



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 07:06 am BST

PDB ID : 5XAG  
Title : Crystal structure of tubulin-stathmin-TTL-Compound Z2 complex  
Authors : Zhang, H.; Luo, C.; Wang, Y.  
Deposited on : 2017-03-12  
Resolution : 2.56 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

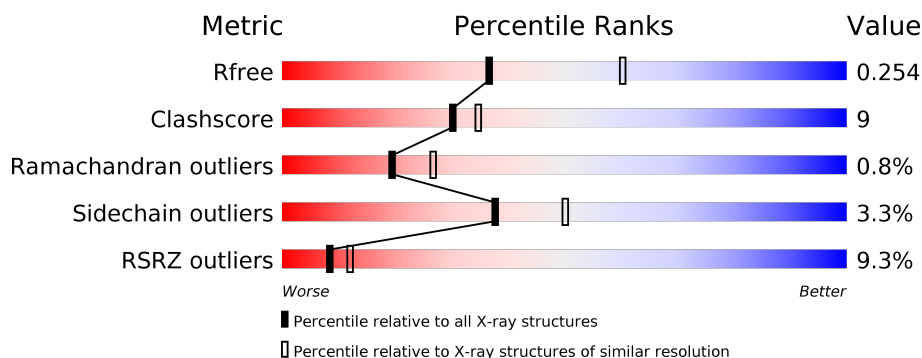
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.56 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))
$R_{free}$	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (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 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	451	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>•</div> </div> </div>
1	C	451	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>16%</div> <div>••</div> </div> </div>
2	B	445	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>• 5%</div> </div> </div>
2	D	445	<div> <div>9%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• 5%</div> </div> </div>
3	E	189	<div> <div>4%</div> <div> <div></div> <div>47%</div> <div>15%</div> <div>• 37%</div> </div> </div>
4	F	378	<div> <div>29%</div> <div> <div></div> <div>57%</div> <div>24%</div> <div>• 16%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	A	504	-	-	-	X
7	GOL	B	505	-	-	X	X
7	GOL	C	505	-	-	-	X
7	GOL	D	503	-	-	-	X

## 2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 17705 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	10	0
			3476	2206	585	660	25			
1	C	440	Total	C	N	O	S	0	9	0
			3482	2204	588	667	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	9	0
			3376	2125	569	655	27			
2	D	421	Total	C	N	O	S	0	3	0
			3321	2089	562	642	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	120	Total	C	N	O	S	0	1	0
			997	616	181	195	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	317	Total	C	N	O	S	0	3	0
			2609	1689	434	472	14			

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



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

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

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).

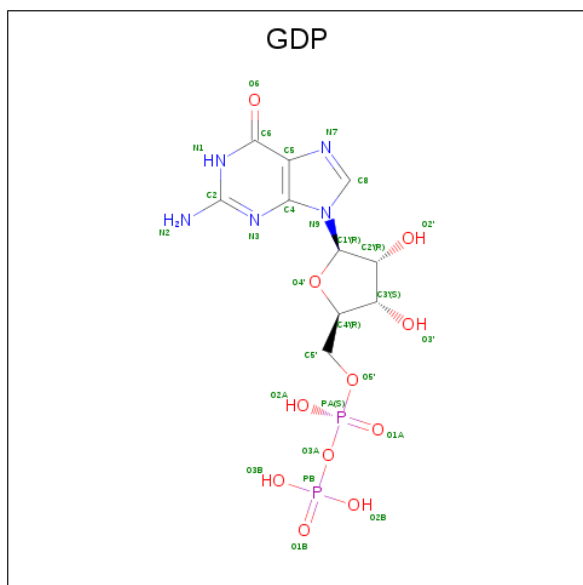


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

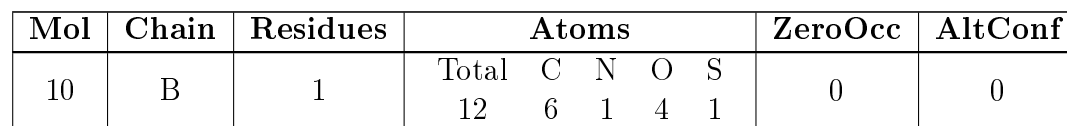
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Ca 1 1	0	0
8	A	1	Total Ca 1 1	0	0
8	C	1	Total Ca 1 1	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



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

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).

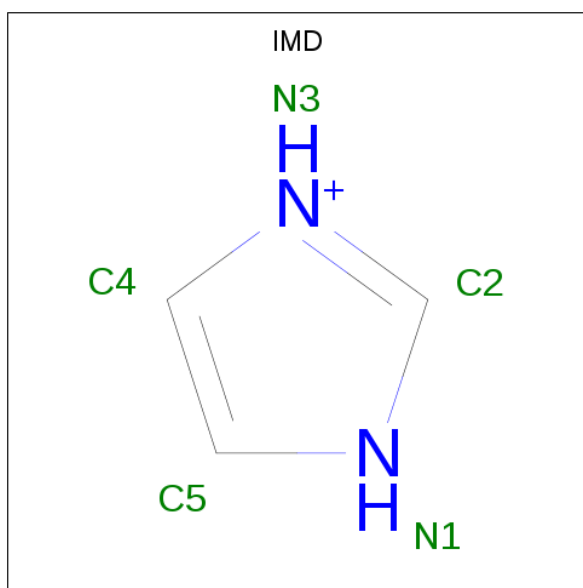


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- ORTEP diagram of the chemical structure of 93X, showing the molecular structure with thermal ellipsoids at the 50% probability level. The structure features a central four-membered ring with a nitrogen atom (N1) and a carbonyl group (C4=O5). It is substituted with two 3,4,5-trimethoxyphenyl groups and a 3-hydroxyphenyl group. The stereochemistry is indicated with wedges and dashes.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total 28	C 20	N 1	O 7	0	0
11	D	1	Total 28	C 20	N 1	O 7	0	0

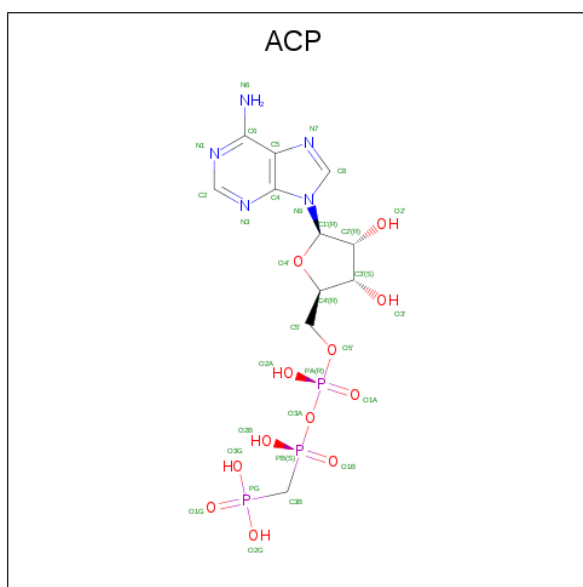


- Molecule 12 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	N	0	0
			5	3	2		
12	C	1	Total	C	N	0	0
			5	3	2		
12	E	1	Total	C	N	0	0
			5	3	2		

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



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

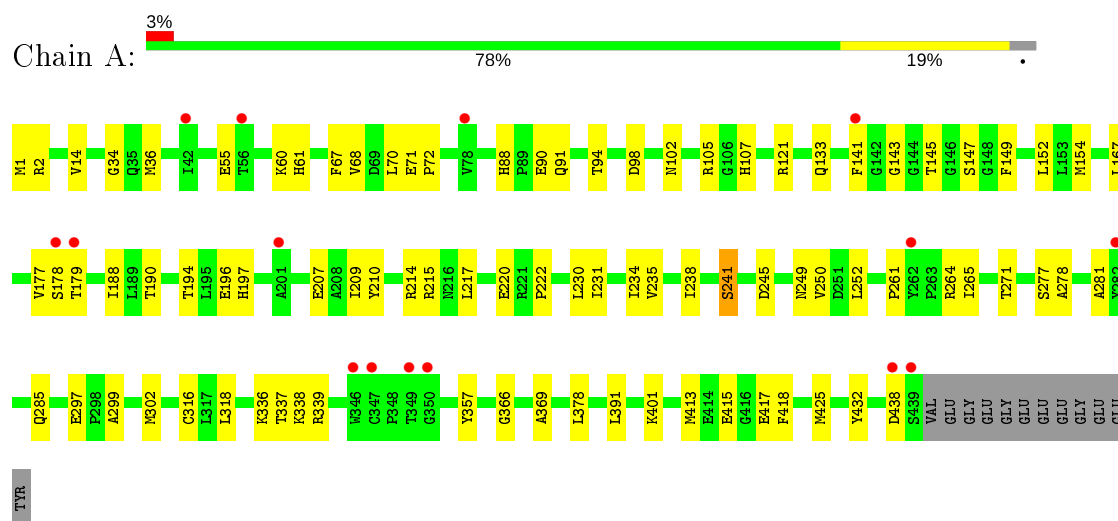
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	20	Total	O	0	0
			20	20		
14	B	20	Total	O	0	0
			20	20		
14	C	48	Total	O	0	0
			48	48		
14	D	9	Total	O	0	0
			9	9		
14	E	15	Total	O	0	0
			15	15		
14	F	18	Total	O	0	0
			18	18		

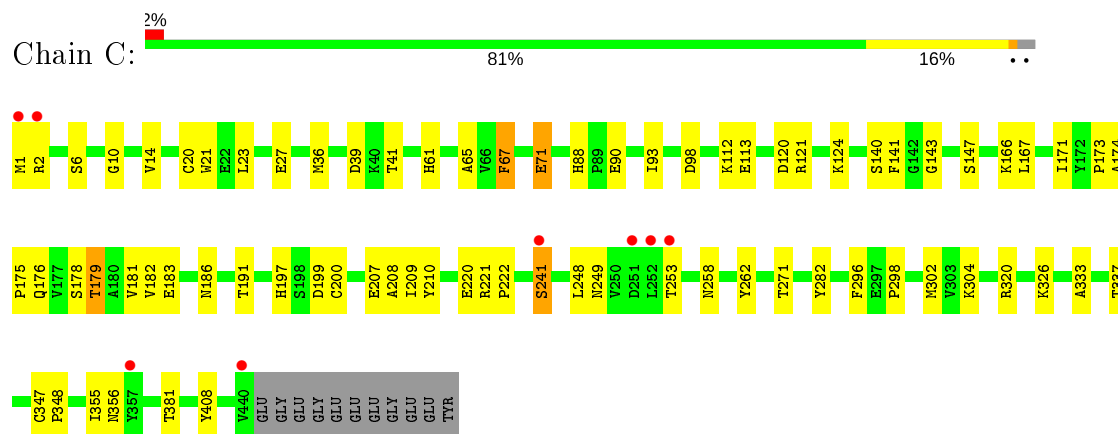
### 3 Residue-property plots [i](#)

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

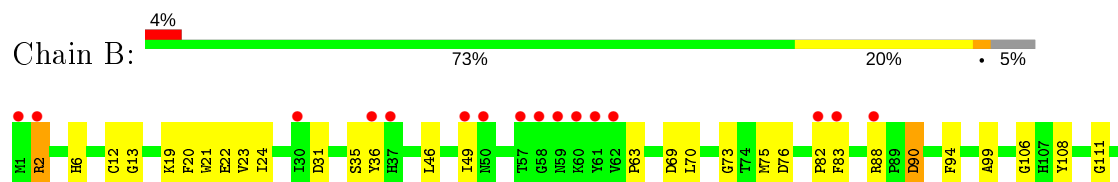
#### • Molecule 1: Tubulin alpha-1B chain

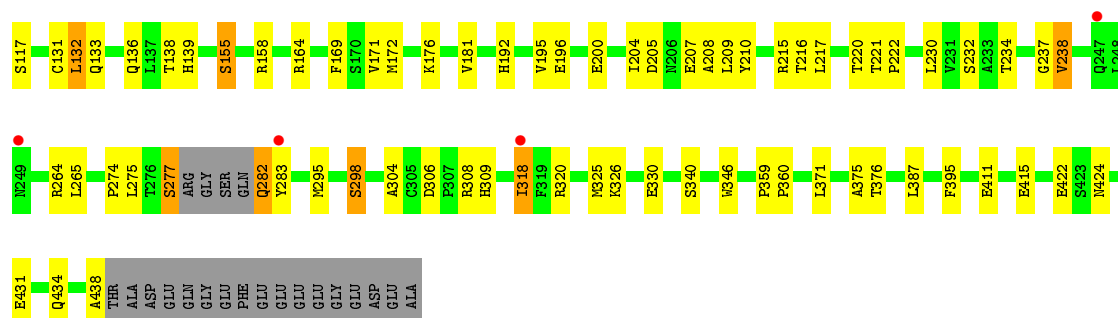


#### • Molecule 1: Tubulin alpha-1B chain

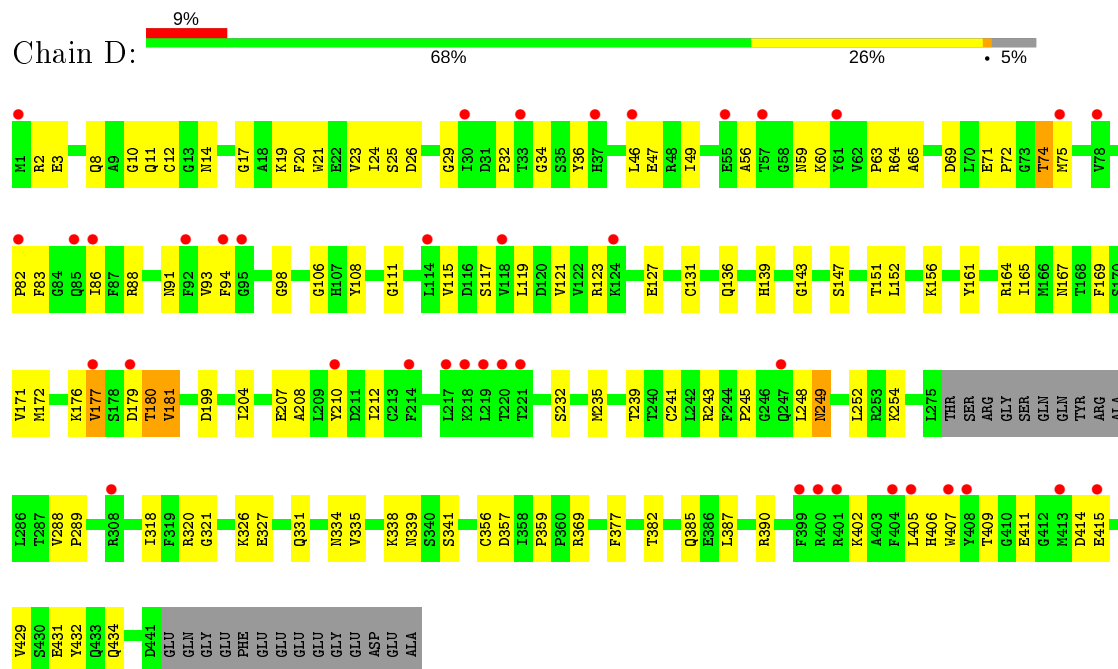


#### • Molecule 2: Tubulin beta-2B chain

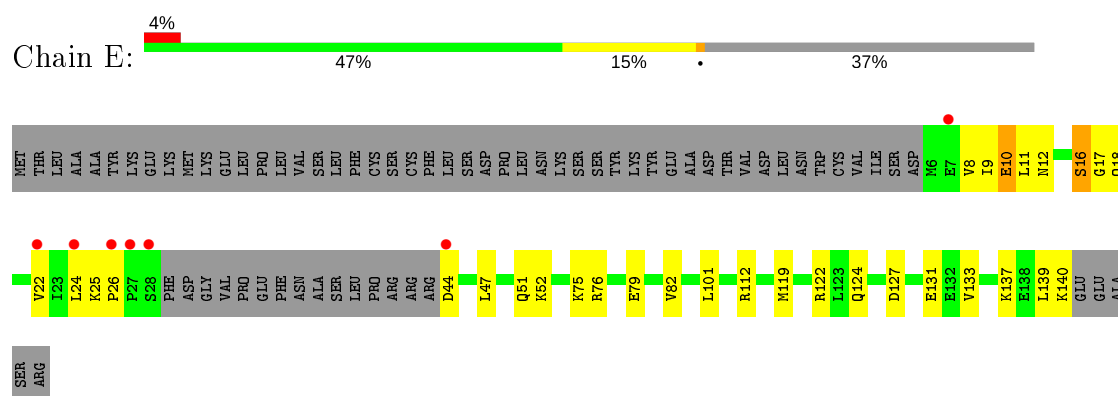




### • Molecule 2: Tubulin beta-2B chain

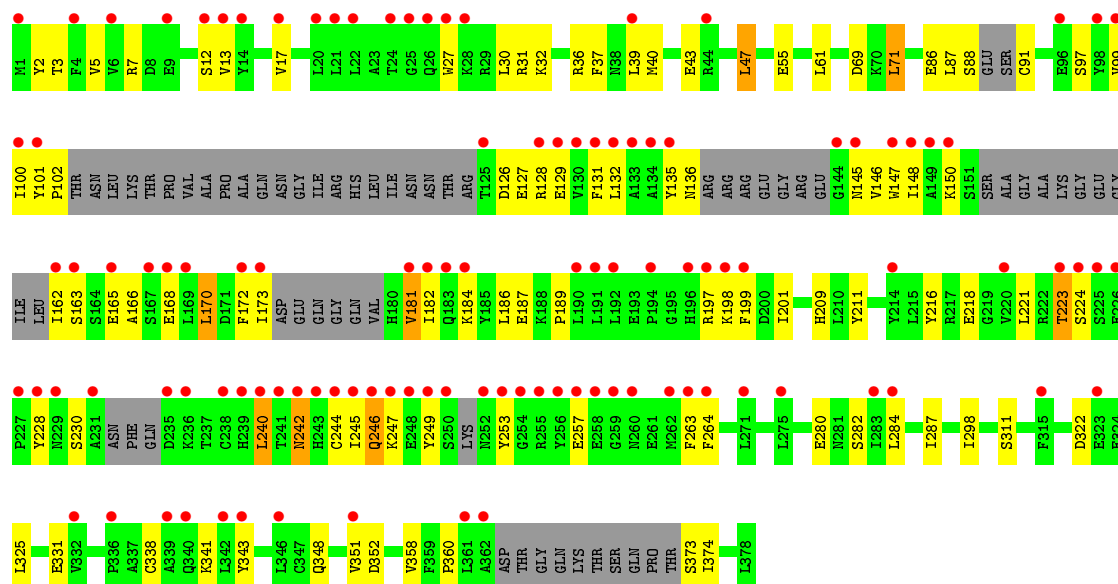


### • Molecule 3: Stathmin-4



### • Molecule 4: Tubulin tyrosine ligase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.27Å 156.12Å 182.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.92 – 2.56 47.92 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.92-2.56) 99.9 (47.92-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.211 , 0.255 0.211 , 0.254	Depositor DCC
$R_{free}$ test set	2000 reflections (2.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.7	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 52.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17705	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GOL, MG, IMD, CA, GTP, 93X, MES, ACP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.43	0/3584	0.60	0/4865
1	C	0.52	1/3584 (0.0%)	0.66	0/4867
2	B	0.46	0/3474	0.62	1/4706 (0.0%)
2	D	0.42	0/3403	0.57	0/4611
3	E	0.50	0/1008	0.56	0/1337
4	F	0.41	1/2674 (0.0%)	0.57	0/3609
All	All	0.46	2/17727 (0.0%)	0.60	1/23995 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	47	LEU	C-N	7.58	1.48	1.34
1	C	20	CYS	CB-SG	-5.15	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	275	LEU	CA-CB-CG	-5.21	103.31	115.30

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	3476	0	3417	55	0
1	C	3482	0	3401	49	1
2	B	3376	0	3265	63	1
2	D	3321	0	3210	74	0
3	E	997	0	1020	22	0
4	F	2609	0	2599	72	0
5	A	32	0	12	2	0
5	C	32	0	12	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	18	0	24	1	0
7	B	18	0	24	6	0
7	C	24	0	32	2	0
7	D	12	0	15	2	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	B	28	0	12	1	0
9	D	28	0	12	2	0
10	B	12	0	12	0	0
11	B	28	0	0	0	0
11	D	28	0	0	1	0
12	C	10	0	10	3	0
12	E	5	0	4	2	0
13	F	31	0	14	1	0
14	A	20	0	0	3	0
14	B	20	0	0	2	0
14	C	48	0	0	0	0
14	D	9	0	0	4	0
14	E	15	0	0	1	0
14	F	18	0	0	9	0
All	All	17705	0	17095	321	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 9.

The worst 5 of 321 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:411:GLU:HA	3:E:137:LYS:HD2	1.61	0.82
4:F:145:ASN:HB3	4:F:147:TRP:HE1	1.45	0.82
1:C:120[B]:ASP:OD2	1:C:124:LYS:NZ	2.13	0.81
4:F:31:ARG:HE	4:F:32:LYS:H	1.28	0.81
2:B:217:LEU:HD22	2:B:277:SER:HB3	1.63	0.81

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)
2:B:411:GLU:OE1	1:C:282:TYR:OH[4_545]	2.17	0.03

## 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	447/451 (99%)	421 (94%)	22 (5%)	4 (1%)	17	24
1	C	447/451 (99%)	431 (96%)	15 (3%)	1 (0%)	47	58
2	B	429/445 (96%)	402 (94%)	24 (6%)	3 (1%)	22	29
2	D	420/445 (94%)	400 (95%)	16 (4%)	4 (1%)	15	21
3	E	117/189 (62%)	105 (90%)	10 (8%)	2 (2%)	9	11
4	F	302/378 (80%)	263 (87%)	37 (12%)	2 (1%)	22	29
All	All	2162/2359 (92%)	2022 (94%)	124 (6%)	16 (1%)	19	29

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	VAL
2	D	177	VAL
3	E	10	GLU
4	F	230	SER

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Mol	Chain	Res	Type
2	D	64	ARG

### 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	380/379 (100%)	372 (98%)	8 (2%)	53	67
1	C	380/379 (100%)	373 (98%)	7 (2%)	59	73
2	B	375/383 (98%)	357 (95%)	18 (5%)	25	34
2	D	367/383 (96%)	355 (97%)	12 (3%)	38	50
3	E	109/171 (64%)	105 (96%)	4 (4%)	34	45
4	F	289/336 (86%)	275 (95%)	14 (5%)	25	34
All	All	1900/2031 (94%)	1837 (97%)	63 (3%)	38	50

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	179	THR
2	D	74	THR
4	F	223	THR
1	C	181	VAL
1	C	347	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	249	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 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	$\# Z  > 2$
7	GOL	B	504	-	5,5,5	0.45	0	5,5,5	0.43	0
7	GOL	D	504	12	5,5,5	0.36	0	5,5,5	0.30	0
7	GOL	C	504	-	5,5,5	0.31	0	5,5,5	0.48	0
12	IMD	E	201	7	3,5,5	0.36	0	4,5,5	0.49	0
11	93X	D	505	-	30,30,30	6.24	11 (36%)	40,43,43	3.97	12 (30%)
9	GDP	D	501	-	24,30,30	1.35	3 (12%)	31,47,47	2.00	8 (25%)
7	GOL	D	503	-	5,5,5	0.33	0	5,5,5	0.38	0
7	GOL	B	505	-	5,5,5	0.38	0	5,5,5	0.58	0
7	GOL	C	505	-	5,5,5	0.42	0	5,5,5	0.09	0
13	ACP	F	402	-	27,33,33	2.50	8 (29%)	32,52,52	1.56	5 (15%)
9	GDP	B	501	6	24,30,30	1.13	1 (4%)	31,47,47	1.91	8 (25%)
7	GOL	A	504	-	5,5,5	0.41	0	5,5,5	0.70	0
7	GOL	A	503	-	5,5,5	0.36	0	5,5,5	0.33	0
12	IMD	C	508	-	3,5,5	0.45	0	4,5,5	0.51	0
10	MES	B	507	-	12,12,12	2.16	1 (8%)	14,16,16	2.22	4 (28%)
5	GTP	C	502	6	26,34,34	1.11	2 (7%)	33,54,54	1.73	7 (21%)
7	GOL	A	506	-	5,5,5	0.38	0	5,5,5	0.40	0
11	93X	B	508	-	30,30,30	6.16	8 (26%)	40,43,43	4.17	15 (37%)
5	GTP	A	501	6	26,34,34	0.99	1 (3%)	33,54,54	1.71	6 (18%)
7	GOL	B	503	-	5,5,5	0.36	0	5,5,5	0.23	0
12	IMD	C	509	-	3,5,5	0.43	0	4,5,5	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	C	506	-	5,5,5	0.54	0	5,5,5	0.57	0
7	GOL	C	501	-	5,5,5	0.36	0	5,5,5	0.31	0

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
7	GOL	B	504	-	-	2/4/4/4	-
7	GOL	D	504	12	-	2/4/4/4	-
7	GOL	C	504	-	-	2/4/4/4	-
12	IMD	E	201	7	-	-	0/1/1/1
11	93X	D	505	-	-	3/18/34/34	0/3/3/3
9	GDP	D	501	-	-	5/12/32/32	0/3/3/3
7	GOL	D	503	-	-	0/4/4/4	-
12	IMD	C	508	-	-	-	0/1/1/1
7	GOL	C	505	-	-	4/4/4/4	-
13	ACP	F	402	-	-	3/15/38/38	0/3/3/3
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
7	GOL	A	504	-	-	4/4/4/4	-
7	GOL	A	503	-	-	4/4/4/4	-
7	GOL	B	505	-	-	4/4/4/4	-
10	MES	B	507	-	-	0/6/14/14	0/1/1/1
5	GTP	C	502	6	-	5/18/38/38	0/3/3/3
7	GOL	A	506	-	-	4/4/4/4	-
11	93X	B	508	-	-	3/18/34/34	0/3/3/3
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3
7	GOL	B	503	-	-	4/4/4/4	-
12	IMD	C	509	-	-	-	0/1/1/1
7	GOL	C	506	-	-	4/4/4/4	-
7	GOL	C	501	-	-	1/4/4/4	-

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	505	93X	C4-N1	24.39	1.75	1.37
11	B	508	93X	C4-N1	24.01	1.74	1.37

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	508	93X	C3-C2	-21.86	1.34	1.57
11	D	505	93X	C3-C2	-21.27	1.35	1.57
13	F	402	ACP	PB-O3A	7.66	1.66	1.58

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	508	93X	C2-N1-C4	-13.19	82.45	95.27
11	D	505	93X	C2-N1-C4	-12.84	82.79	95.27
11	B	508	93X	C3-C2-N1	12.43	98.01	86.56
11	D	505	93X	C3-C2-N1	11.63	97.28	86.56
11	D	505	93X	C3-C4-N1	-10.99	81.99	93.08

There are no chirality outliers.

5 of 62 torsion outliers are listed below:

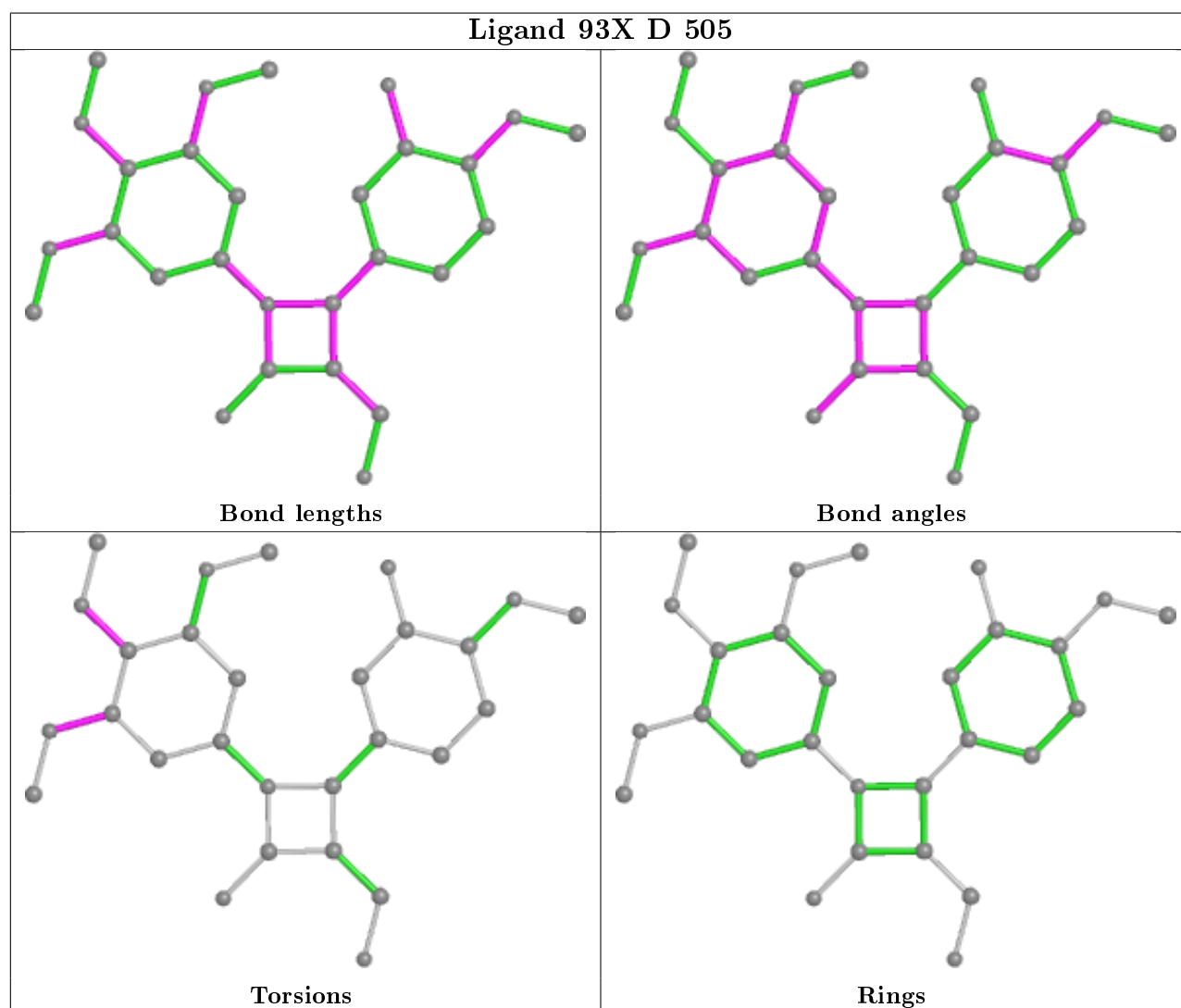
Mol	Chain	Res	Type	Atoms
7	D	504	GOL	O1-C1-C2-C3
7	C	504	GOL	O1-C1-C2-O2
7	C	504	GOL	O1-C1-C2-C3
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A

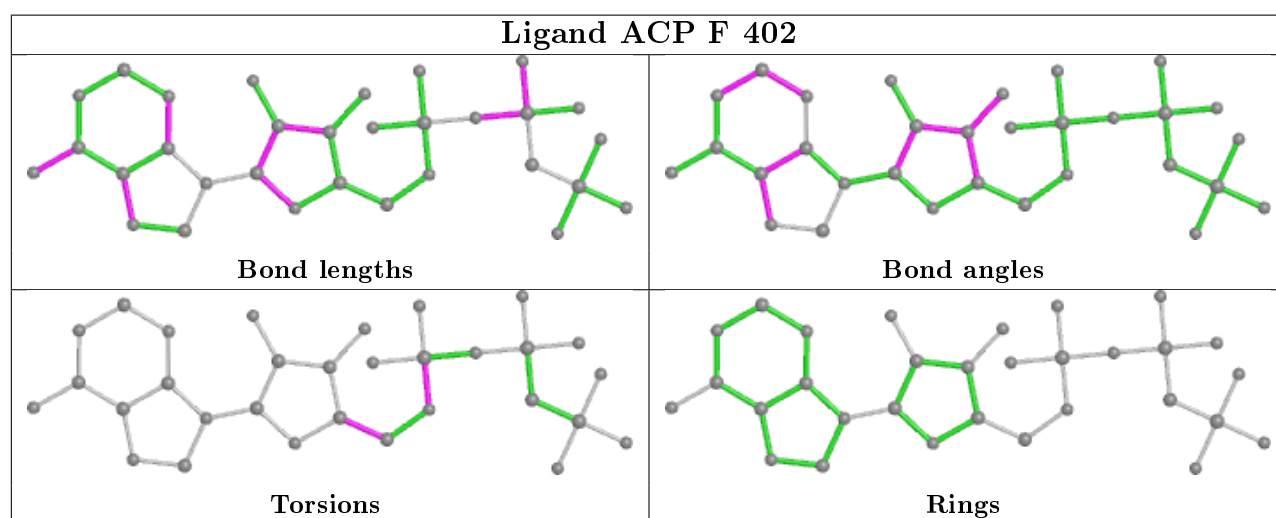
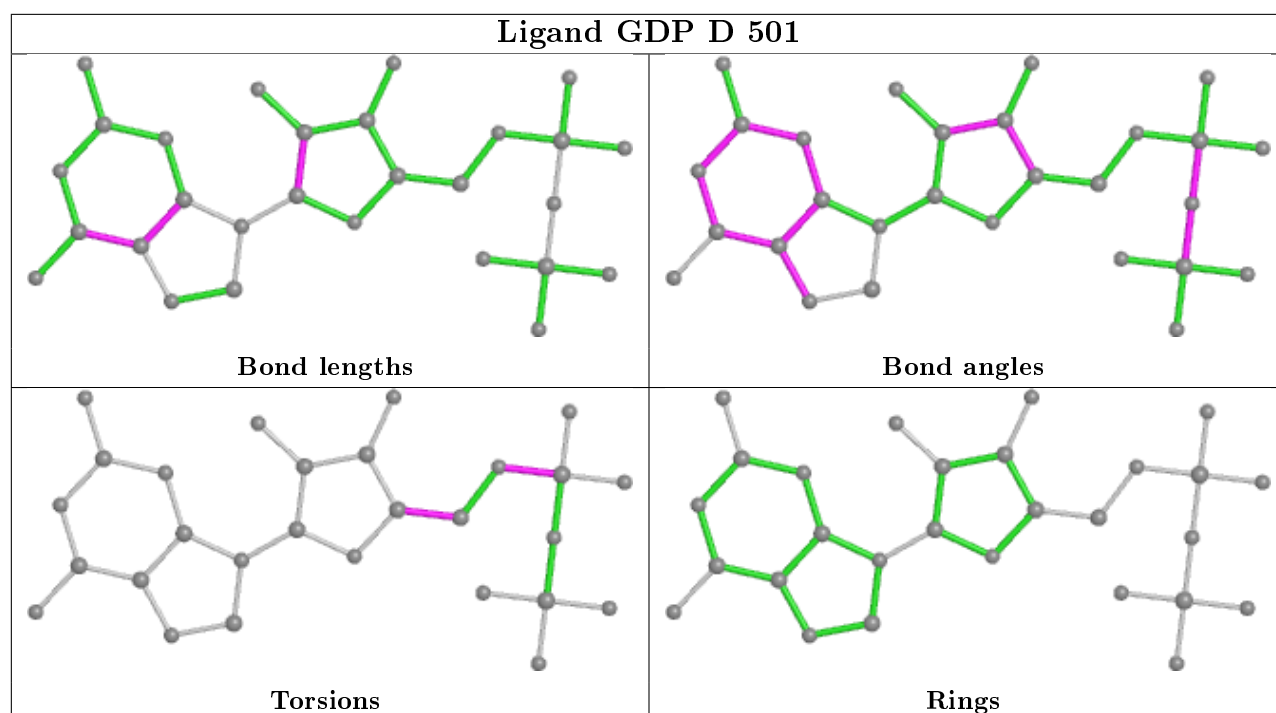
There are no ring outliers.

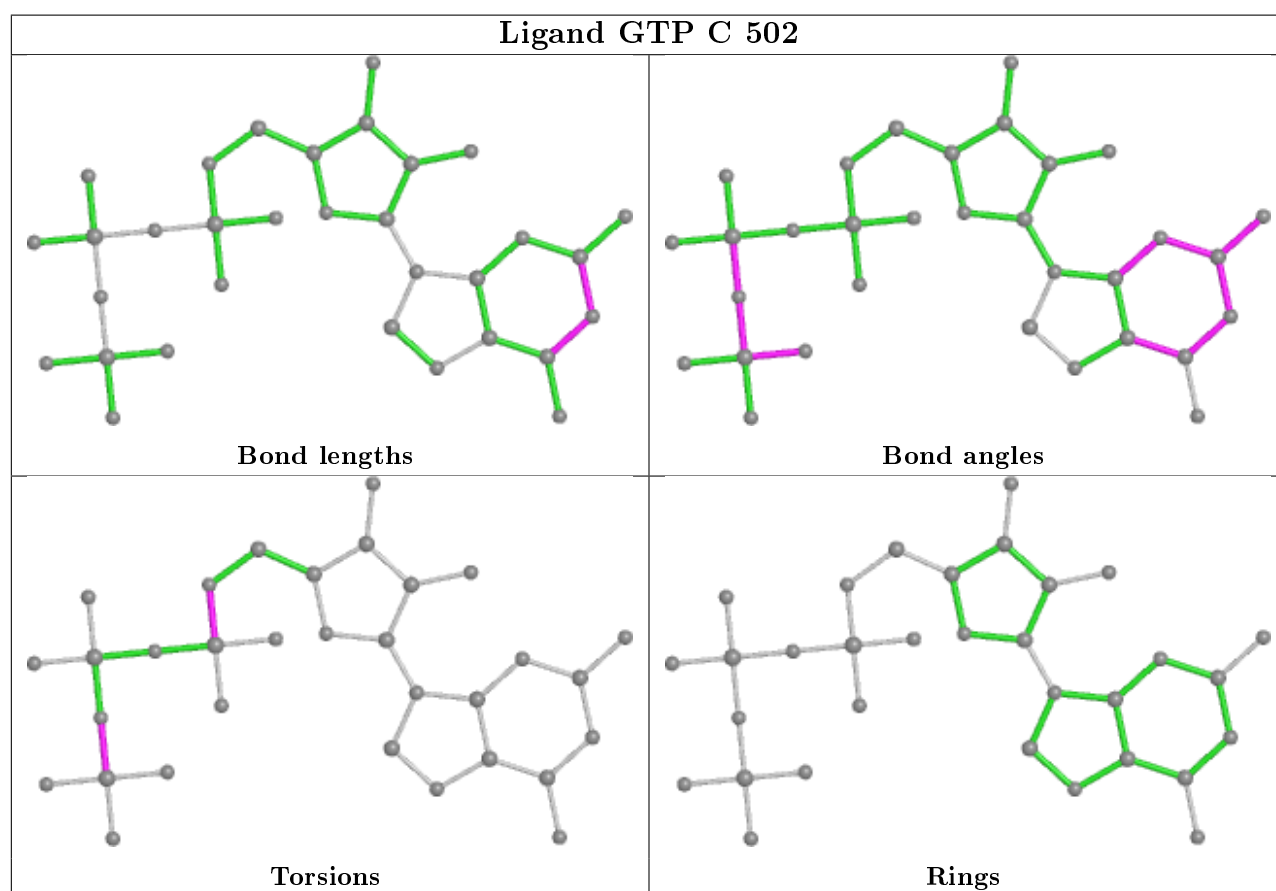
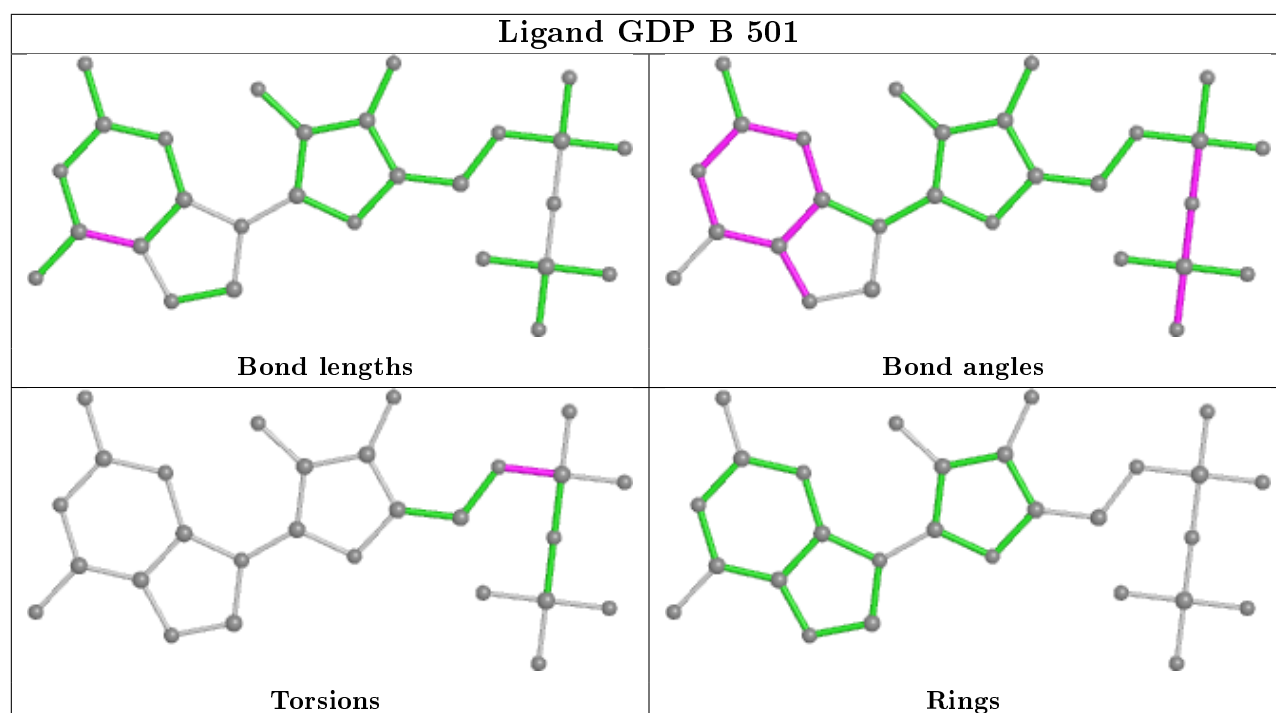
14 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	201	IMD	2	0
11	D	505	93X	1	0
9	D	501	GDP	2	0
7	D	503	GOL	2	0
7	B	505	GOL	6	0
13	F	402	ACP	1	0
9	B	501	GDP	1	0
12	C	508	IMD	2	0
5	C	502	GTP	2	0
7	A	506	GOL	1	0
5	A	501	GTP	2	0
12	C	509	IMD	1	0
7	C	506	GOL	1	0
7	C	501	GOL	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.

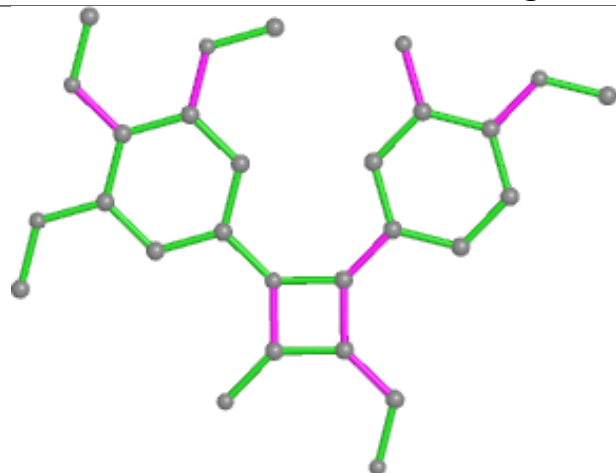




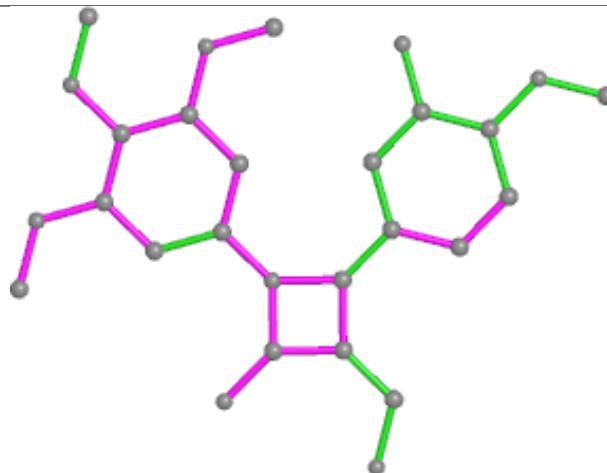




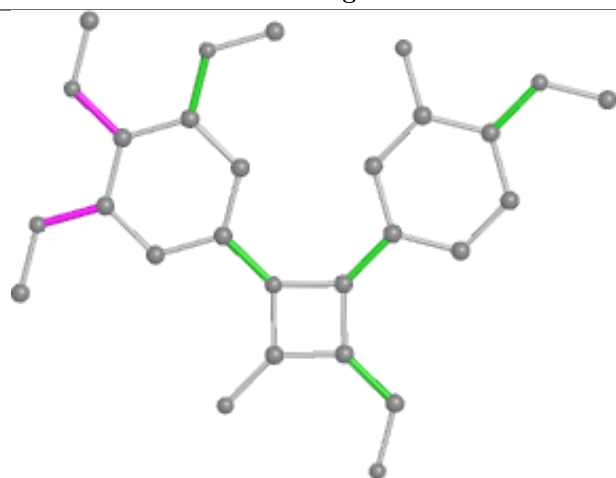
## Ligand 93X B 508



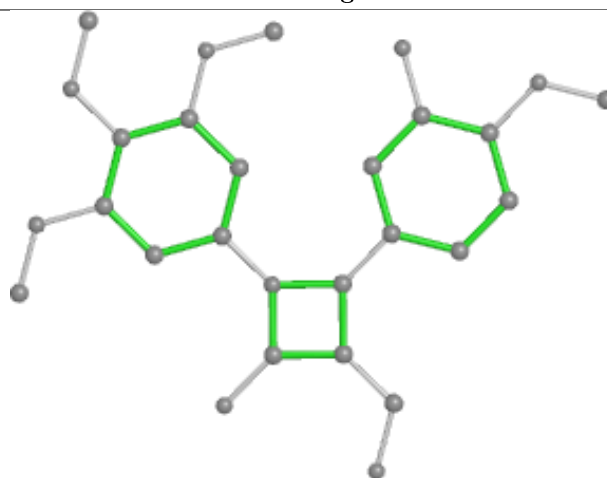
Bond lengths



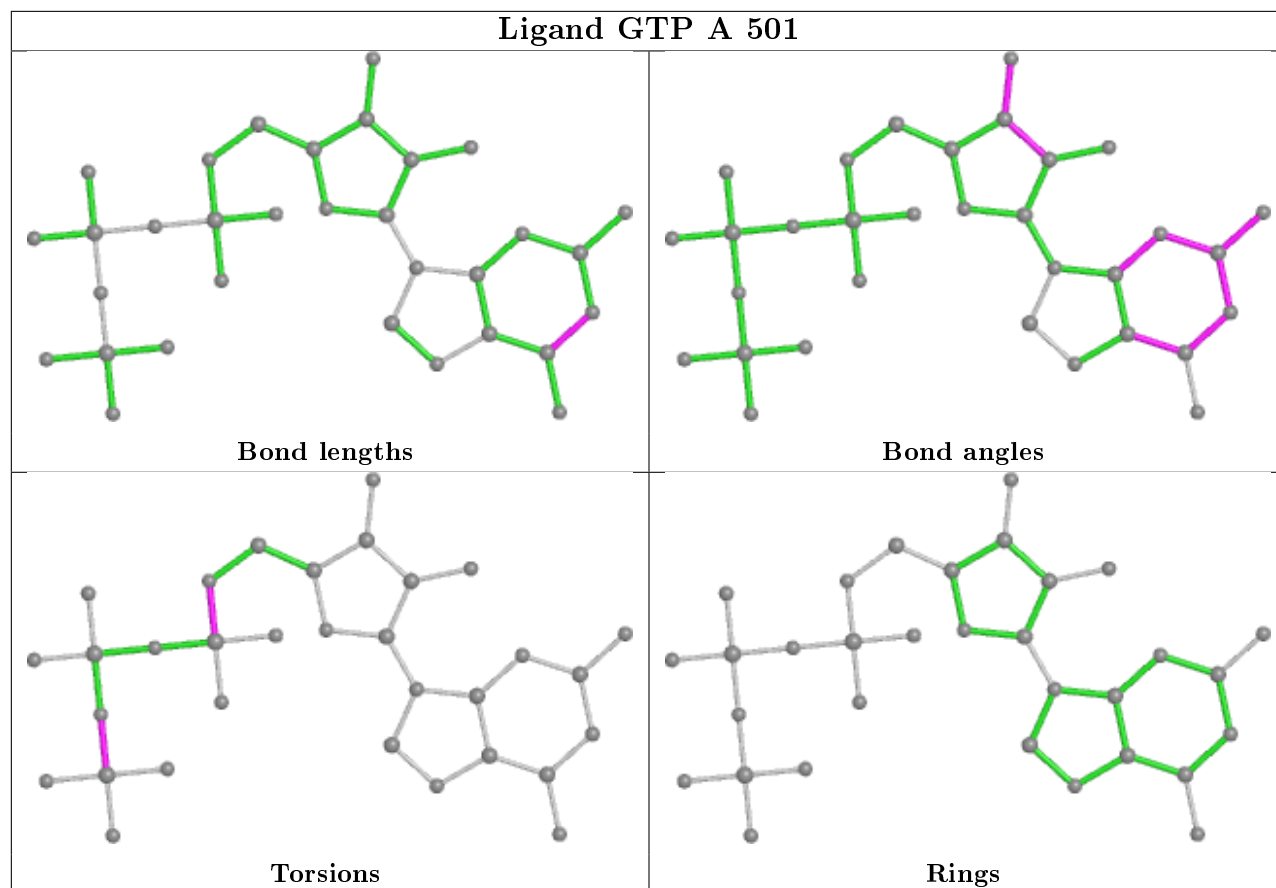
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	439/451 (97%)	0.34	15 (3%) 45 54	48, 71, 104, 153	0
1	C	440/451 (97%)	0.02	8 (1%) 68 75	40, 55, 82, 106	0
2	B	424/445 (95%)	0.28	20 (4%) 31 40	38, 64, 102, 176	0
2	D	421/445 (94%)	0.59	39 (9%) 8 12	48, 85, 122, 181	4 (0%)
3	E	120/189 (63%)	0.35	7 (5%) 23 29	50, 80, 115, 154	0
4	F	317/378 (83%)	1.55	111 (35%) 0 0	55, 100, 170, 220	0
All	All	2161/2359 (91%)	0.49	200 (9%) 8 12	38, 73, 124, 220	4 (0%)

The worst 5 of 200 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	244	CYS	15.4
4	F	245	ILE	10.9
4	F	133	ALA	9.2
4	F	249	TYR	8.4
4	F	248	GLU	7.6

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

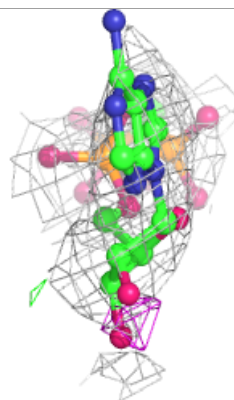
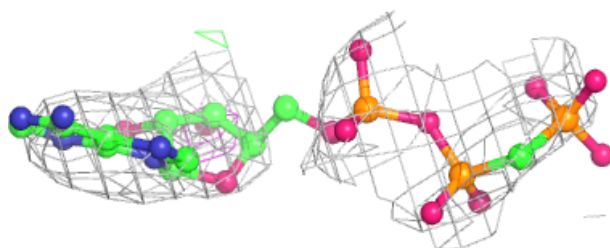
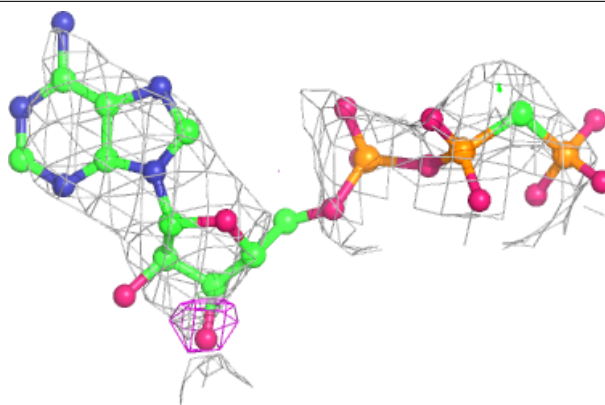
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
7	GOL	A	504	6/6	0.50	0.45	111,113,114,115	0
7	GOL	B	505	6/6	0.58	0.77	100,107,115,123	0
7	GOL	D	503	6/6	0.66	0.57	139,142,144,145	0
6	MG	D	502	1/1	0.68	0.13	95,95,95,95	0
7	GOL	B	504	6/6	0.70	0.38	77,95,99,102	0
13	ACP	F	402	31/31	0.70	0.33	86,147,176,178	0
7	GOL	B	503	6/6	0.71	0.37	82,96,105,110	0
7	GOL	C	505	6/6	0.74	0.74	108,114,117,119	0
7	GOL	A	506	6/6	0.74	0.26	86,93,98,101	0
7	GOL	C	501	6/6	0.80	0.36	78,88,91,93	0
12	IMD	C	509	5/5	0.82	0.36	110,112,113,114	0
7	GOL	D	504	6/6	0.83	0.31	101,109,113,118	0
7	GOL	C	504	6/6	0.85	0.23	91,98,99,101	0
7	GOL	C	506	6/6	0.86	0.23	79,86,88,88	0
12	IMD	E	201	5/5	0.86	0.33	123,124,128,129	0
7	GOL	A	503	6/6	0.89	0.21	89,92,95,99	0
9	GDP	D	501	28/28	0.90	0.17	79,90,101,102	0
12	IMD	C	508	5/5	0.91	0.18	66,73,74,78	0
8	CA	A	505	1/1	0.92	0.08	97,97,97,97	0
6	MG	F	401	1/1	0.92	0.23	119,119,119,119	0
6	MG	B	502	1/1	0.95	0.40	51,51,51,51	0
11	93X	B	508	28/28	0.95	0.24	34,62,74,83	0
11	93X	D	505	28/28	0.96	0.19	55,66,75,83	0
6	MG	C	503	1/1	0.96	0.28	52,52,52,52	0
10	MES	B	507	12/12	0.96	0.15	52,69,81,85	0
8	CA	C	507	1/1	0.96	0.07	112,112,112,112	0
9	GDP	B	501	28/28	0.97	0.21	36,46,54,66	0
6	MG	A	502	1/1	0.98	0.26	80,80,80,80	0
5	GTP	A	501	32/32	0.98	0.23	49,55,60,62	0
8	CA	B	506	1/1	0.98	0.08	118,118,118,118	0
5	GTP	C	502	32/32	0.98	0.20	43,51,57,60	0

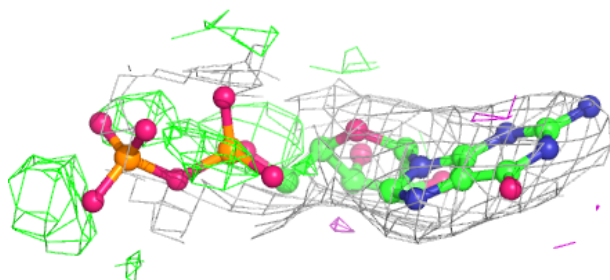
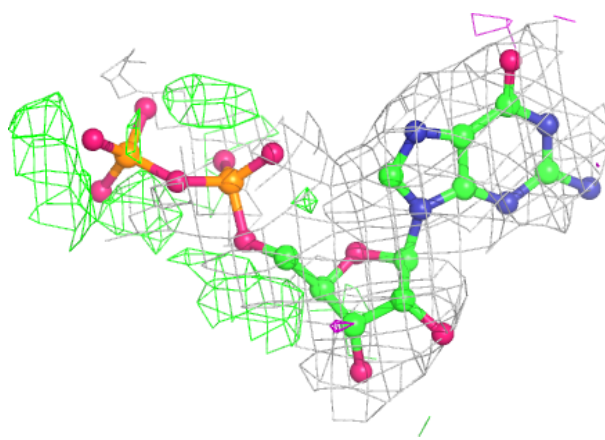
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ACP F 402:**

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

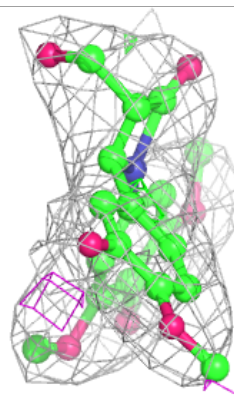
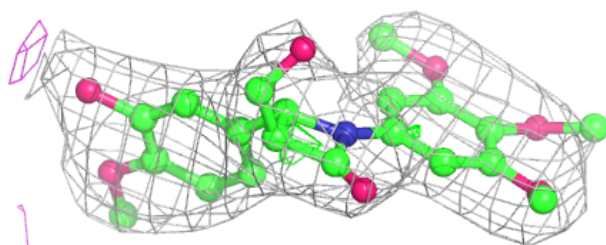
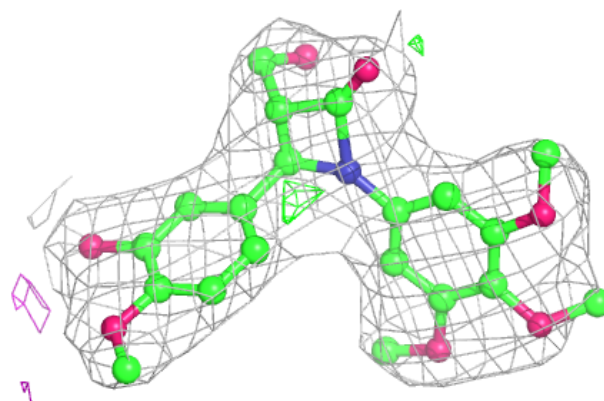
**Electron density around GDP D 501:**

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

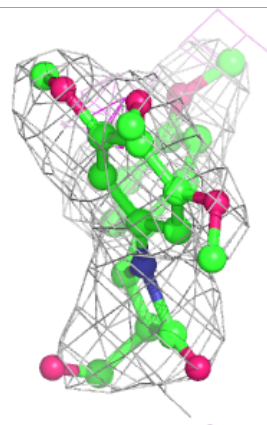
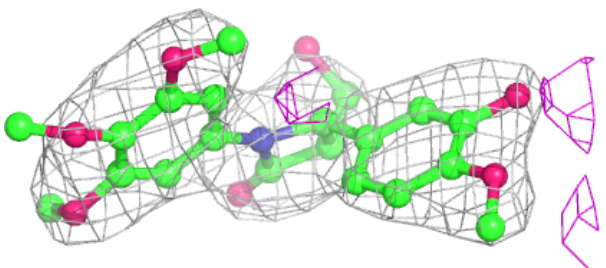
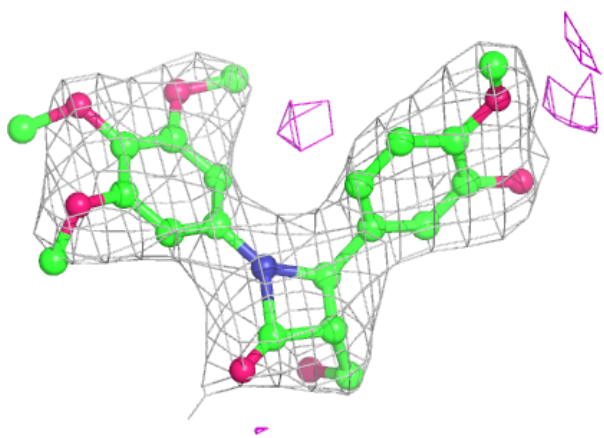


**Electron density around 93X B 508:**

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

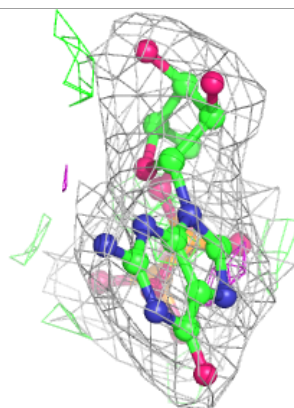
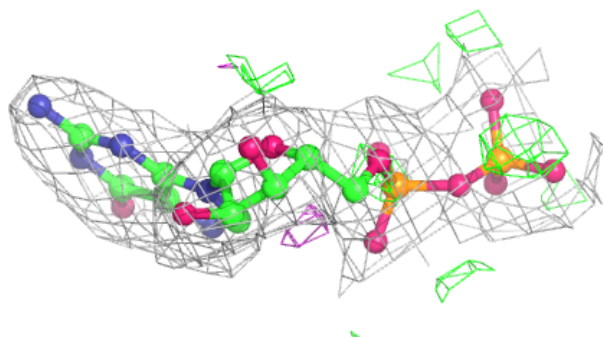
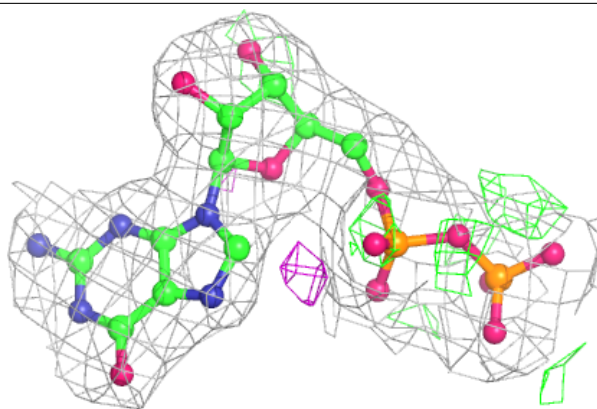
**Electron density around 93X D 505:**

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

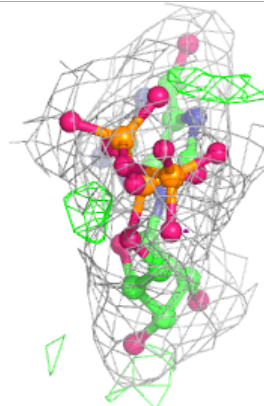
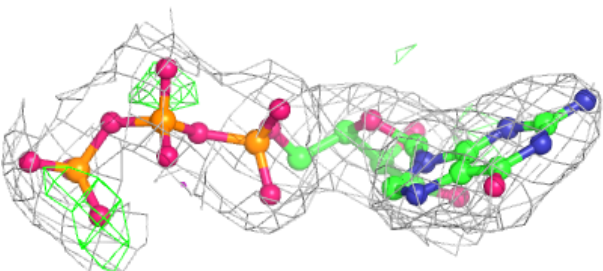
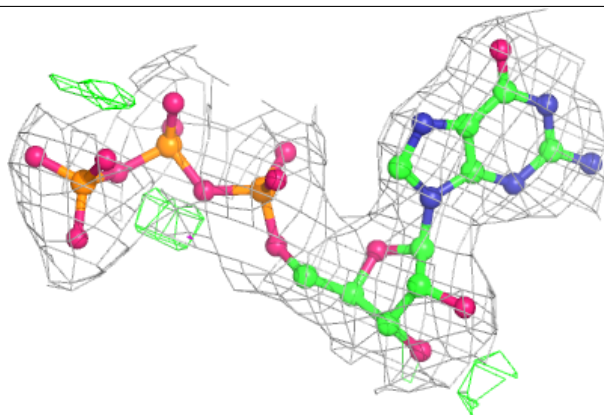


**Electron density around GDP B 501:**

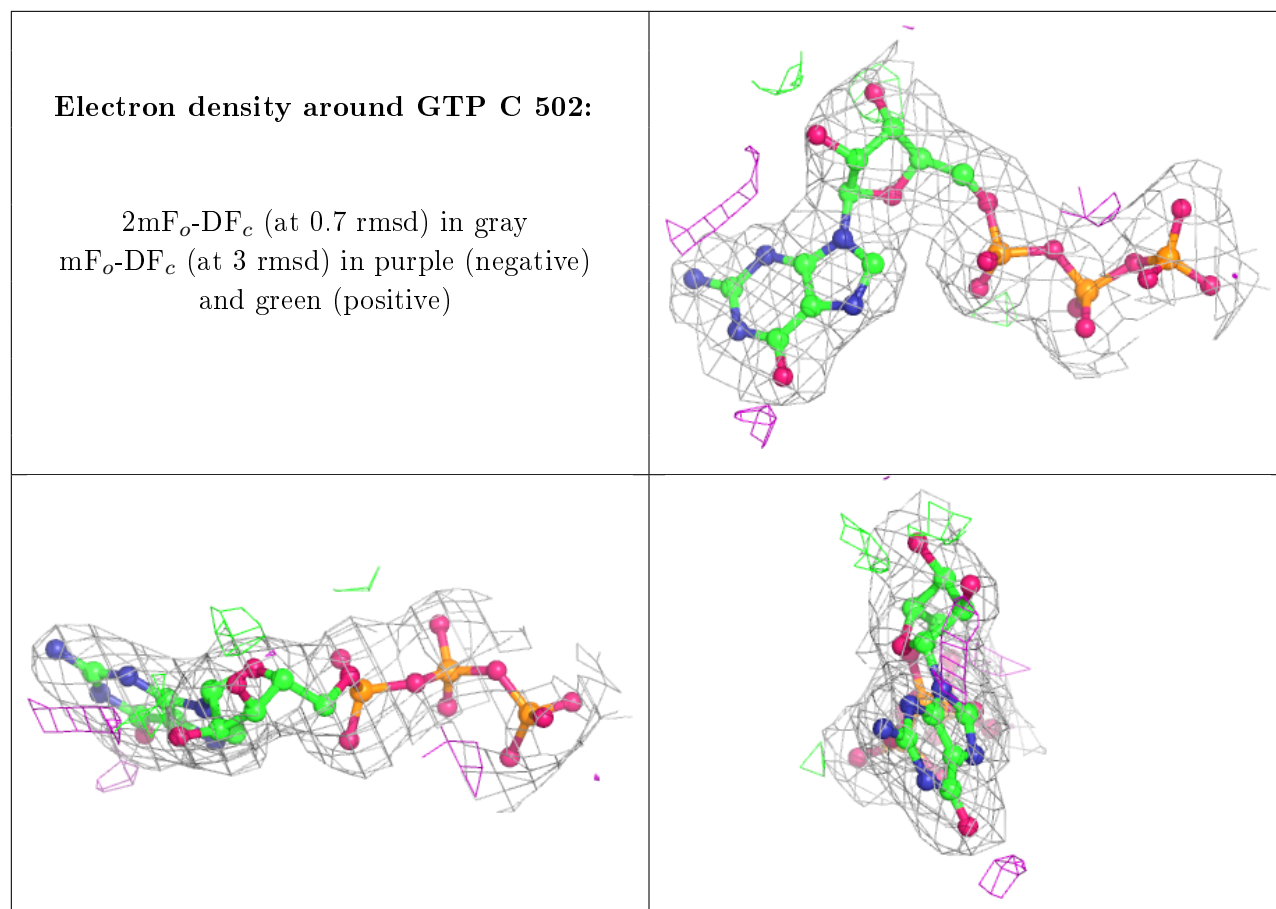
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**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)







## 6.5 Other polymers ⓘ

There are no such residues in this entry.