



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 15, 2022 – 03:20 pm GMT

PDB ID : 6Y4N  
Title : Structure of Tubulin Tyrosine Ligase in Complex with Tb116  
Authors : Gavrilyuk, J.; Nocek, B.; Rigol, S.; Nicolaou, K.C.; Stoll, V.  
Deposited on : 2020-02-21  
Resolution : 2.85 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.

The types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

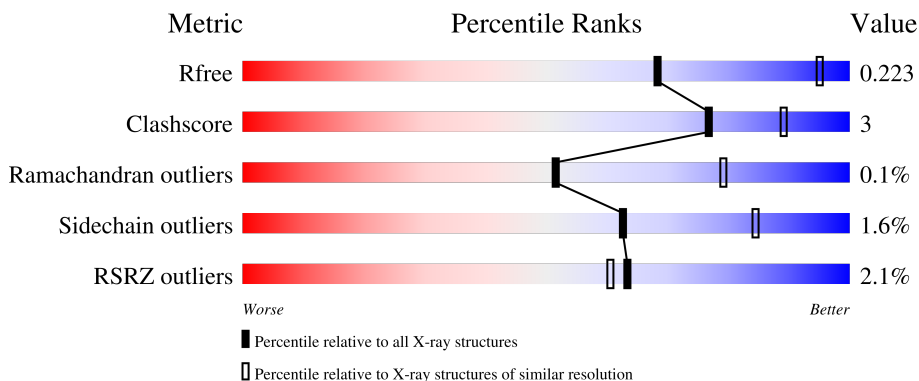
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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.



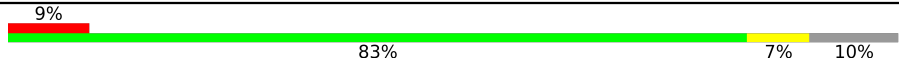
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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  $\geq 3$ , 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	93%
1	C	451	88% 9%
2	B	445	89% 8%
2	D	445	2% 90% 6%
3	E	143	80% 6% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '9%', a large green segment labeled '83%', a yellow segment labeled '7%', and a grey segment on the right labeled '10%'.</p>

## 2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 18400 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
			Total	C	N	O	S			
1	A	439	Total	C	N	O	S	0	0	0
			3430	2170	583	655	22			
1	C	440	Total	C	N	O	S	0	5	0
			3484	2202	594	665	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	431	Total	C	N	O	S	0	2	0
			3401	2134	582	658	27			
2	D	428	Total	C	N	O	S	0	1	0
			3367	2112	578	651	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	47	MET	-	expression tag	UNP P63043
E	48	ALA	-	expression tag	UNP P63043

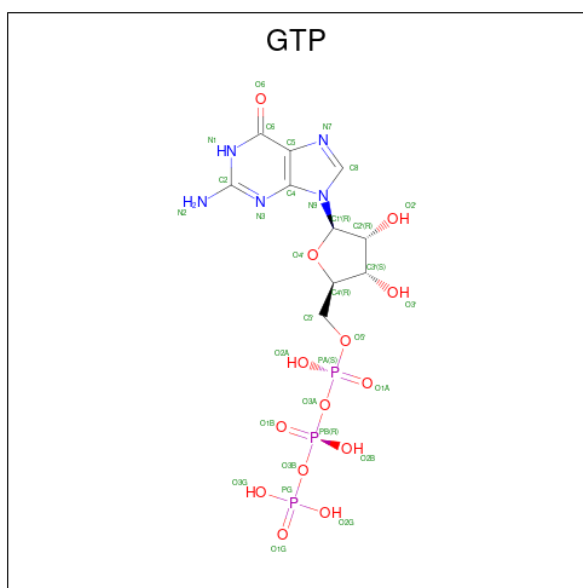
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	346	Total	C	N	O	S	0	1	0
			2851	1826	488	522	15			

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
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
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		
5	D	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
			Total	Mg		
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



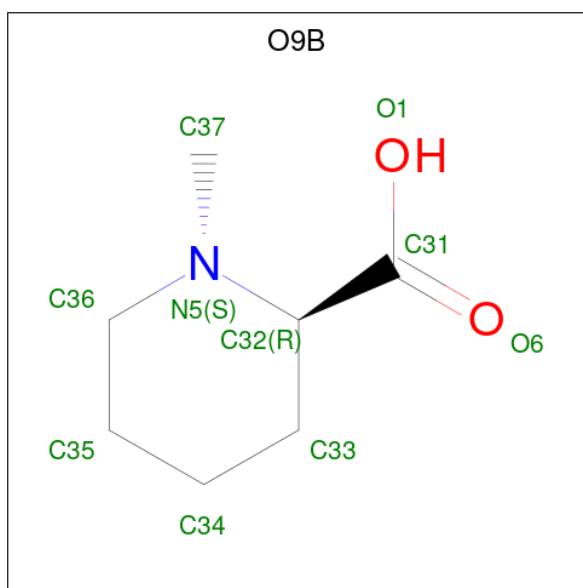
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



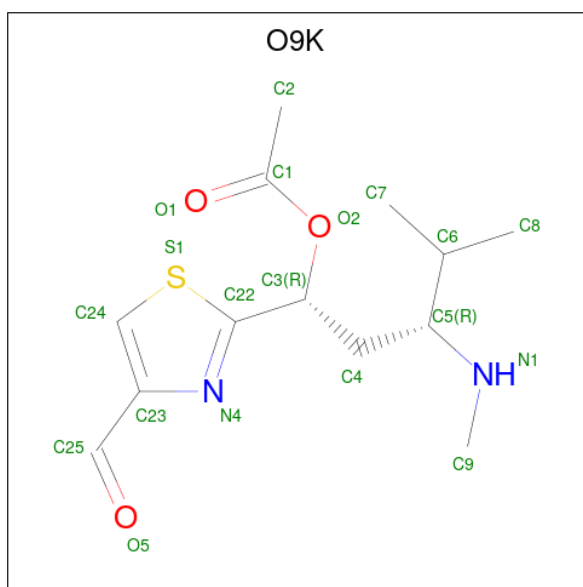
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
9	B	1	12	6	1	4	1	0	0

- Molecule 10 is (2 {R})-1-methylpiperidine-2-carboxylic acid (three-letter code: O9B) (formula:  $C_7H_{13}NO_2$ ).



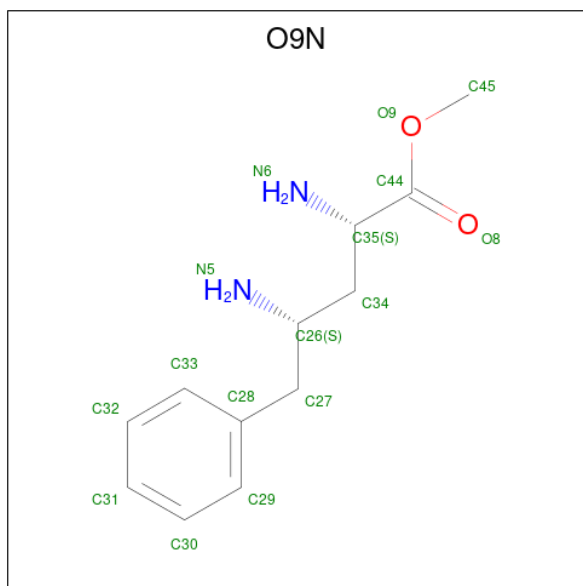
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	B	1	9	7	1	1	0	0

- Molecule 11 is [(1 {R},3 {R})-1-(4-methanoyl-1,3-thiazol-2-yl)-4-methyl-3-(methylamino)pentyl] ethanoate (three-letter code: O9K) (formula:  $C_{13}H_{20}N_2O_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
11	B	1	19	13	2	3	1	0	0

- Molecule 12 is methyl (2 {S},4 {S})-2,4-bis(azanyl)-5-phenyl-pentanoate (three-letter code: O9N) (formula:  $C_{12}H_{18}N_2O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
12	B	1	16	12	2	2	0	0

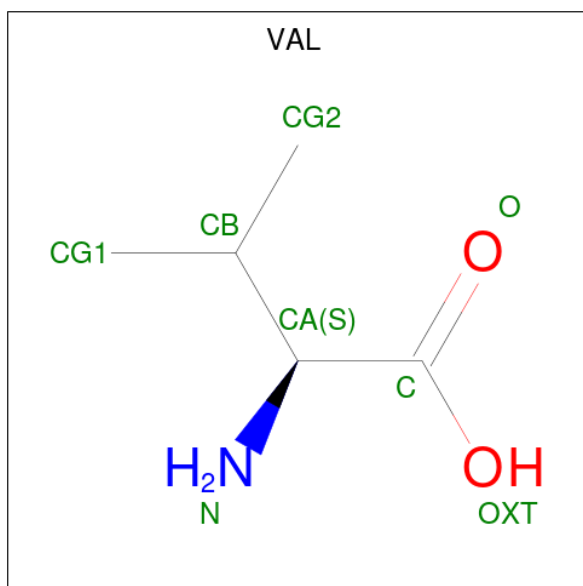
- Molecule 13 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).





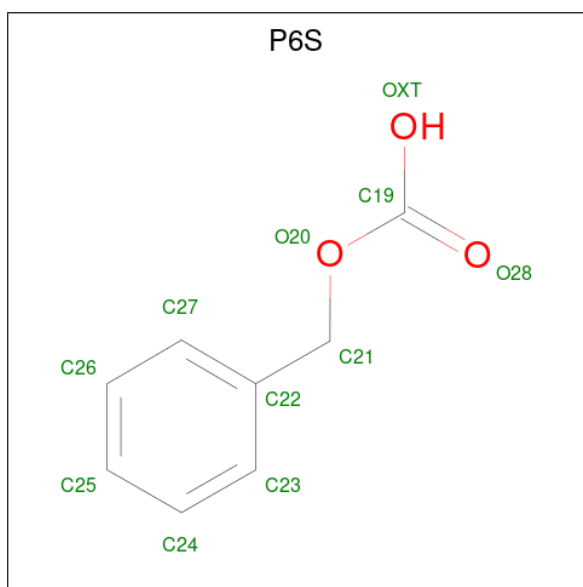
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 14 is VALINE (three-letter code: VAL) (formula:  $C_5H_{11}NO_2$ ).



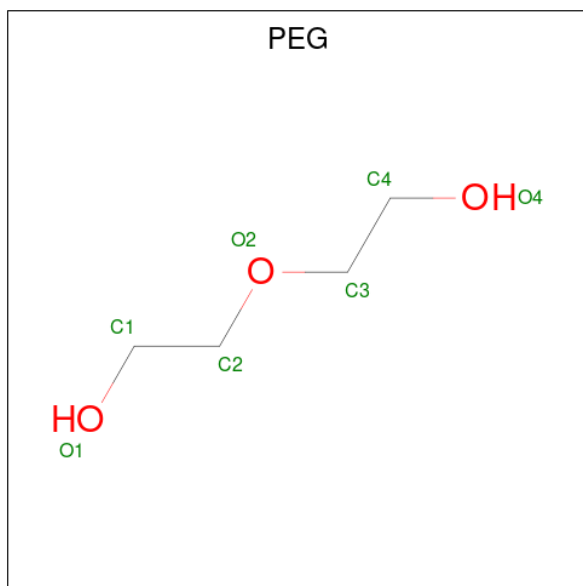
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 15 is benzyl hydrogen carbonate (three-letter code: P6S) (formula:  $C_8H_8O_3$ ).



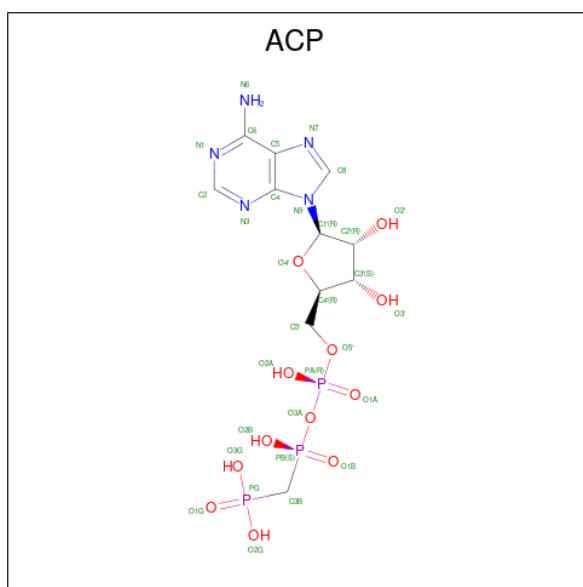
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C	O	0	0
			10	8	2		

- Molecule 16 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 17 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
			Total	C	N	O	P		
17	F	1	31	11	5	12	3	0	0

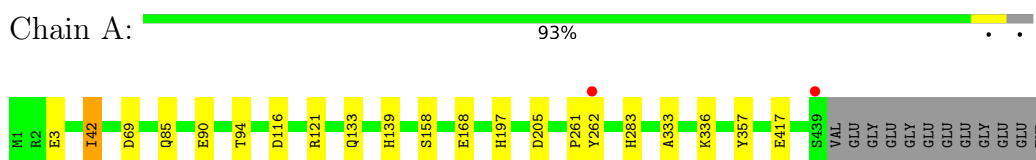
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	116	Total	O	0	0
			116	116		
18	B	143	Total	O	0	0
			143	143		
18	C	174	Total	O	0	0
			174	174		
18	D	67	Total	O	0	1
			67	67		
18	E	31	Total	O	0	0
			31	31		
18	F	70	Total	O	0	0
			70	70		

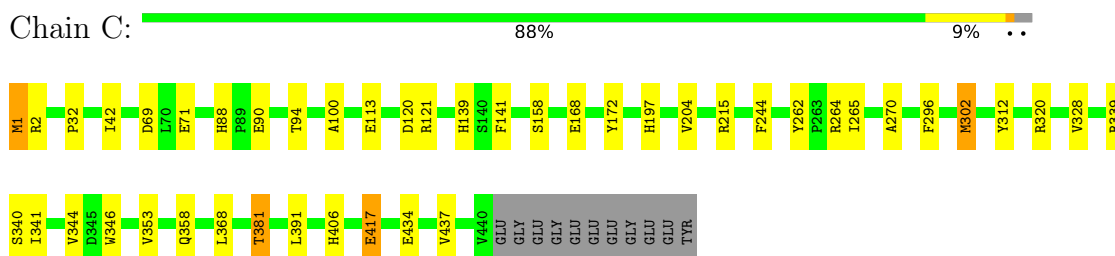
### 3 Residue-property plots [i](#)

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.

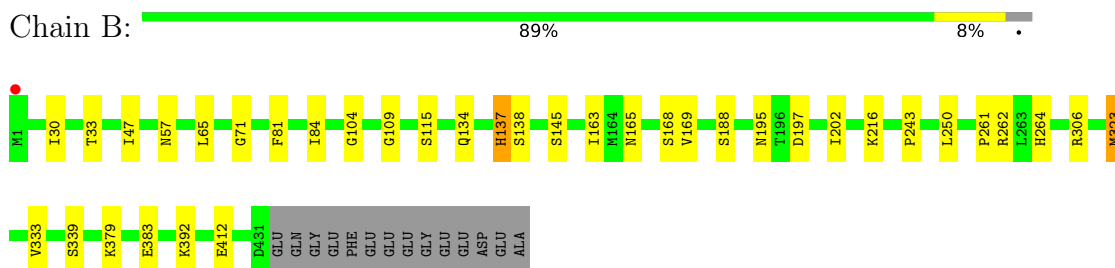
- Molecule 1: Tubulin alpha-1B chain



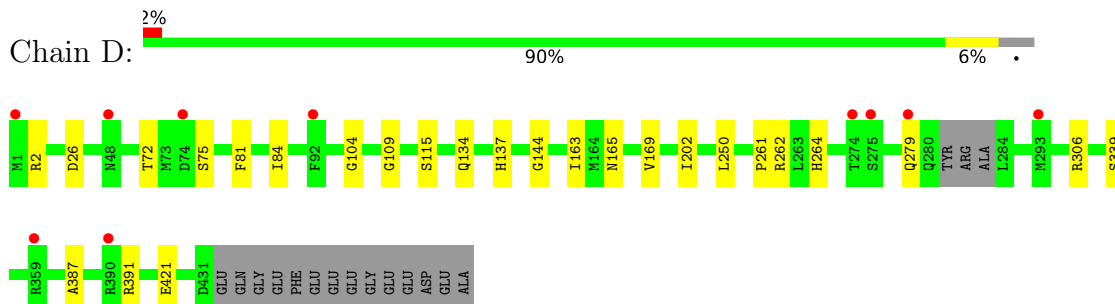
- Molecule 1: Tubulin alpha-1B chain




- Molecule 2: Tubulin beta chain

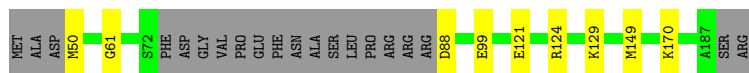


- Molecule 2: Tubulin beta chain




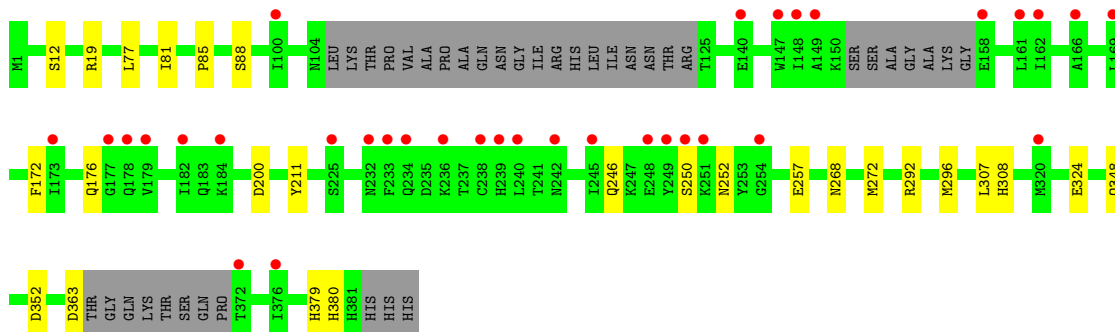
- Molecule 3: Stathmin-4

Chain E:  80% 6% 14%



- Molecule 4: Tubulin-Tyrosine Ligase

Chain F:  9% 83% 7% 10%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.28Å 154.97Å 183.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.93 – 2.85 78.93 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (78.93-2.85) 100.0 (78.93-2.85)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.86Å)	Xtrriage
Refinement program	BUSTER 2.11.7 (6-FEB-2020)	Depositor
R, $R_{free}$	0.183 , 0.220 0.183 , 0.223	Depositor DCC
$R_{free}$ test set	3527 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.8	Xtrriage
Anisotropy	0.328	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: GTP, P6S, PEG, O9N, O9B, O9K, MES, PGE, CA, ACP, GDP, MG

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	0/3508	0.61	0/4762
1	C	0.45	0/3563	0.61	0/4837
2	B	0.43	0/3476	0.59	0/4709
2	D	0.40	0/3440	0.58	0/4659
3	E	0.44	0/1022	0.53	0/1356
4	F	0.42	0/2916	0.58	0/3939
All	All	0.43	0/17925	0.59	0/24262

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	3430	0	3339	15	0
1	C	3484	0	3386	31	0
2	B	3401	0	3275	24	0
2	D	3367	0	3246	15	0
3	E	1014	0	1029	9	0
4	F	2851	0	2808	13	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
5	D	32	0	12	0	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	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
9	B	12	0	13	2	0
10	B	9	0	0	0	0
11	B	19	0	0	0	0
12	B	16	0	0	0	0
13	C	10	0	14	4	0
14	C	7	0	8	0	0
15	C	10	0	0	0	0
16	D	7	0	10	0	0
17	F	31	0	14	0	0
18	A	116	0	0	8	0
18	B	143	0	0	11	0
18	C	174	0	0	11	0
18	D	67	0	0	6	0
18	E	31	0	0	7	0
18	F	70	0	0	4	0
All	All	18400	0	17190	106	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 3.

The worst 5 of 106 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)
3:E:149:MET:HB3	18:E:223:HOH:O	1.42	1.14
1:C:215:ARG:HB2	18:C:1208:HOH:O	1.68	0.91
3:E:149:MET:CB	18:E:223:HOH:O	2.06	0.88
1:C:113:GLU:HG3	18:C:1197:HOH:O	1.72	0.88
1:A:261:PRO:HD2	18:A:1147:HOH:O	1.74	0.86

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	437/451 (97%)	422 (97%)	15 (3%)	0	100	100
1	C	443/451 (98%)	430 (97%)	13 (3%)	0	100	100
2	B	431/445 (97%)	418 (97%)	12 (3%)	1 (0%)	47	75
2	D	425/445 (96%)	412 (97%)	12 (3%)	1 (0%)	47	75
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	339/384 (88%)	325 (96%)	14 (4%)	0	100	100
All	All	2194/2319 (95%)	2126 (97%)	66 (3%)	2 (0%)	51	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	279	GLN
2	B	71	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/379 (98%)	367 (99%)	3 (1%)	81	93
1	C	376/379 (99%)	365 (97%)	11 (3%)	42	72
2	B	372/381 (98%)	366 (98%)	6 (2%)	62	84
2	D	369/381 (97%)	367 (100%)	2 (0%)	88	96
3	E	110/127 (87%)	108 (98%)	2 (2%)	59	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	F	313/342 (92%)	306 (98%)	7 (2%)	52 79
All	All	1910/1989 (96%)	1879 (98%)	31 (2%)	62 84

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	302[B]	MET
4	F	252	ASN
1	C	368	LEU
4	F	324	GLU
4	F	12	SER

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

Mol	Chain	Res	Type
2	D	137	HIS
2	D	264	HIS
4	F	260	ASN
4	F	180	HIS
2	B	190	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 7 are monoatomic - leaving 13 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
8	GDP	B	1001	6	24,30,30	0.70	1 (4%)	30,47,47	0.58	0
10	O9B	B	1004	14	7,9,10	0.48	0	7,11,13	0.84	0
12	O9N	B	1006	15,11	16,16,16	0.24	0	18,20,20	0.74	1 (5%)
17	ACP	F	1001	6	27,33,33	1.42	5 (18%)	32,52,52	1.26	5 (15%)
5	GTP	A	1001	6	26,34,34	0.89	1 (3%)	32,54,54	0.57	0
5	GTP	C	1001	6	26,34,34	0.89	1 (3%)	32,54,54	0.58	0
11	O9K	B	1005	14,12	16,19,19	0.28	0	12,25,25	0.98	1 (8%)
13	PGE	C	1004	-	9,9,9	0.24	0	8,8,8	0.28	0
5	GTP	D	1001	6	26,34,34	0.80	0	32,54,54	0.70	1 (3%)
14	VAL	C	1005	10,11	4,6,7	0.60	0	6,7,9	0.91	0
15	P6S	C	1006	12	9,10,11	0.23	0	10,11,13	0.24	0
16	PEG	D	1003	-	6,6,6	0.17	0	5,5,5	0.08	0
9	MES	B	1003	-	12,12,12	0.70	0	14,16,16	0.51	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
8	GDP	B	1001	6	-	4/12/32/32	0/3/3/3
10	O9B	B	1004	14	-	0/1/13/15	0/1/1/1
12	O9N	B	1006	15,11	-	2/14/14/14	0/1/1/1
17	ACP	F	1001	6	-	5/15/38/38	0/3/3/3
5	GTP	A	1001	6	-	7/18/38/38	0/3/3/3
5	GTP	C	1001	6	-	8/18/38/38	0/3/3/3
11	O9K	B	1005	14,12	-	1/14/20/20	0/1/1/1
13	PGE	C	1004	-	-	5/7/7/7	-
5	GTP	D	1001	6	-	3/18/38/38	0/3/3/3
14	VAL	C	1005	10,11	-	1/5/6/8	-
15	P6S	C	1006	12	-	1/4/4/5	0/1/1/1
16	PEG	D	1003	-	-	0/4/4/4	-
9	MES	B	1003	-	-	4/6/14/14	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	F	1001	ACP	PG-O2G	3.28	1.62	1.54
17	F	1001	ACP	PG-O3G	3.10	1.62	1.54
5	C	1001	GTP	C5-C6	-2.66	1.42	1.47
17	F	1001	ACP	PB-O3A	2.60	1.61	1.58
5	A	1001	GTP	C5-C6	-2.60	1.42	1.47

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	F	1001	ACP	N3-C2-N1	-3.60	123.05	128.68
5	D	1001	GTP	O5'-PA-O1A	2.38	118.36	109.07
17	F	1001	ACP	PB-O3A-PA	-2.28	125.33	132.56
17	F	1001	ACP	O2G-PG-O1G	-2.21	106.54	112.39
17	F	1001	ACP	C4-C5-N7	-2.20	107.11	109.40

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1001	GTP	C5'-O5'-PA-O1A
5	C	1001	GTP	C5'-O5'-PA-O1A
5	D	1001	GTP	C5'-O5'-PA-O1A
8	B	1001	GDP	C5'-O5'-PA-O1A
9	B	1003	MES	C8-C7-N4-C5

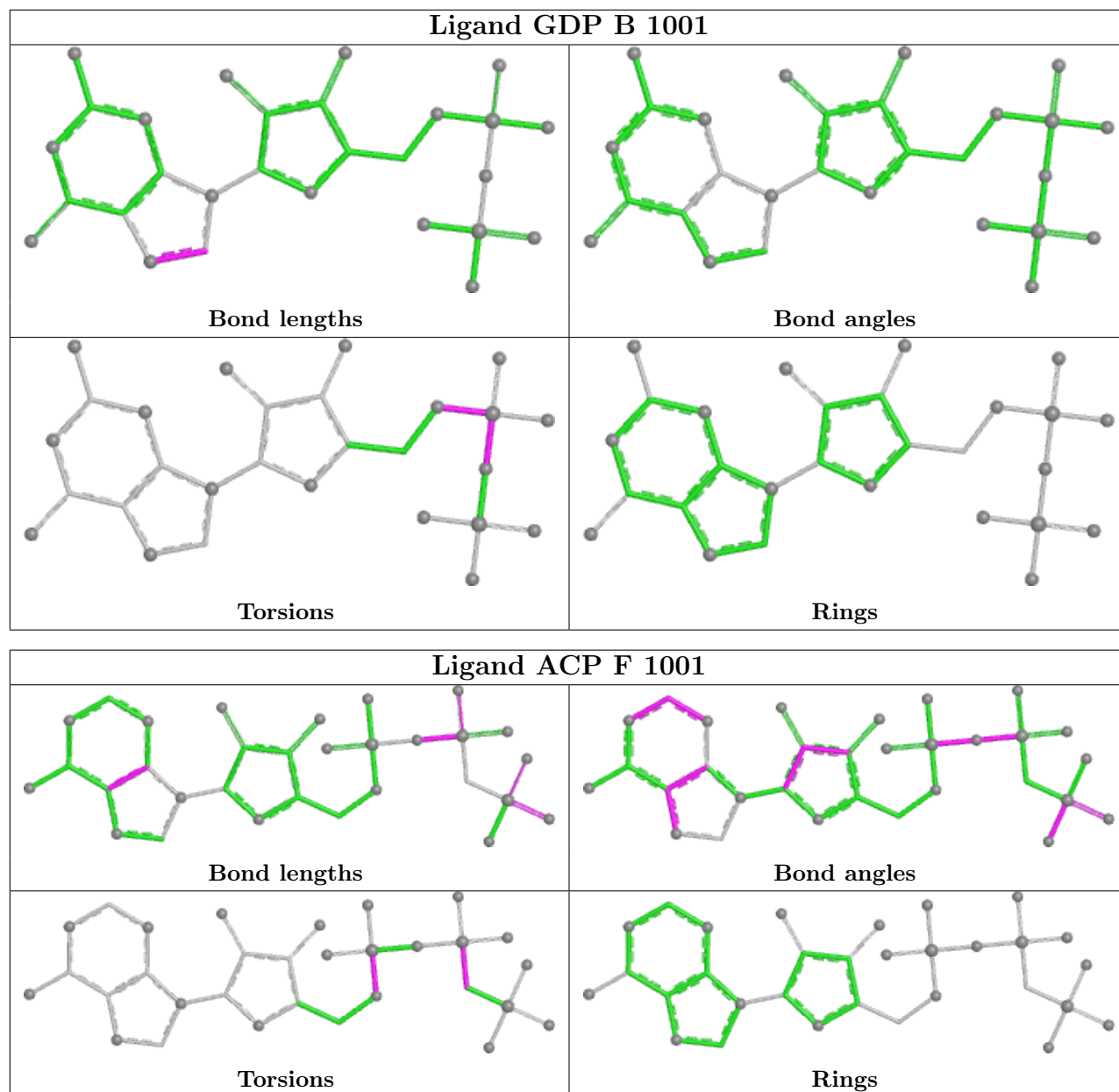
There are no ring outliers.

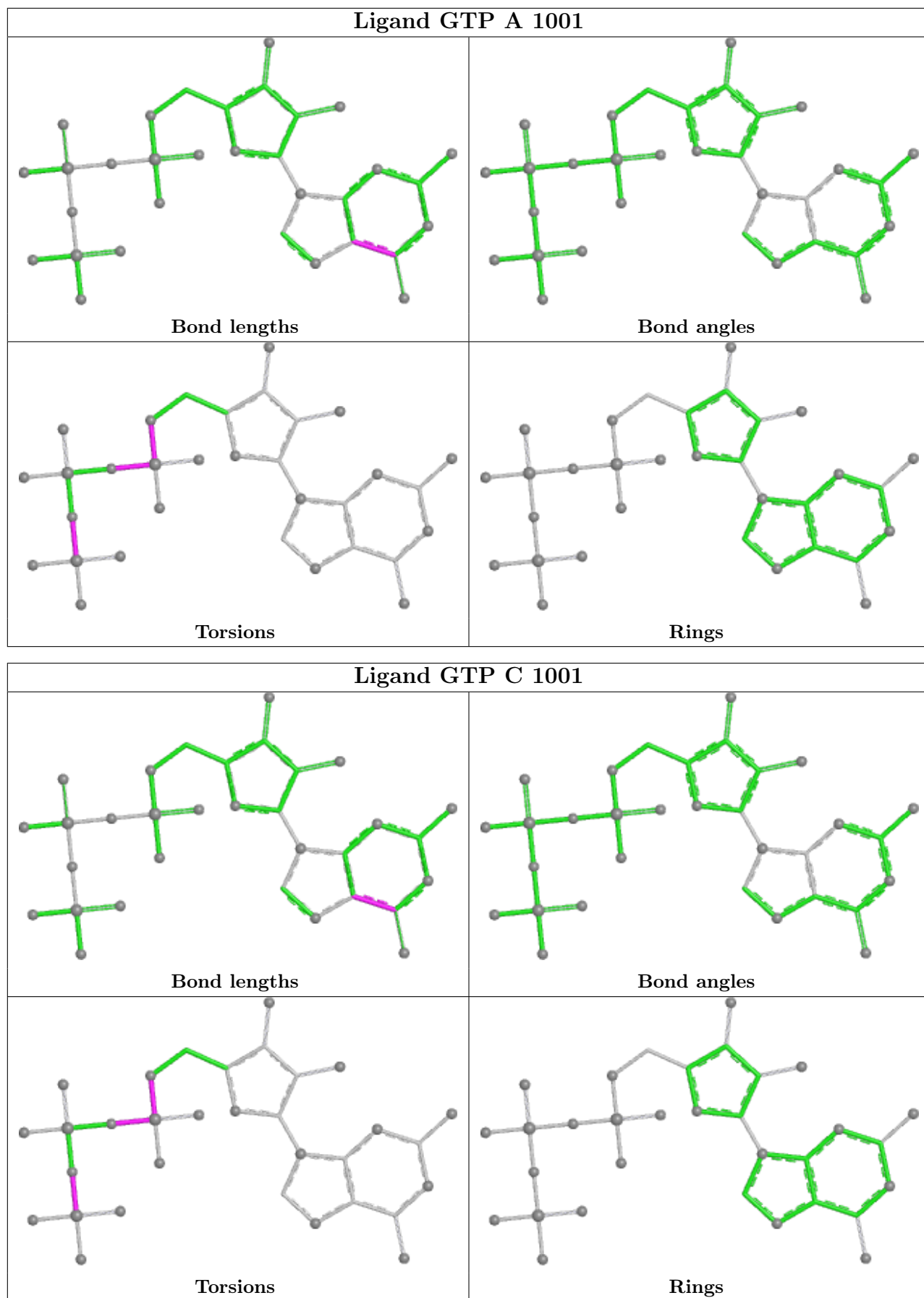
2 monomers are involved in 6 short contacts:

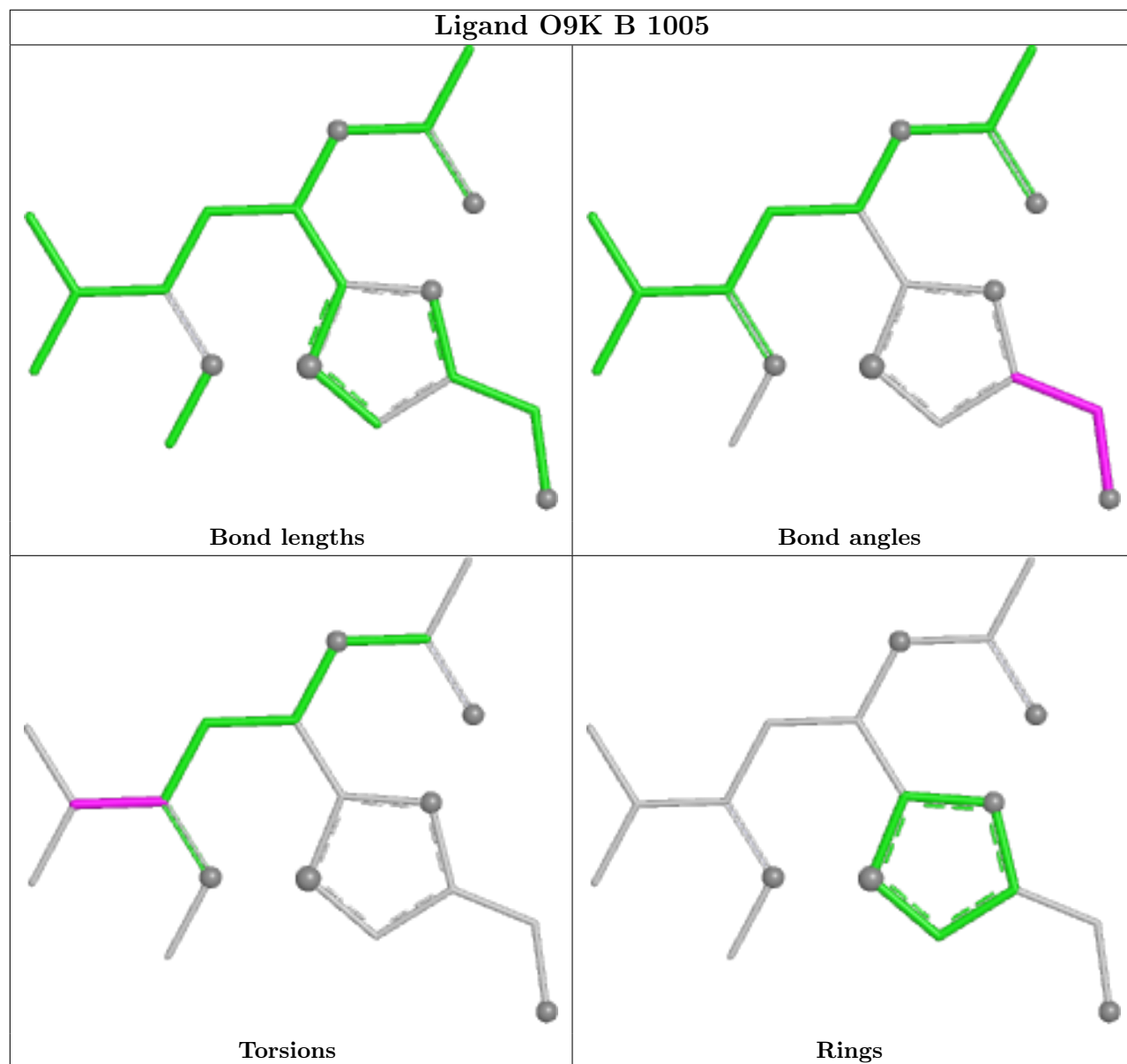
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	1004	PGE	4	0
9	B	1003	MES	2	0

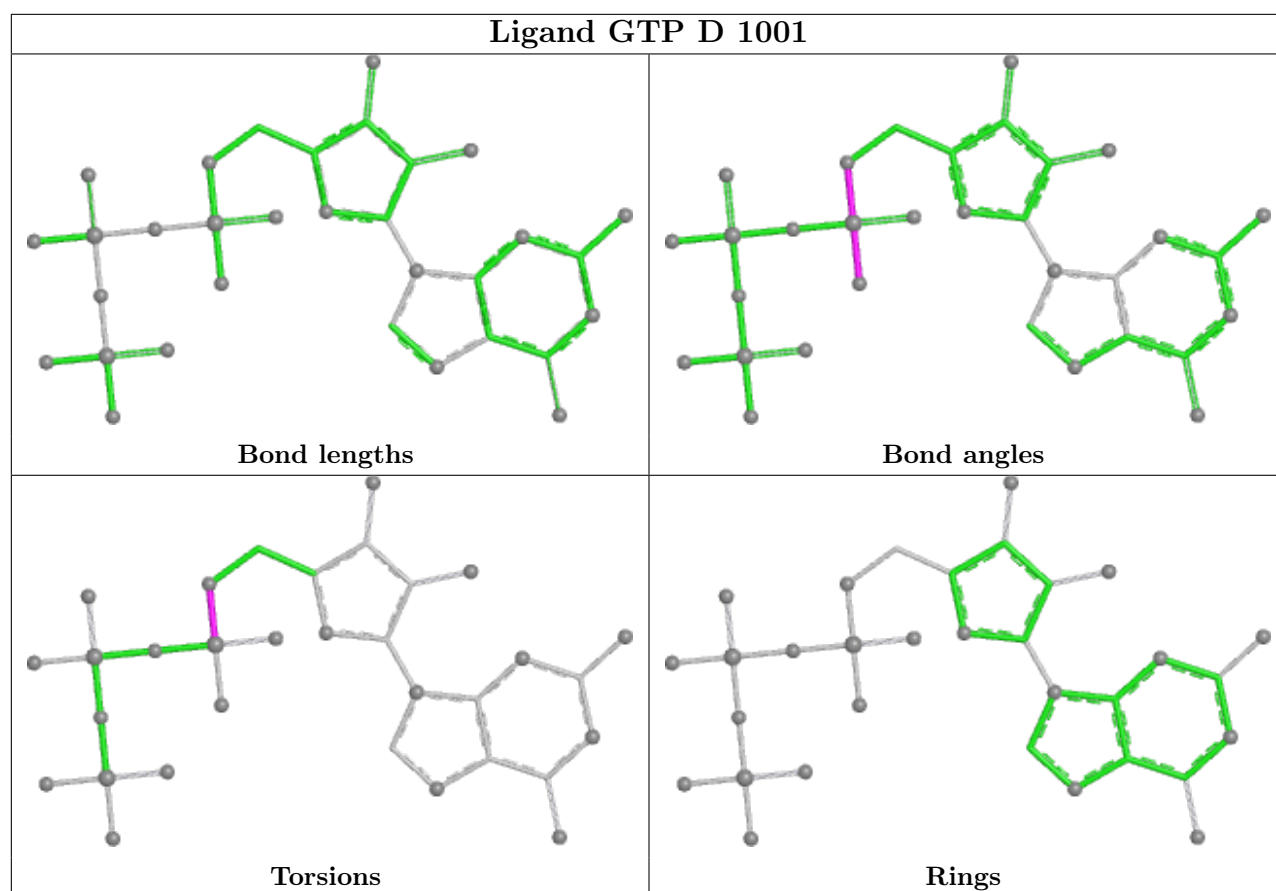
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









### 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%)	0.06	2 (0%) 91 90	37, 57, 83, 98	0
1	C	440/451 (97%)	-0.02	0 100 100	32, 48, 65, 87	0
2	B	431/445 (96%)	-0.01	1 (0%) 95 95	33, 49, 79, 99	0
2	D	428/445 (96%)	0.27	10 (2%) 60 57	45, 69, 92, 123	0
3	E	123/143 (86%)	0.06	0 100 100	46, 66, 92, 107	0
4	F	346/384 (90%)	0.63	34 (9%) 7 5	45, 76, 143, 179	0
All	All	2207/2319 (95%)	0.16	47 (2%) 63 60	32, 59, 98, 179	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	MET	4.9
4	F	182	ILE	4.4
4	F	234	GLN	4.2
4	F	100	ILE	3.8
2	D	279	GLN	3.8

### 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 monosaccharides in this entry.

## 6.4 Ligands

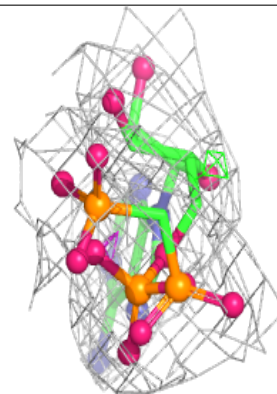
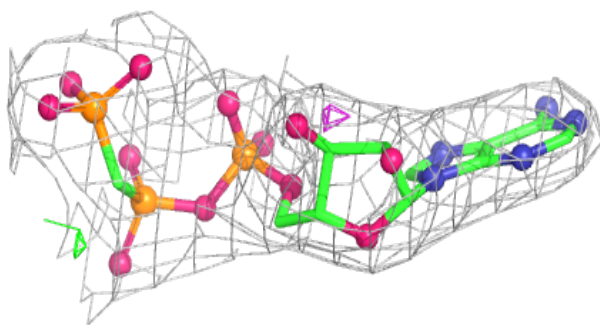
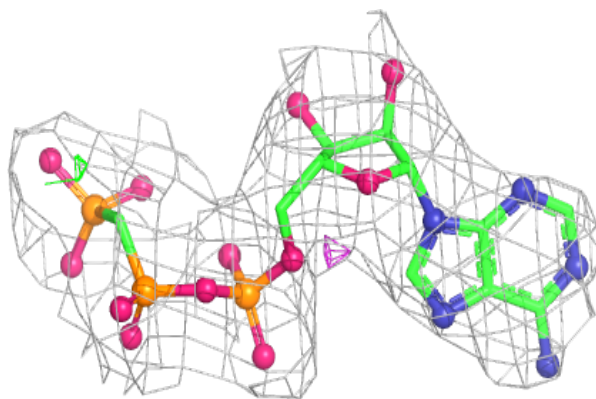
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
16	PEG	D	1003	7/7	0.61	0.24	93,93,94,94	0
13	PGE	C	1004	10/10	0.87	0.29	70,70,71,71	0
12	O9N	B	1006	16/16	0.90	0.21	58,59,69,69	0
15	P6S	C	1006	10/11	0.92	0.38	71,74,74,74	0
6	MG	B	1002	1/1	0.94	0.23	58,58,58,58	0
6	MG	F	1002	1/1	0.94	0.06	68,68,68,68	0
17	ACP	F	1001	31/31	0.94	0.21	91,94,105,105	0
6	MG	A	1002	1/1	0.96	0.12	45,45,45,45	0
11	O9K	B	1005	19/19	0.97	0.20	47,54,57,57	0
6	MG	D	1002	1/1	0.97	0.04	64,64,64,64	0
9	MES	B	1003	12/12	0.97	0.19	65,65,68,68	0
5	GTP	A	1001	32/32	0.98	0.16	44,46,48,48	0
5	GTP	D	1001	32/32	0.98	0.17	65,68,75,75	0
7	CA	A	1003	1/1	0.98	0.15	80,80,80,80	0
14	VAL	C	1005	7/8	0.98	0.21	44,45,46,47	0
7	CA	C	1003	1/1	0.98	0.16	64,64,64,64	0
6	MG	C	1002	1/1	0.98	0.08	42,42,42,42	0
10	O9B	B	1004	9/10	0.98	0.19	42,43,46,46	0
8	GDP	B	1001	28/28	0.99	0.19	38,39,40,41	0
5	GTP	C	1001	32/32	0.99	0.18	41,43,45,46	0

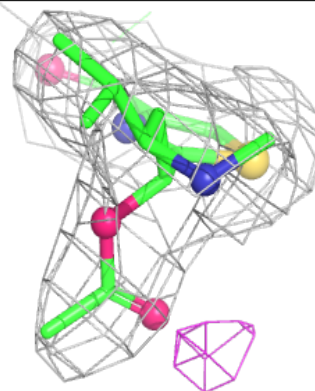
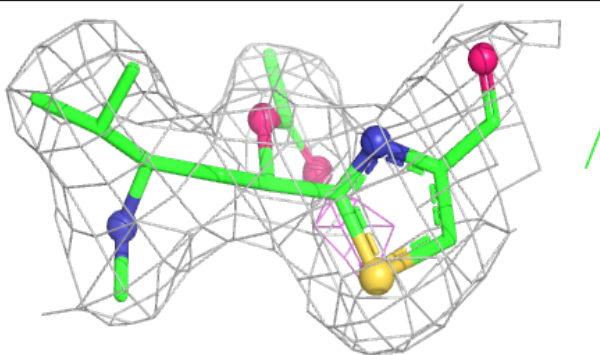
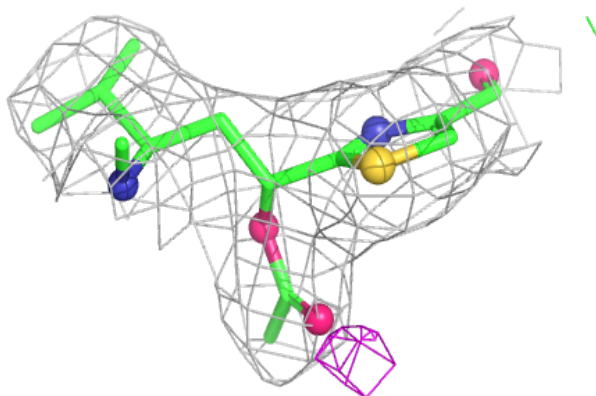
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ACP F 1001:**

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

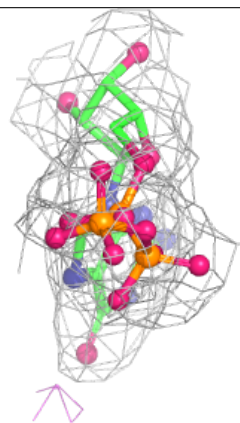
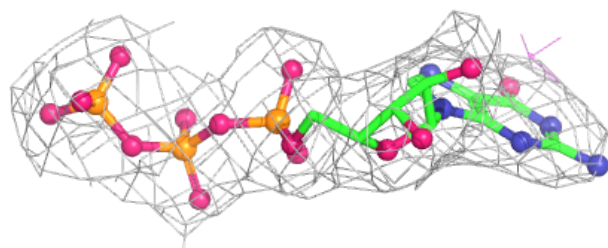
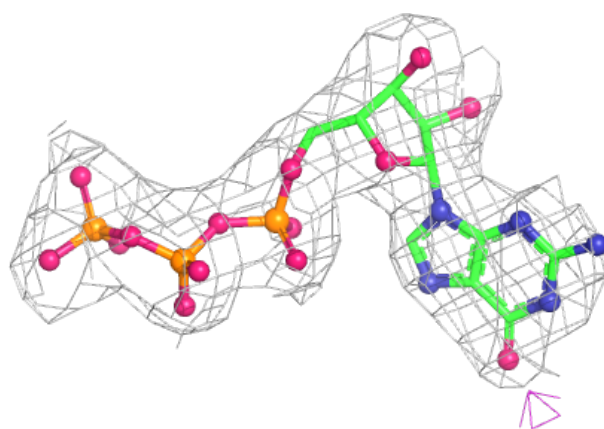
**Electron density around O9K B 1005:**

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

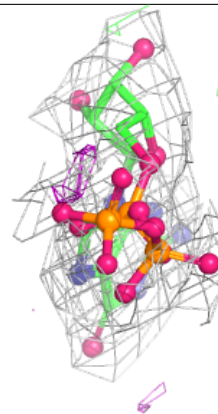
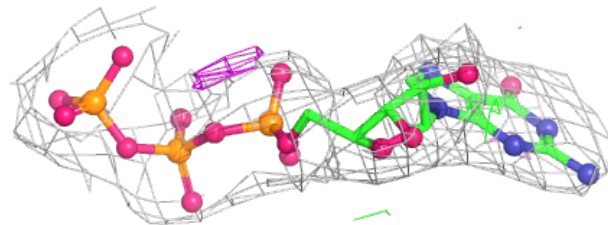
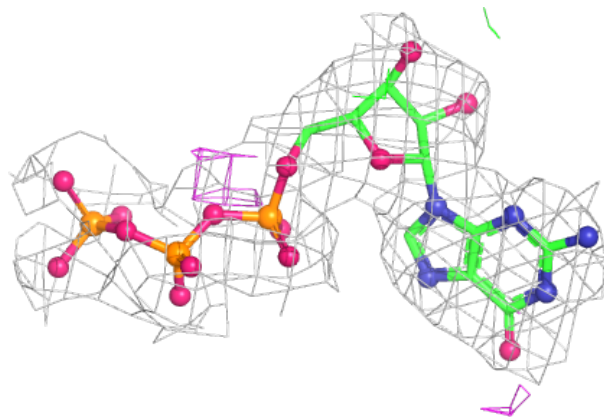


**Electron density around GTP A 1001:**

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

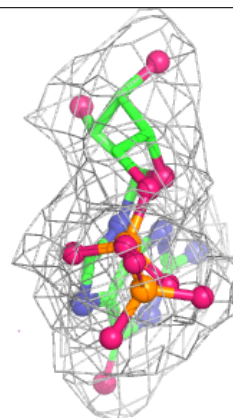
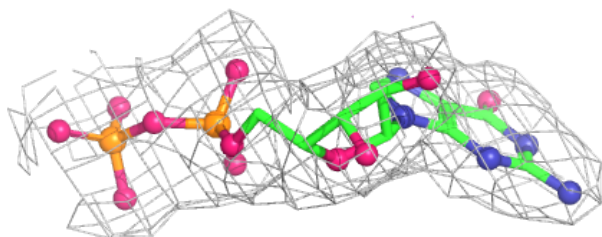
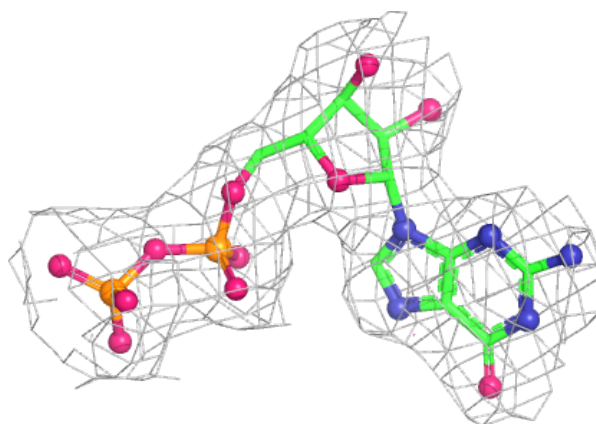
**Electron density around GTP D 1001:**

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

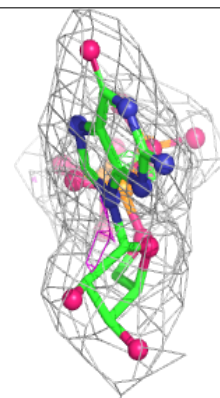
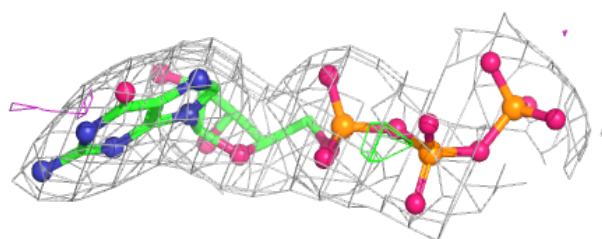
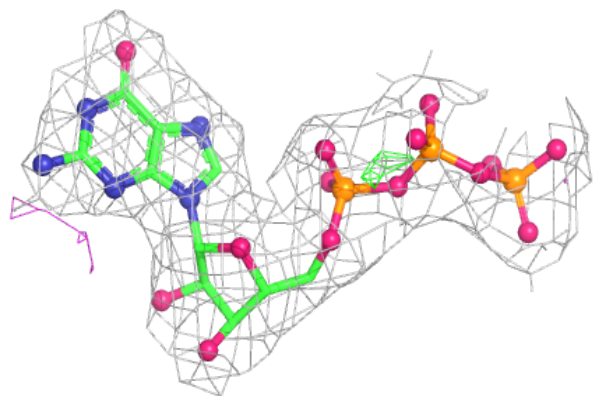


**Electron density around GDP B 1001:**

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

**Electron density around GTP C 1001:**

$2mF_o-DF_c$  (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.