2-N1	-5.25	120.22	127.22
6	A	501	GTP	N3-C2-N1	-5.01	120.54	127.22
9	D	501	GDP	C2-N3-C4	4.58	120.58	115.36
9	B	501	GDP	C6-N1-C2	4.55	123.16	115.93
9	B	501	GDP	C6-C5-C4	-4.33	116.66	120.80

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

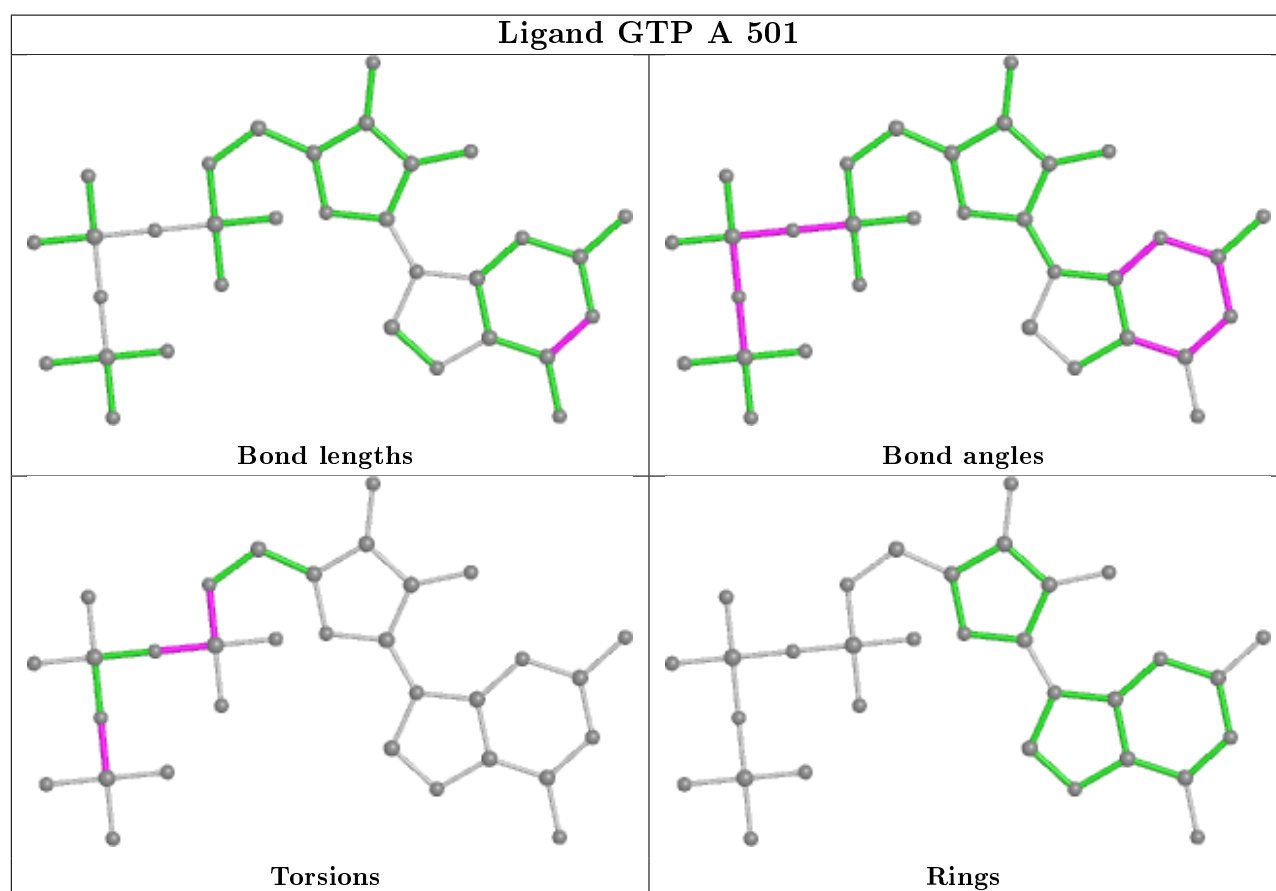
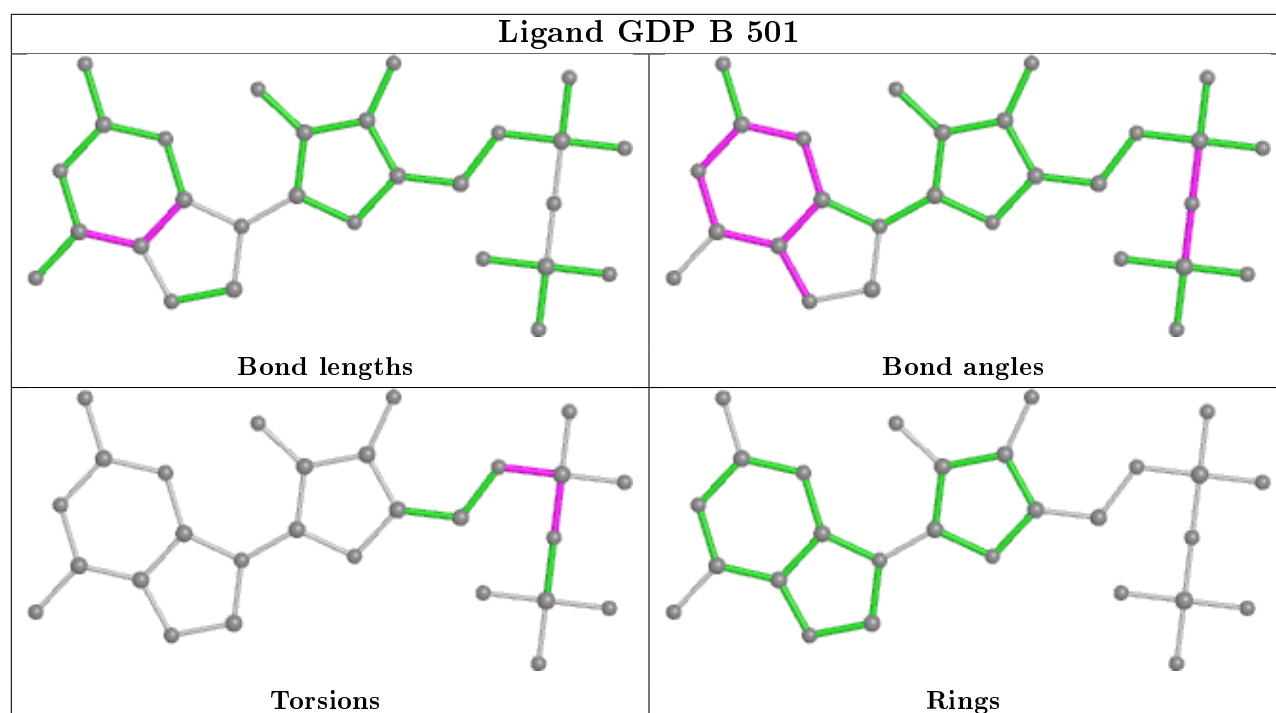
Mol	Chain	Res	Type	Atoms
10	F	401	ACP	PB-C3B-PG-O1G
10	F	401	ACP	PB-C3B-PG-O2G
10	F	401	ACP	PB-C3B-PG-O3G
10	F	401	ACP	C5'-O5'-PA-O1A
10	F	401	ACP	C5'-O5'-PA-O2A

There are no ring outliers.

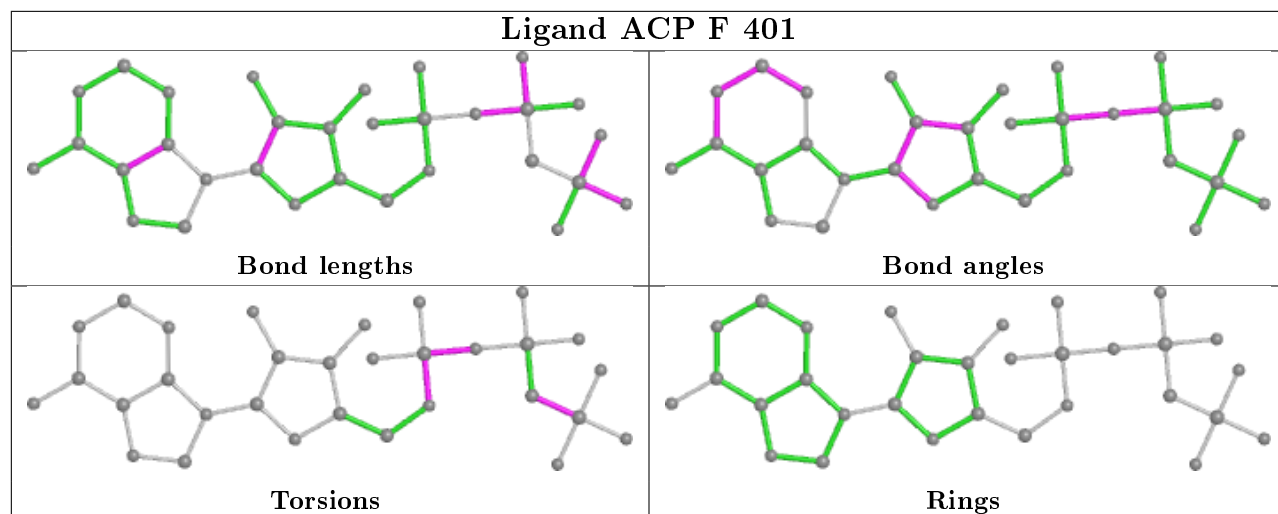
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	501	GTP	1	0
10	F	401	ACP	2	0
6	C	501	GTP	1	0
9	D	501	GDP	1	0

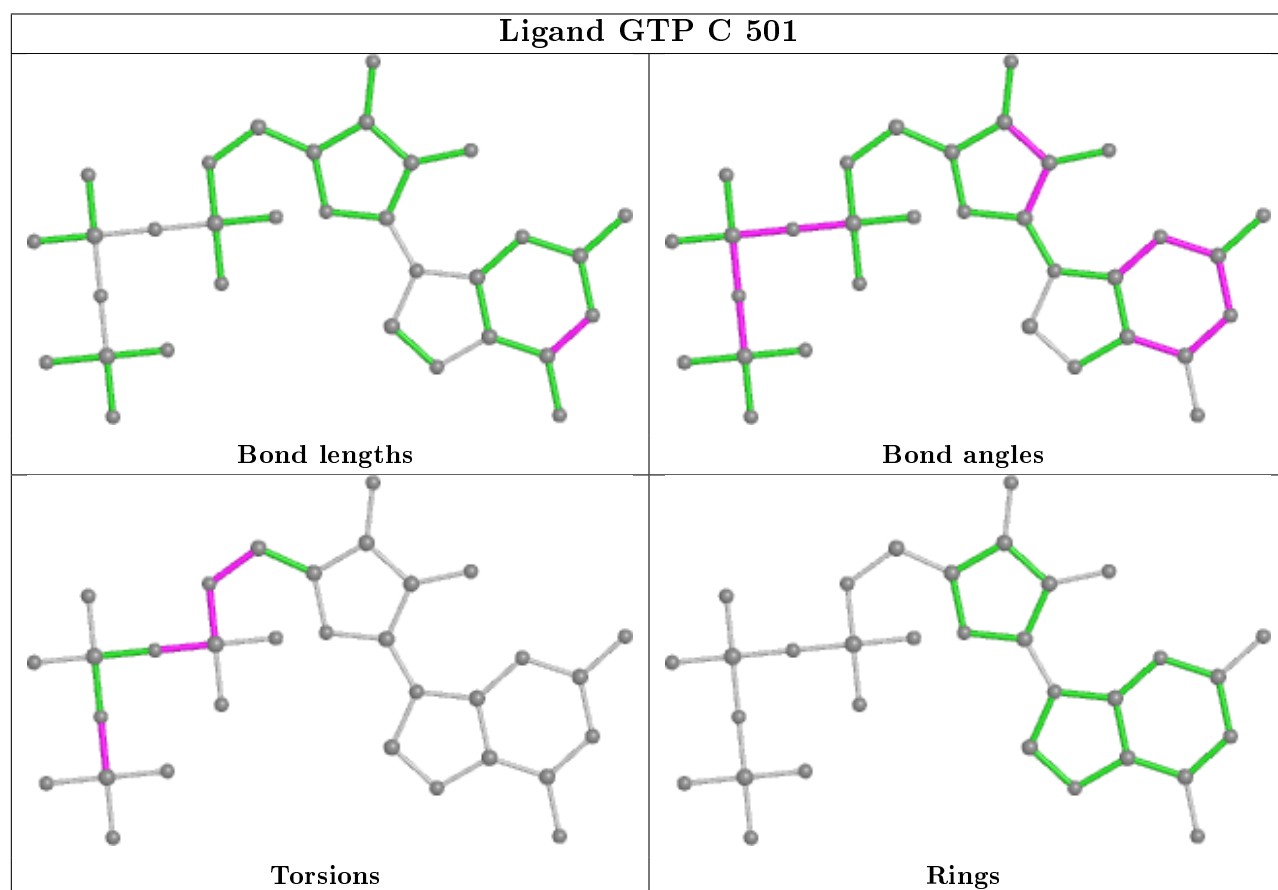
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

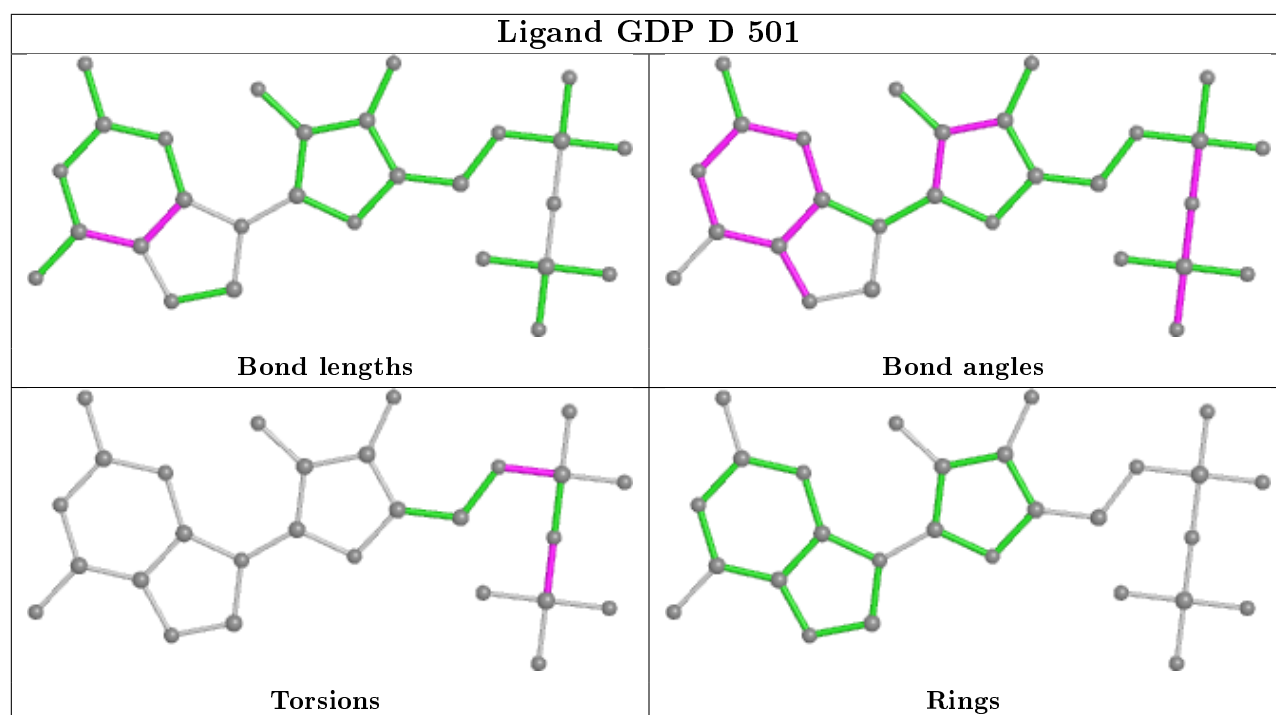


## Ligand ACP F 401



## Ligand GTP C 501





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	439/440 (99%)	0.66	20 (4%) 32 45	45, 66, 105, 160	0
1	C	440/440 (100%)	0.55	14 (3%) 47 59	36, 53, 80, 115	0
2	B	428/445 (96%)	0.53	10 (2%) 60 70	42, 59, 87, 123	1 (0%)
2	D	422/445 (94%)	0.80	45 (10%) 6 9	48, 72, 99, 123	2 (0%)
3	E	123/138 (89%)	0.94	17 (13%) 2 4	50, 76, 113, 147	0
4	F	344/378 (91%)	2.04	132 (38%) 0 0	57, 94, 170, 275	0
5	L	1/5 (20%)	1.04	0 100 100	49, 49, 49, 49	0
All	All	2197/2291 (95%)	0.87	238 (10%) 5 9	36, 67, 127, 275	3 (0%)

The worst 5 of 238 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	11.1
4	F	177	GLY	9.6
4	F	233	PHE	9.5
4	F	173	ILE	9.2
4	F	253	TYR	8.7

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	3WT	L	3	13/14	0.96	0.18	45,61,73,73	0
5	3WU	L	4	12/13	0.96	0.13	43,53,69,69	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

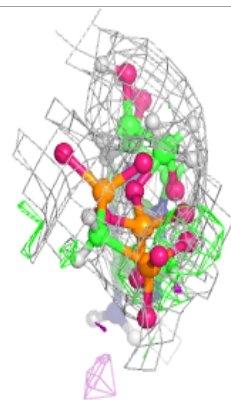
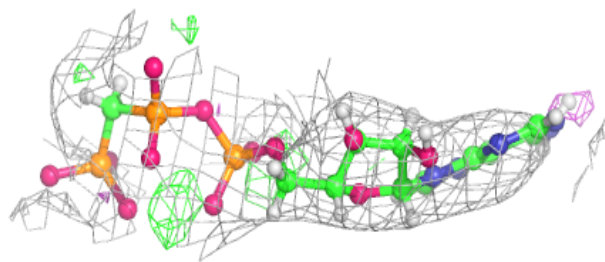
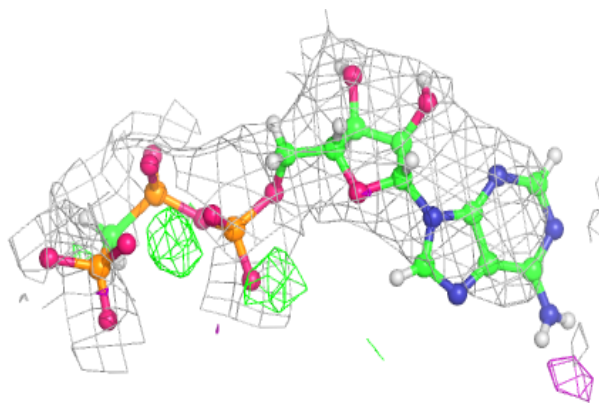
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	CA	A	503	1/1	0.68	0.09	115,115,115,115	0
7	MG	B	503	1/1	0.77	0.26	72,72,72,72	0
7	MG	A	502	1/1	0.78	0.25	56,56,56,56	0
7	MG	C	502	1/1	0.81	0.37	48,48,48,48	0
10	ACP	F	401	31/31	0.82	0.21	104,133,172,179	0
7	MG	C	503	1/1	0.94	0.14	82,82,82,82	0
7	MG	B	502	1/1	0.94	0.17	76,76,76,76	0
9	GDP	D	501	28/28	0.95	0.16	61,75,98,118	0
6	GTP	A	501	32/32	0.96	0.20	45,55,75,84	0
9	GDP	B	501	28/28	0.98	0.19	40,49,72,81	0
6	GTP	C	501	32/32	0.98	0.23	38,47,61,80	0

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

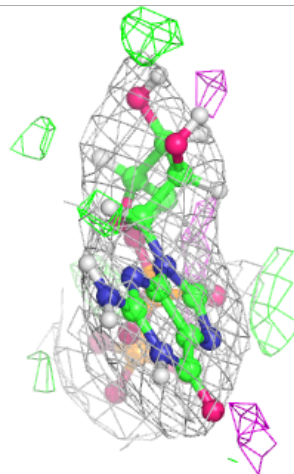
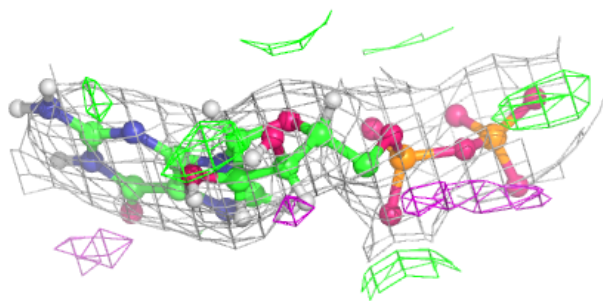
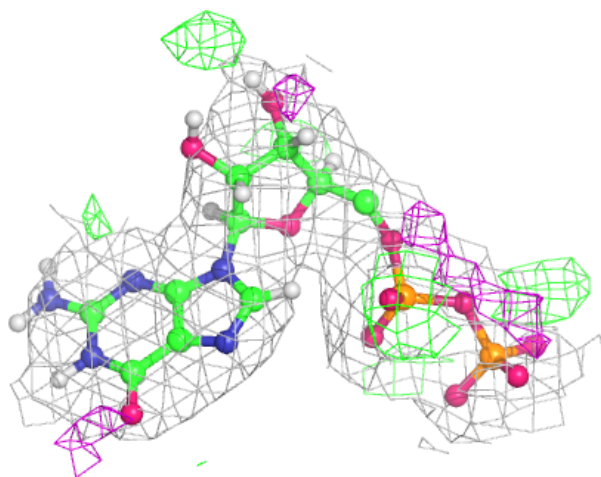
**Electron density around ACP F 401:**

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



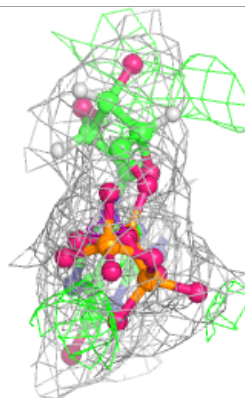
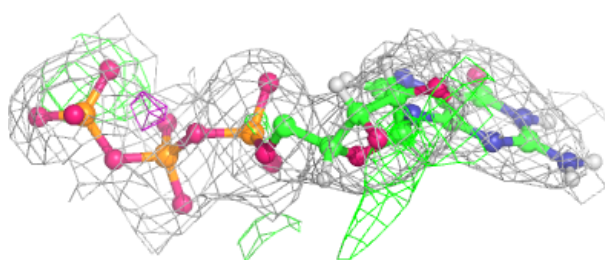
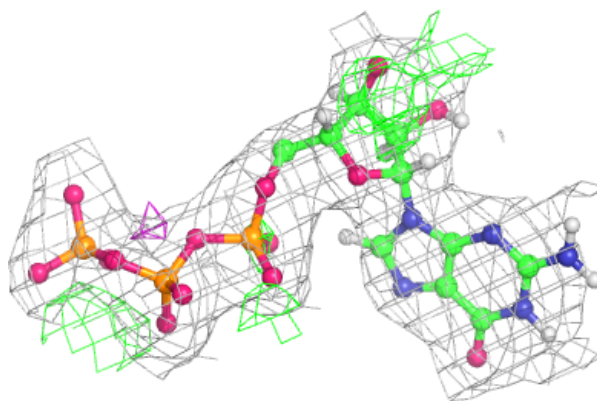
**Electron density around GDP D 501:**

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

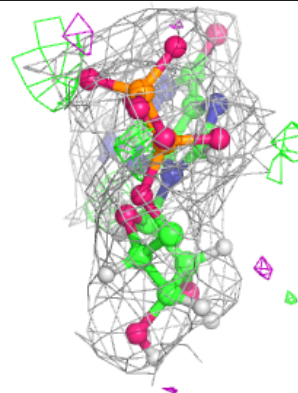
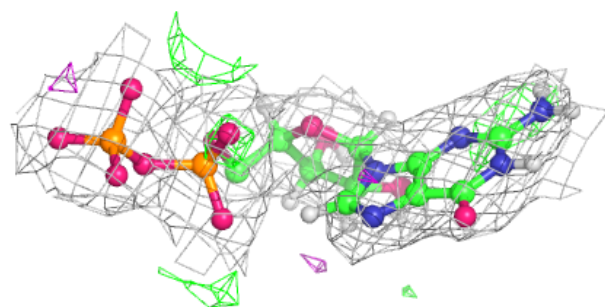
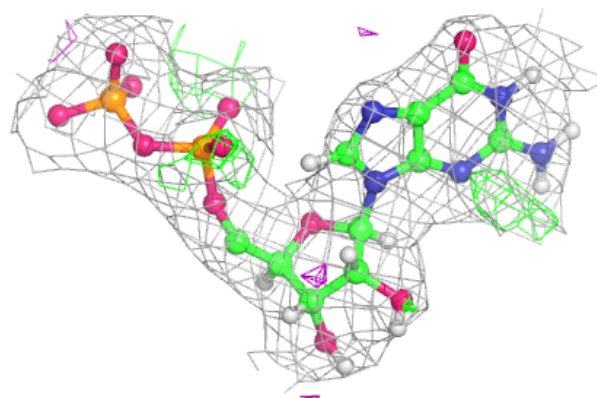


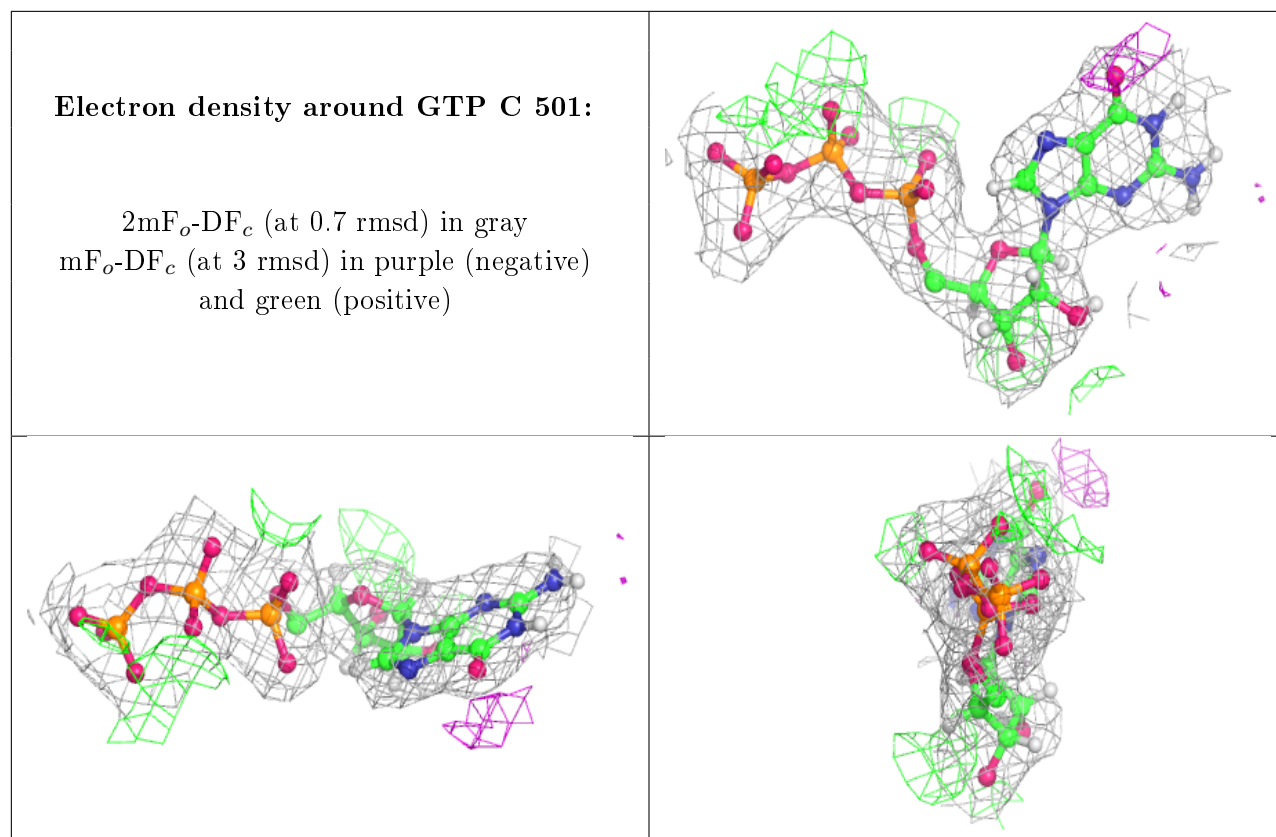
**Electron density around GTP A 501:**

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

**Electron density around GDP B 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.