



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 22, 2023 – 10:42 AM JST

PDB ID : 7CEK  
Title : Crystal structure of T2R-TTL-BML-284 complex  
Authors : Chen, L.J.; Chen, Q.; Yu, Y.; Yang, J.H.  
Deposited on : 2020-06-23  
Resolution : 2.70 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

<http://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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

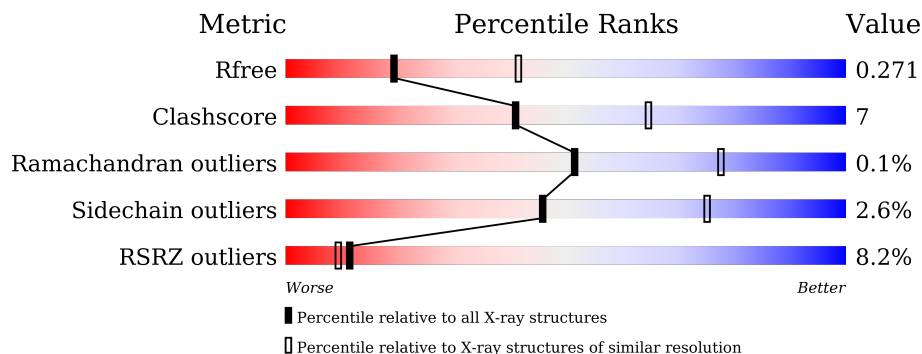
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	450	 4% (poor fit), 84% (0-1 outliers), 13% (2 outliers), 0% (3+ outliers), 0% (not modelled)
1	C	450	 0% (poor fit), 81% (0-1 outliers), 16% (2 outliers), 0% (3+ outliers), 0% (not modelled)
2	B	445	 4% (poor fit), 80% (0-1 outliers), 15% (2 outliers), 0% (3+ outliers), 0% (not modelled)
2	D	445	 6% (poor fit), 79% (0-1 outliers), 16% (2 outliers), 0% (3+ outliers), 5% (not modelled)
3	E	143	 7% (poor fit), 66% (0-1 outliers), 20% (2 outliers), 0% (3+ outliers), 14% (not modelled)
4	F	384	 27% (poor fit), 69% (0-1 outliers), 19% (2 outliers), 0% (3+ outliers), 9% (not modelled)

## 2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 34902 atoms, of which 17075 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	H	N	O	S			
1	A	438	6768	2173	3334	583	655	23	0	2	0
1	C	440	6839	2196	3373	587	660	23	0	6	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	425	6593	2111	3234	574	647	27	0	3	0
2	D	423	6520	2089	3195	564	644	28	0	1	0

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	E	123	2061	631	1036	185	204	5	0	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	F	349	5650	1825	2801	488	522	14	0	0	0

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

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

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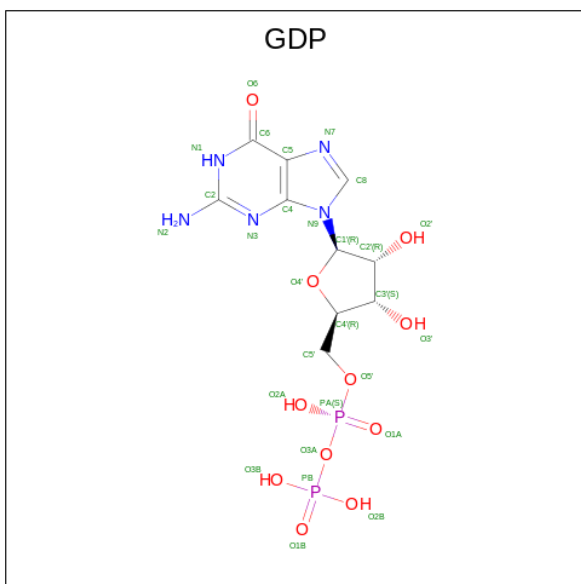
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Mg 1 1	0	0
6	F	1	Total Mg 1 1	0	0

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

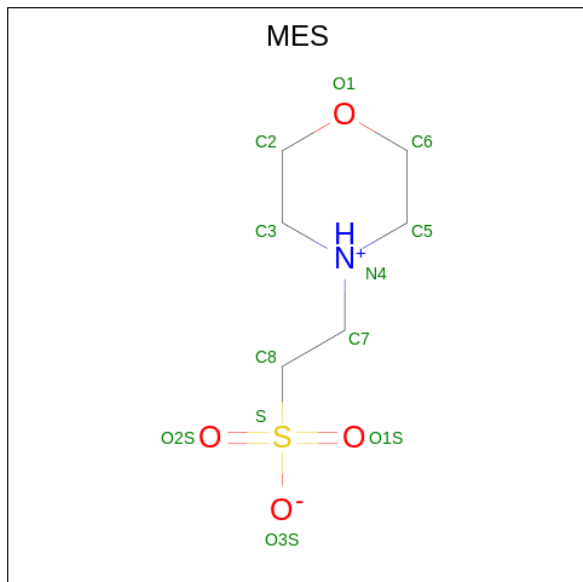
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	2	Total Ca 2 2	0	0
7	C	1	Total Ca 1 1	0	0
7	D	1	Total Ca 1 1	0	0
7	E	1	Total Ca 1 1	0	0

- 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>).



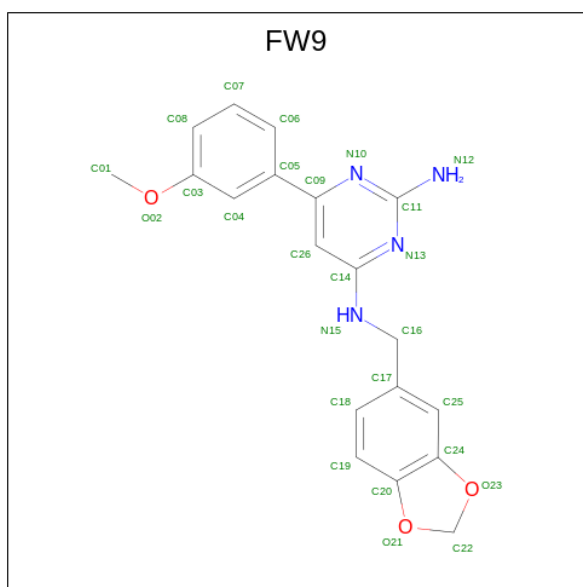
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C H N O P 38 10 10 5 11 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



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

- Molecule 10 is N4-(1,3-benzodioxol-5-ylmethyl)-6-(3-methoxyphenyl)pyrimidine-2,4-diamine (three-letter code: FW9) (formula:  $C_{19}H_{18}N_4O_3$ ) (labeled as "Ligand of Interest" by depositor).

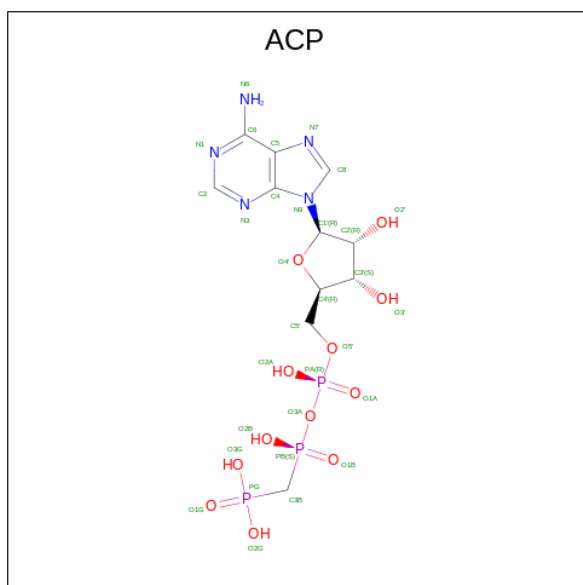


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			44	19	18	4	3		
10	D	1	Total	C	H	N	O	0	0
			44	19	18	4	3		

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	1	Total	Cl	0	0
			1	1		

- Molecule 12 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
12	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	34	Total	O	0	0
			34	34		
13	B	25	Total	O	0	0
			25	25		
13	C	54	Total	O	0	0
			54	54		

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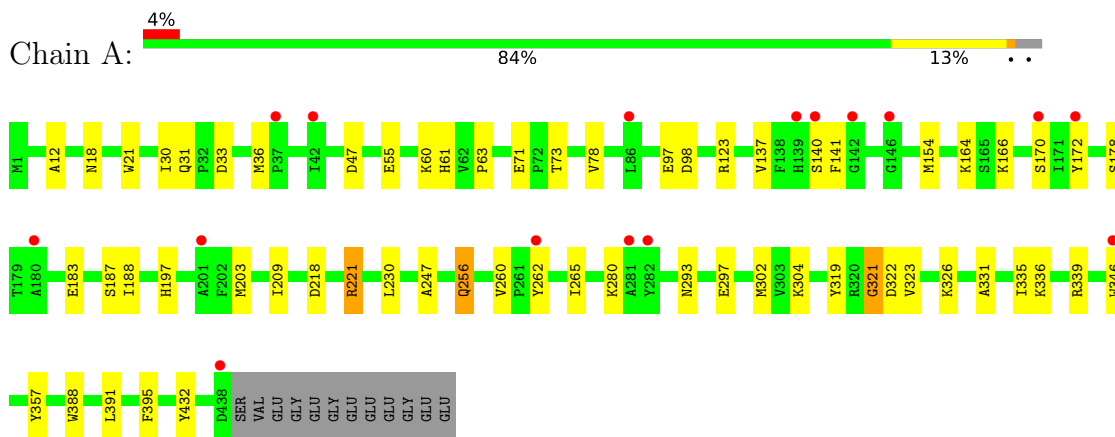
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
13	D	15	Total 15	O 15	0	0
13	E	1	Total 1	O 1	0	0
13	F	9	Total 9	O 9	0	0



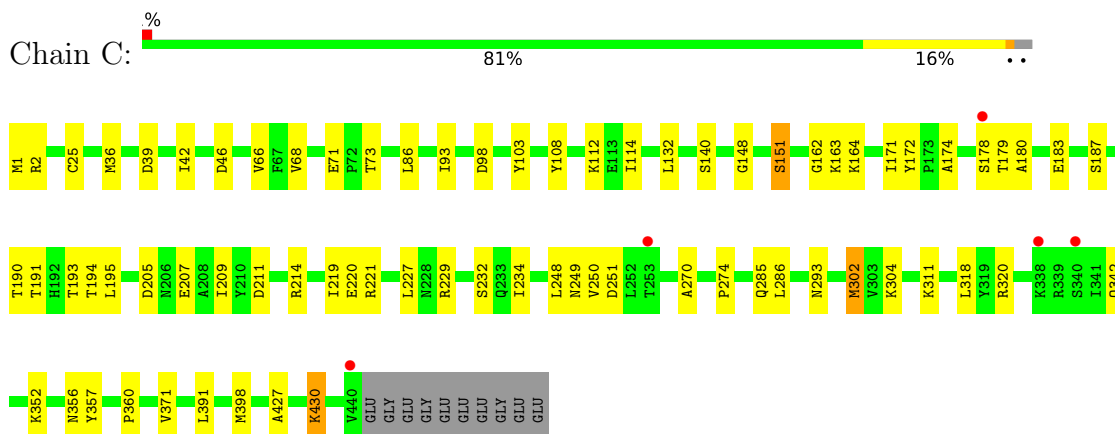
### 3 Residue-property plots [i](#)

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.

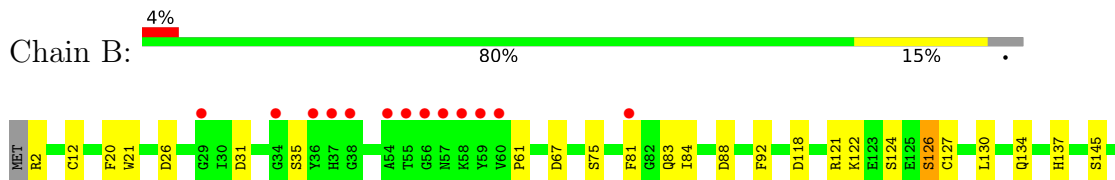
- Molecule 1: Tubulin alpha-1B chain

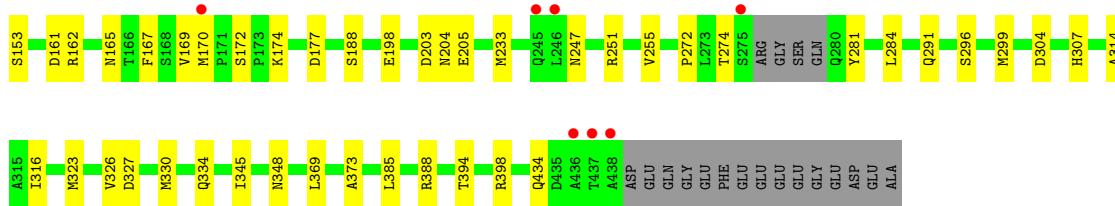


- Molecule 1: Tubulin alpha-1B chain

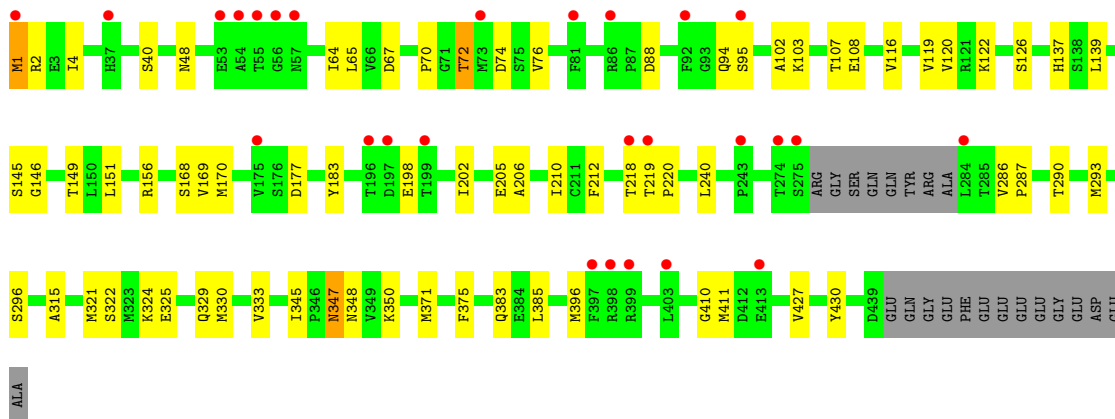


- Molecule 2: Tubulin beta chain

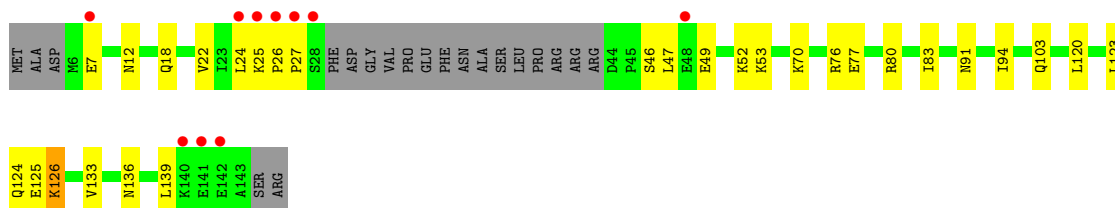




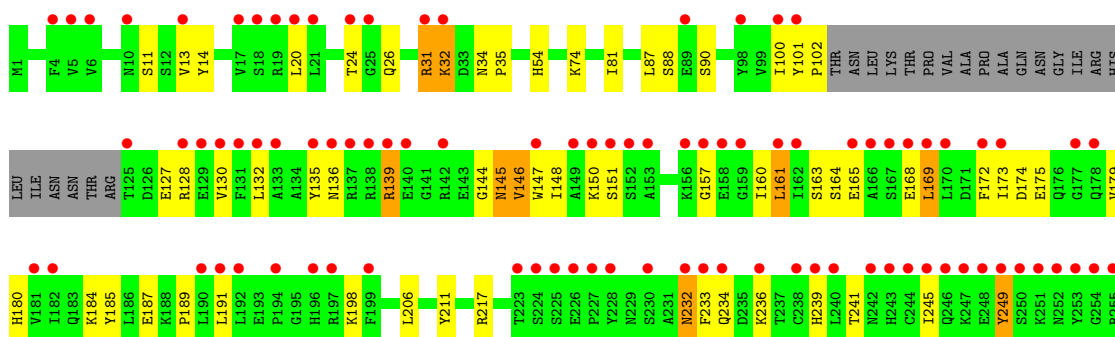
• Molecule 2: Tubulin beta chain

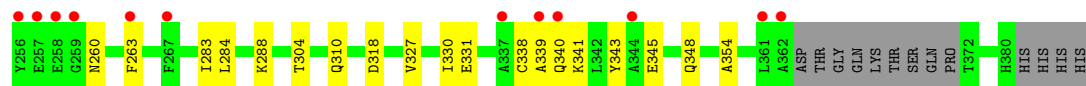


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.57Å 158.08Å 181.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.26 – 2.70 48.26 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.26-2.70) 99.7 (48.26-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.228 , 0.271 0.228 , 0.271	Depositor DCC
$R_{free}$ test set	1008 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.8	Xtrriage
Anisotropy	0.285	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	34902	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: CL, MG, FW9, CA, MES, GTP, ACP, GDP

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	0.34	0/3515	0.49	0/4772
1	C	0.38	2/3560 (0.1%)	0.49	0/4835
2	B	0.31	0/3442	0.46	0/4662
2	D	0.32	0/3401	0.48	0/4607
3	E	0.34	0/1036	0.43	0/1375
4	F	0.37	1/2914 (0.0%)	0.57	5/3936 (0.1%)
All	All	0.35	3/17868 (0.0%)	0.49	5/24187 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
4	F	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	GLN	CA-CB	-7.44	1.37	1.53
4	F	161	LEU	CG-CD2	7.10	1.78	1.51
1	C	342	GLN	CB-CG	-6.98	1.33	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	169	LEU	CD1-CG-CD2	10.04	140.63	110.50
4	F	161	LEU	CB-CG-CD1	8.05	124.69	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	161	LEU	CB-CG-CD2	-8.03	97.35	111.00
4	F	161	LEU	CD1-CG-CD2	6.03	128.59	110.50
4	F	169	LEU	CB-CG-CD2	-5.79	101.16	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	GLY	Peptide
4	F	145	ASN	Peptide

## 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	3434	3334	3345	33	0
1	C	3466	3373	3386	47	1
2	B	3359	3234	3244	41	0
2	D	3325	3195	3206	49	0
3	E	1025	1036	1039	21	1
4	F	2849	2801	2816	69	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	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	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
8	B	28	10	12	3	0
9	B	12	12	12	0	0
10	B	26	18	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	26	18	0	0	0
11	D	1	0	0	0	0
12	F	31	14	14	2	0
13	A	34	0	0	0	0
13	B	25	0	0	2	0
13	C	54	0	0	0	0
13	D	15	0	0	3	0
13	E	1	0	0	1	0
13	F	9	0	0	0	0
All	All	17827	17075	17110	247	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 7.

The worst 5 of 247 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:161:LEU:CG	4:F:161:LEU:CD2	1.78	1.58
4:F:161:LEU:HD22	4:F:172:PHE:CD1	1.95	1.01
3:E:125:GLU:OE2	13:E:301:HOH:O	1.83	0.97
4:F:169:LEU:N	4:F:169:LEU:HD23	1.81	0.92
4:F:161:LEU:CD2	4:F:161:LEU:CB	2.47	0.92

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:GLN:NE2	3:E:91:ASN:OD1[4_455]	2.09	0.11

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/450 (97%)	421 (96%)	17 (4%)	0	100	100
1	C	444/450 (99%)	428 (96%)	16 (4%)	0	100	100
2	B	424/445 (95%)	406 (96%)	18 (4%)	0	100	100
2	D	420/445 (94%)	399 (95%)	19 (4%)	2 (0%)	29	54
3	E	121/143 (85%)	115 (95%)	6 (5%)	0	100	100
4	F	343/384 (89%)	326 (95%)	16 (5%)	1 (0%)	41	66
All	All	2190/2317 (94%)	2095 (96%)	92 (4%)	3 (0%)	51	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	72	THR
4	F	146	VAL
2	D	220	PRO

### 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	371/378 (98%)	362 (98%)	9 (2%)	49	77
1	C	377/378 (100%)	367 (97%)	10 (3%)	44	74
2	B	370/383 (97%)	362 (98%)	8 (2%)	52	79
2	D	367/383 (96%)	355 (97%)	12 (3%)	38	67
3	E	112/127 (88%)	108 (96%)	4 (4%)	35	64
4	F	311/342 (91%)	303 (97%)	8 (3%)	46	75
All	All	1908/1991 (96%)	1857 (97%)	51 (3%)	46	74

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	40	SER
2	D	205	GLU

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Mol	Chain	Res	Type
4	F	249	TYR
2	D	74	ASP
2	D	151	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
4	F	252	ASN
4	F	232	ASN
2	B	334	GLN
2	D	105	HIS
2	B	83	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	GTP	D	504	6	26,34,34	1.16	2 (7%)	32,54,54	1.58	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GTP	C	501	6	26,34,34	1.08	2 (7%)	32,54,54	1.53	5 (15%)
9	MES	B	503	-	12,12,12	2.10	1 (8%)	14,16,16	1.78	3 (21%)
5	GTP	A	501	6	26,34,34	1.11	2 (7%)	32,54,54	1.59	5 (15%)
10	FW9	D	503	-	29,29,29	1.40	4 (13%)	39,40,40	1.11	4 (10%)
8	GDP	B	501	6	24,30,30	1.03	2 (8%)	30,47,47	1.47	7 (23%)
10	FW9	B	506	-	29,29,29	1.30	3 (10%)	39,40,40	0.96	2 (5%)
12	ACP	F	402	6	27,33,33	2.67	7 (25%)	32,52,52	1.69	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	D	504	6	-	5/18/38/38	0/3/3/3
5	GTP	C	501	6	-	4/18/38/38	0/3/3/3
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
5	GTP	A	501	6	-	5/18/38/38	0/3/3/3
10	FW9	D	503	-	-	2/11/17/17	0/4/4/4
8	GDP	B	501	6	-	4/12/32/32	0/3/3/3
10	FW9	B	506	-	-	0/11/17/17	0/4/4/4
12	ACP	F	402	6	-	6/15/38/38	0/3/3/3

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	402	ACP	O4'-C1'	8.41	1.52	1.41
9	B	503	MES	C8-S	-6.86	1.67	1.77
12	F	402	ACP	PB-O3A	6.62	1.65	1.58
5	D	504	GTP	C5-C6	-3.92	1.39	1.47
10	D	503	FW9	C14-N15	3.89	1.42	1.36

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	402	ACP	C3'-C2'-C1'	4.84	108.27	100.98
9	B	503	MES	C5-N4-C3	4.80	119.62	108.83
12	F	402	ACP	N3-C2-N1	-4.09	122.29	128.68
5	C	501	GTP	PB-O3B-PG	-3.72	120.05	132.83

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*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	402	ACP	C4-C5-N7	-3.57	105.68	109.40

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

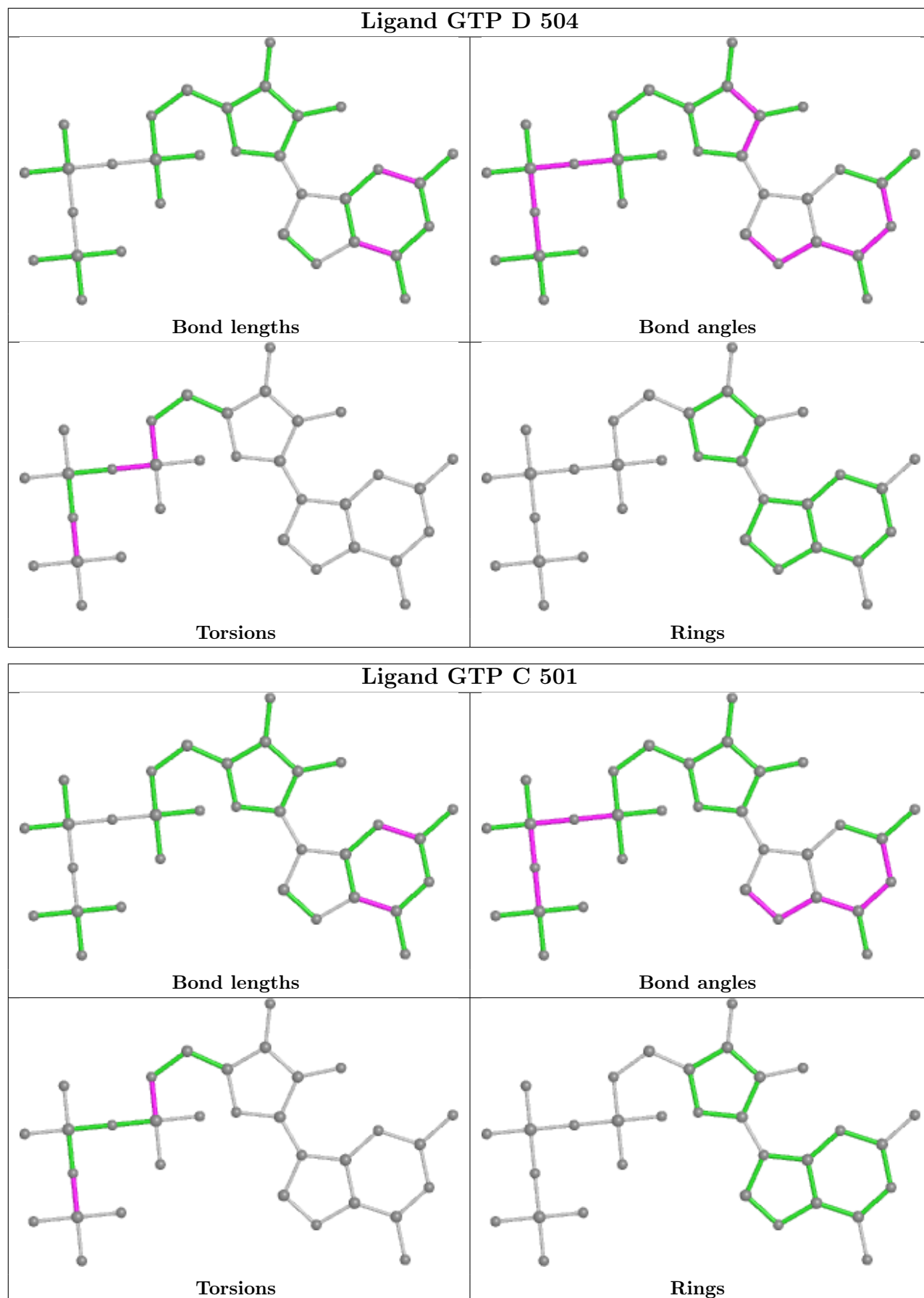
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A

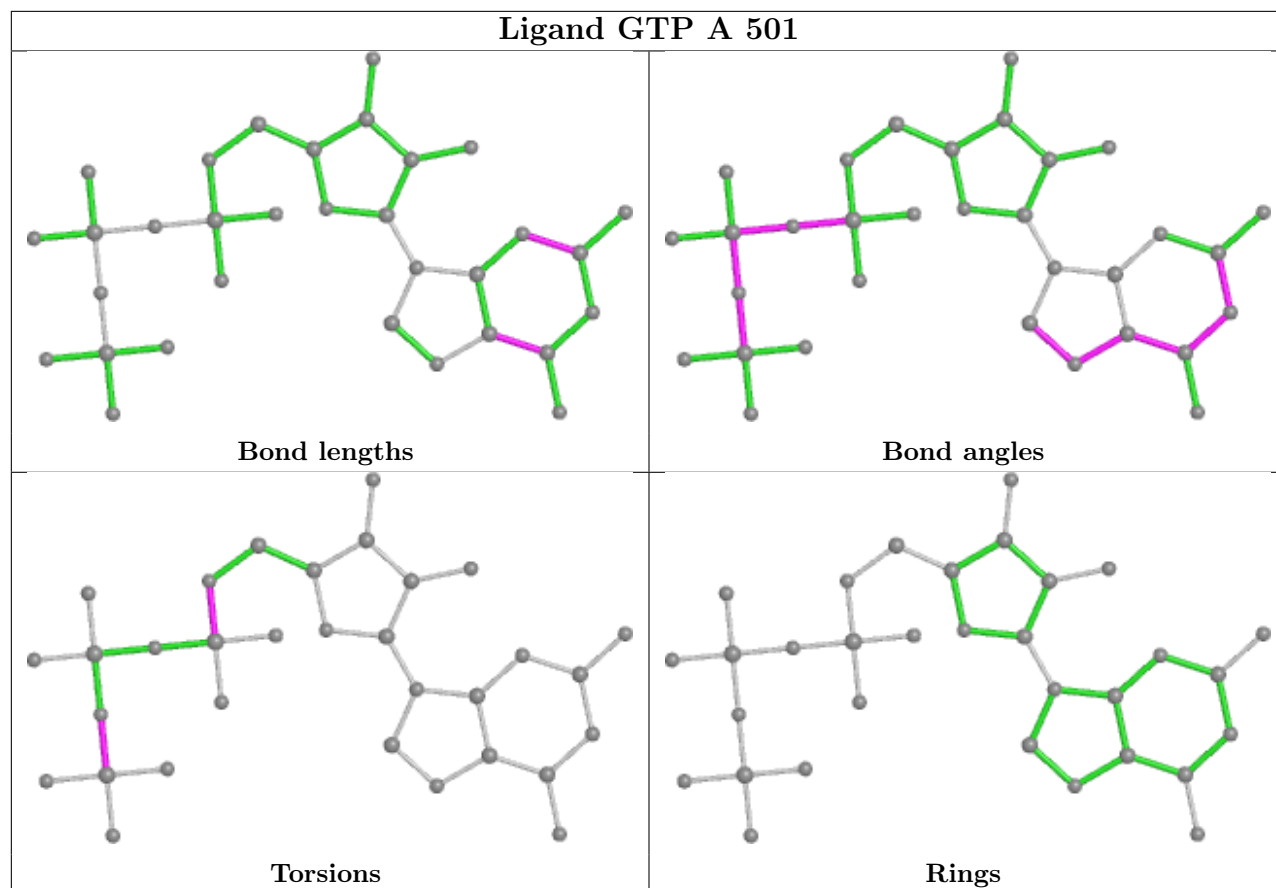
There are no ring outliers.

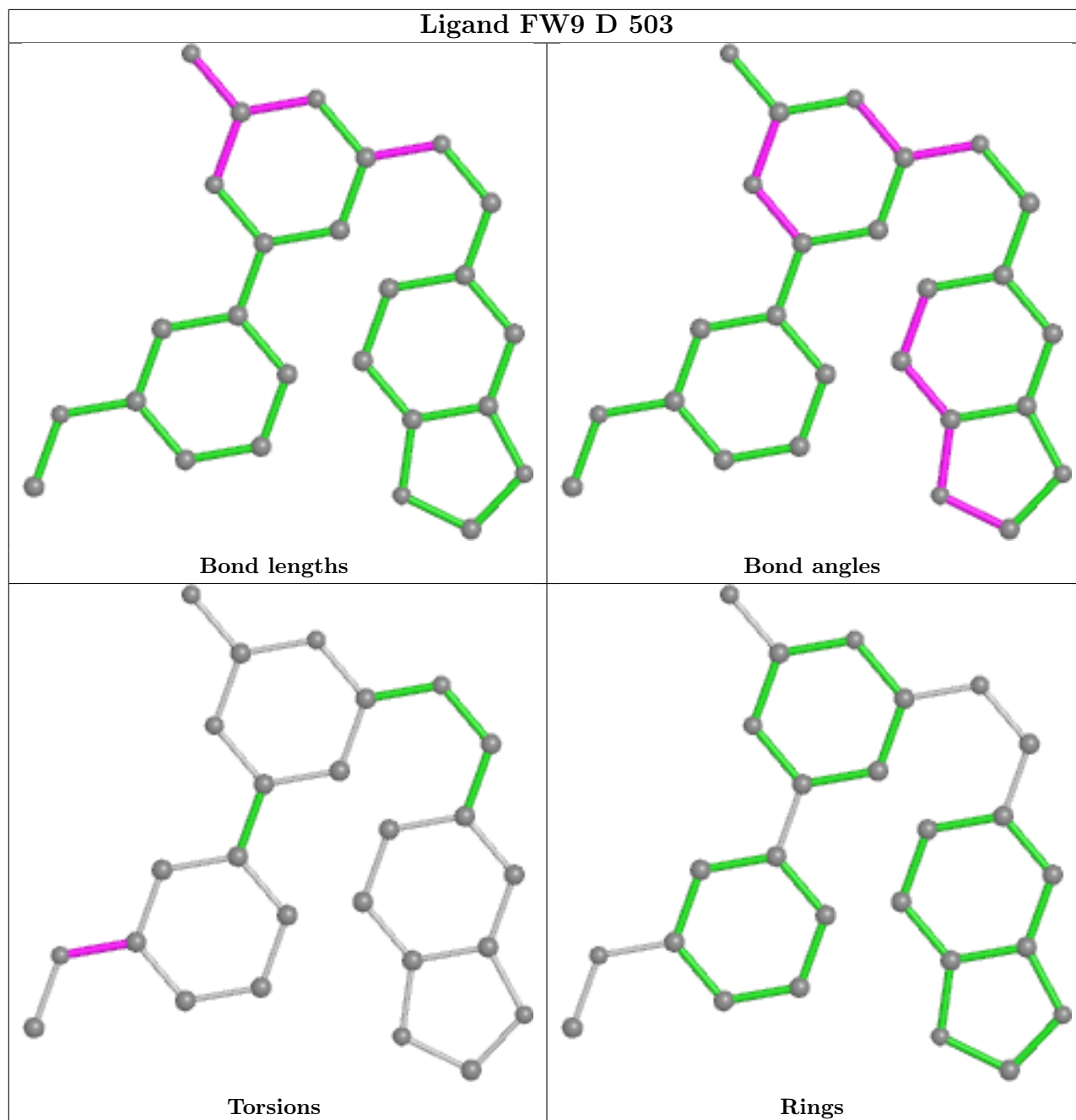
3 monomers are involved in 6 short contacts:

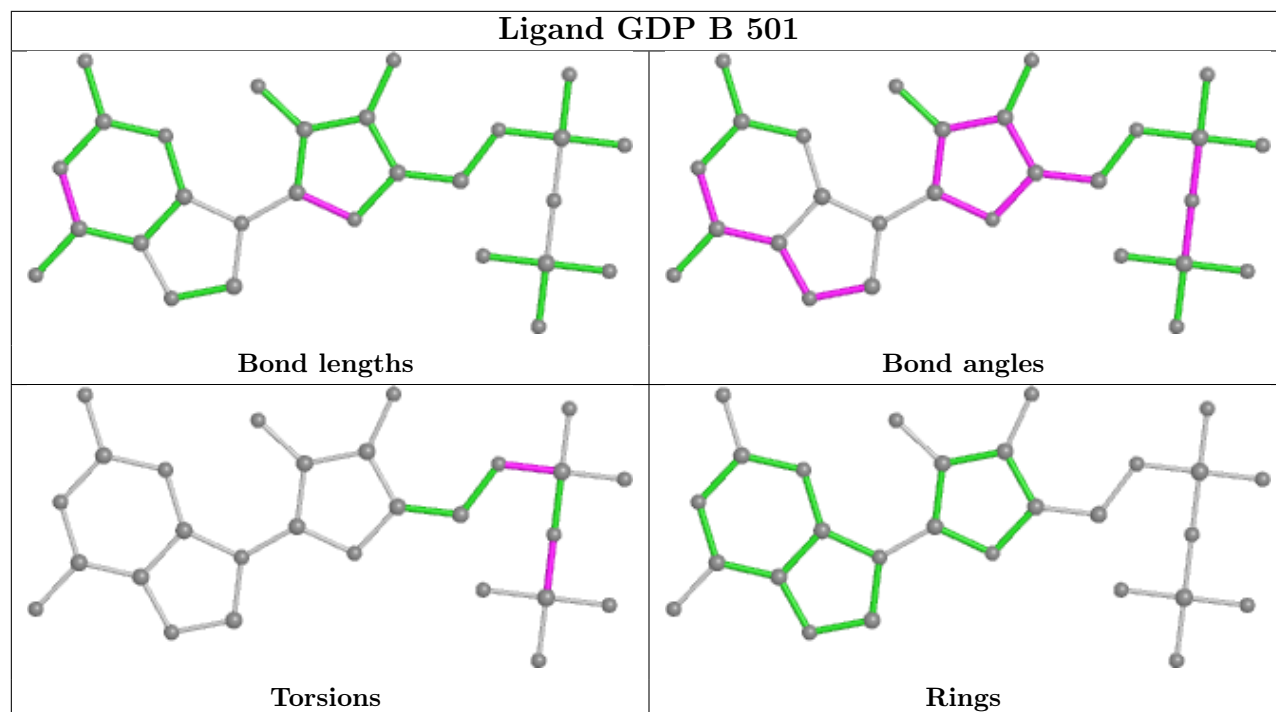
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	501	GDP	3	0
10	B	506	FW9	1	0
12	F	402	ACP	2	0

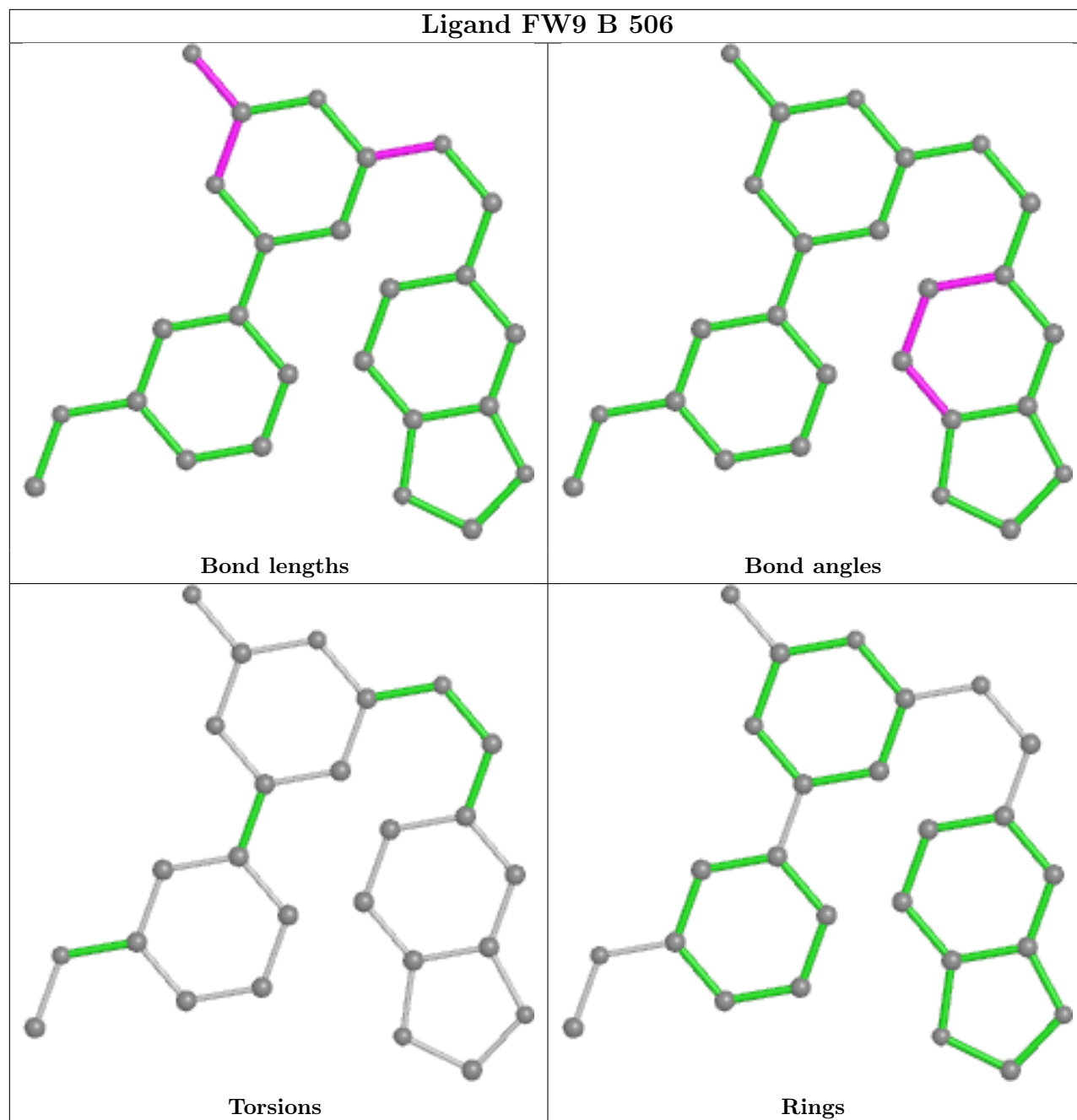
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



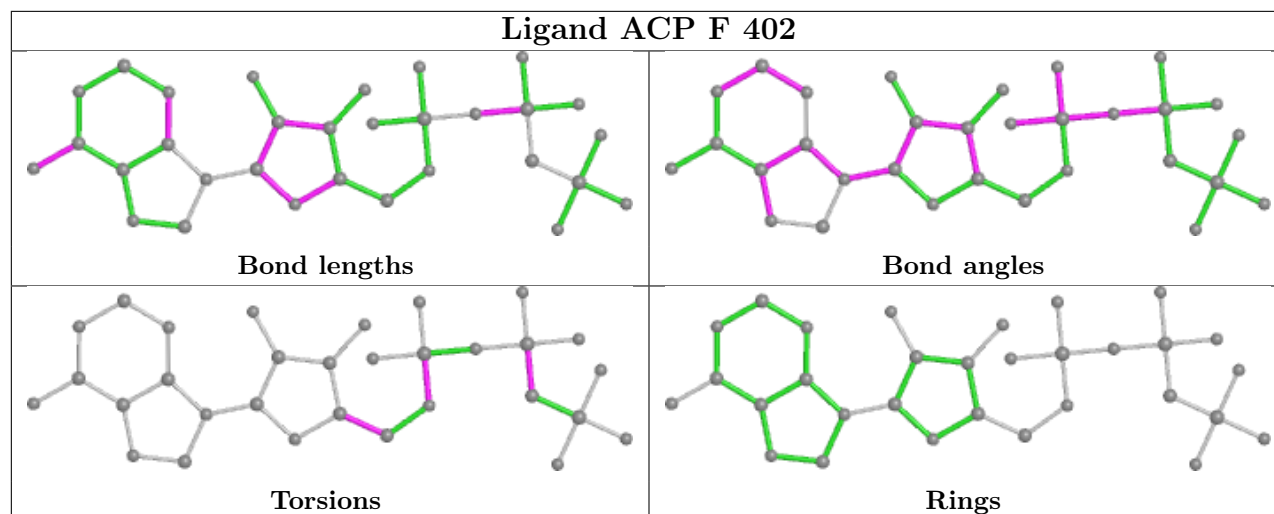












## 5.7 Other polymers [i](#)

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	438/450 (97%)	0.43	16 (3%) 41 41	47, 61, 78, 109	0
1	C	440/450 (97%)	0.25	5 (1%) 80 82	38, 52, 69, 78	0
2	B	425/445 (95%)	0.47	20 (4%) 31 30	43, 61, 84, 99	0
2	D	423/445 (95%)	0.57	27 (6%) 19 18	51, 72, 89, 98	0
3	E	123/143 (86%)	0.55	10 (8%) 12 10	53, 69, 93, 109	0
4	F	349/384 (90%)	1.24	103 (29%) 0 0	58, 82, 130, 139	0
All	All	2198/2317 (94%)	0.56	181 (8%) 11 9	38, 65, 103, 139	0

The worst 5 of 181 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	161	LEU	9.5
4	F	173	ILE	7.3
2	D	275	SER	7.2
4	F	169	LEU	6.9
4	F	249	TYR	6.6

### 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 monosaccharides in this entry.

## 6.4 Ligands

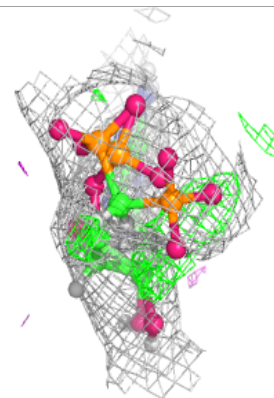
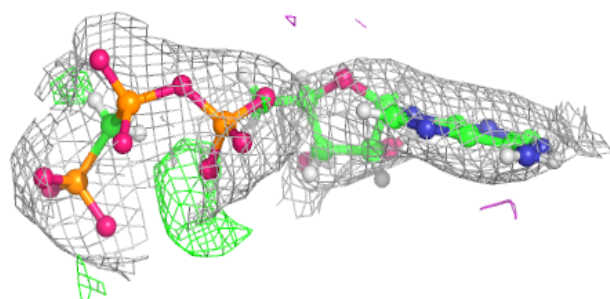
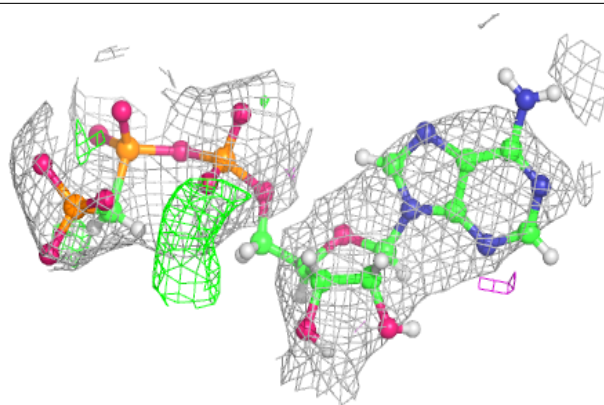
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
7	CA	D	502	1/1	0.68	0.10	98,98,98,98	0
7	CA	B	504	1/1	0.82	0.08	97,97,97,97	0
12	ACP	F	402	31/31	0.83	0.20	99,108,133,133	0
7	CA	E	201	1/1	0.85	0.12	95,95,95,95	0
7	CA	B	505	1/1	0.87	0.09	88,88,88,88	0
11	CL	D	505	1/1	0.89	1.25	118,118,118,118	0
6	MG	F	401	1/1	0.89	0.16	106,106,106,106	0
10	FW9	B	506	26/26	0.90	0.26	55,67,81,89	0
6	MG	D	501	1/1	0.91	0.08	79,79,79,79	0
10	FW9	D	503	26/26	0.91	0.25	58,66,80,82	0
5	GTP	D	504	32/32	0.94	0.16	66,73,86,94	0
8	GDP	B	501	28/28	0.95	0.27	46,55,66,77	0
9	MES	B	503	12/12	0.95	0.14	55,67,75,76	0
7	CA	A	503	1/1	0.95	0.07	79,79,79,79	0
5	GTP	A	501	32/32	0.97	0.28	47,55,67,73	0
5	GTP	C	501	32/32	0.98	0.22	38,49,61,71	0
7	CA	C	503	1/1	0.98	0.11	66,66,66,66	0
6	MG	A	502	1/1	0.98	0.26	53,53,53,53	0
6	MG	B	502	1/1	0.98	0.27	55,55,55,55	0
6	MG	C	502	1/1	0.98	0.25	44,44,44,44	0

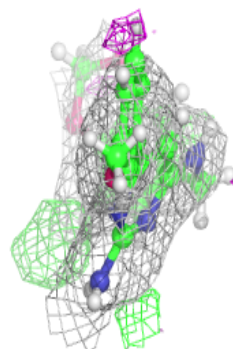
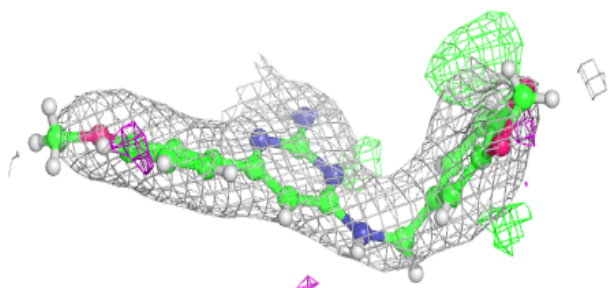
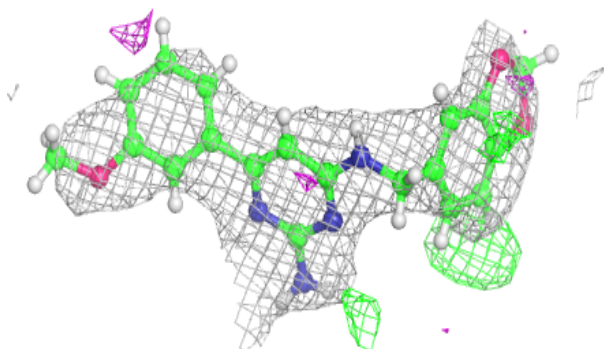
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

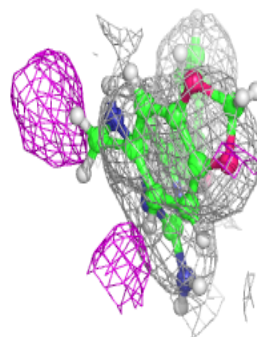
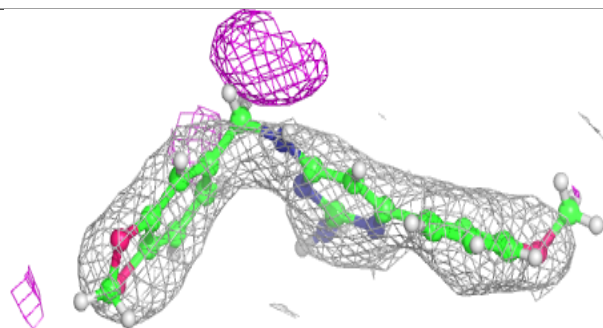
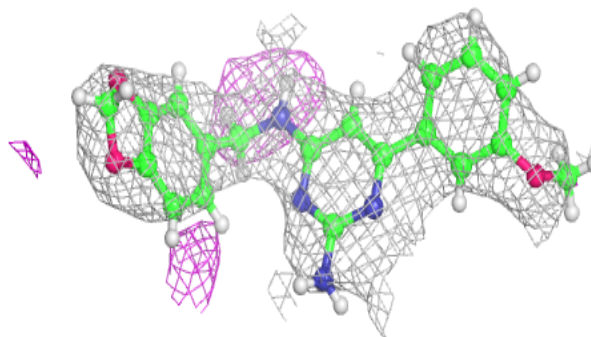
**Electron density around FW9 B 506:**

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

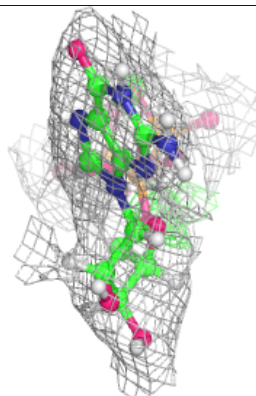
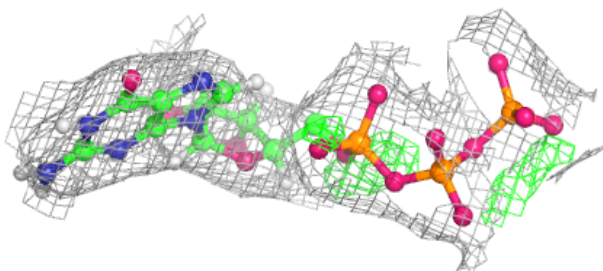
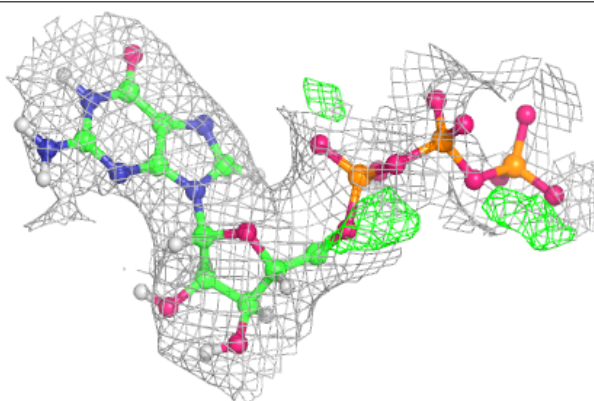


**Electron density around FW9 D 503:**

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

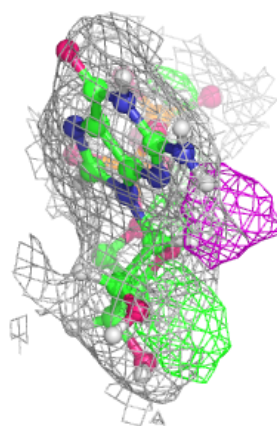
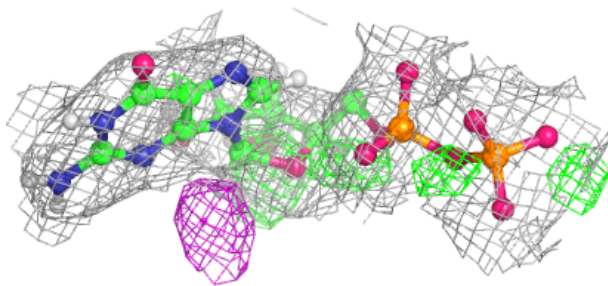
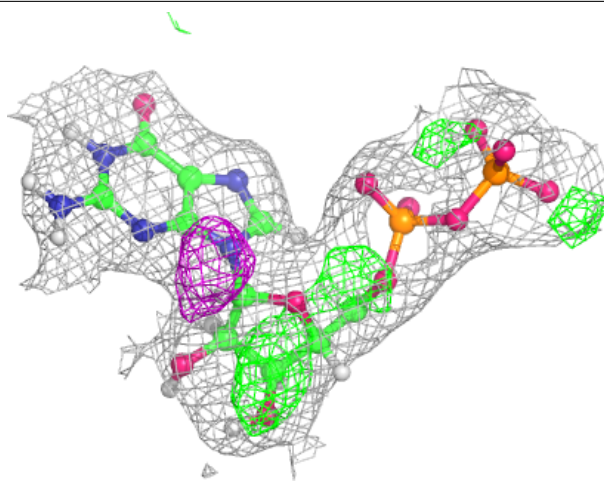
**Electron density around GTP D 504:**

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

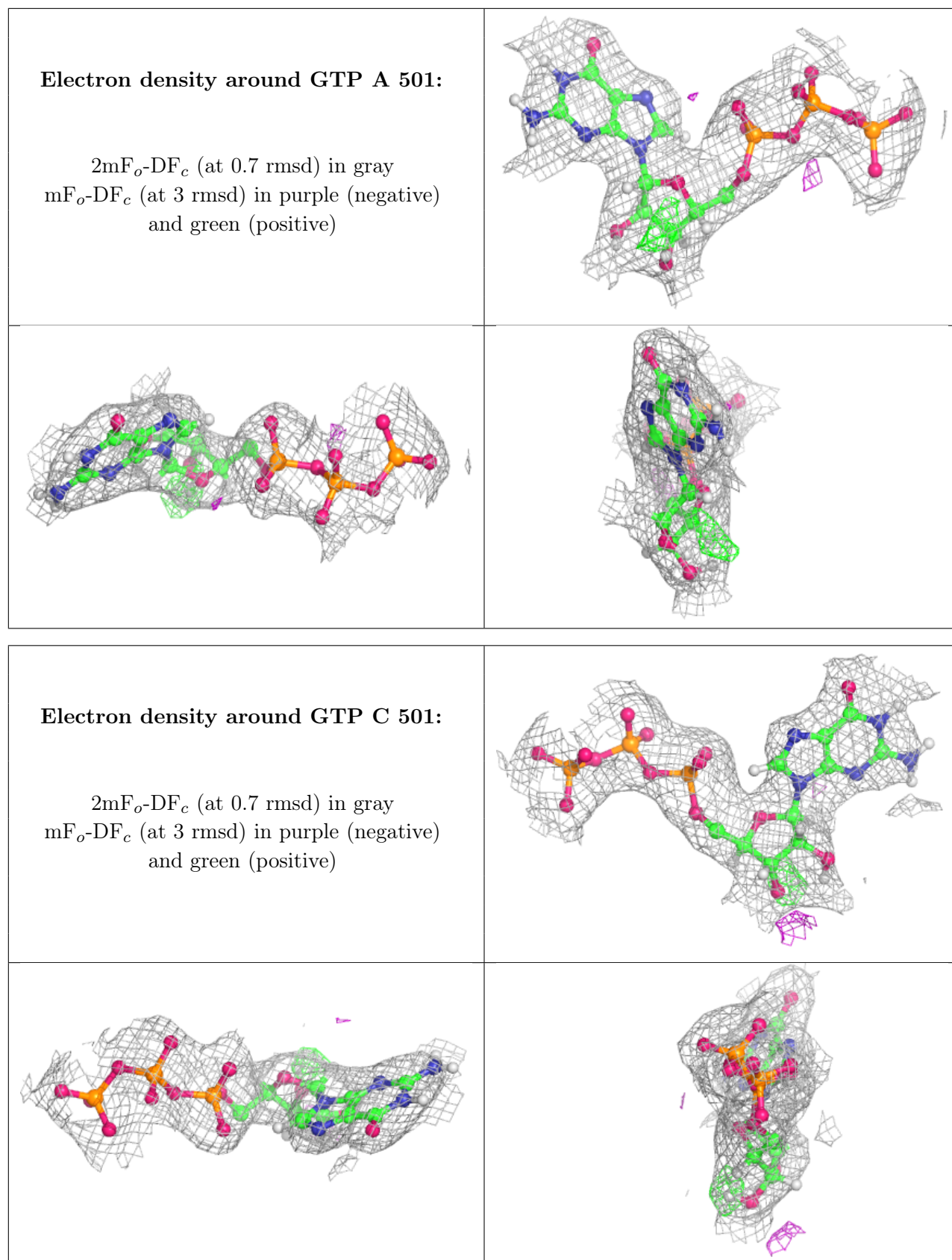


**Electron density around GDP B 501:**

$2mF_o-DF_c$  (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.