



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 08:33 PM EDT

PDB ID : 7CEK / pdb_00007cek
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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

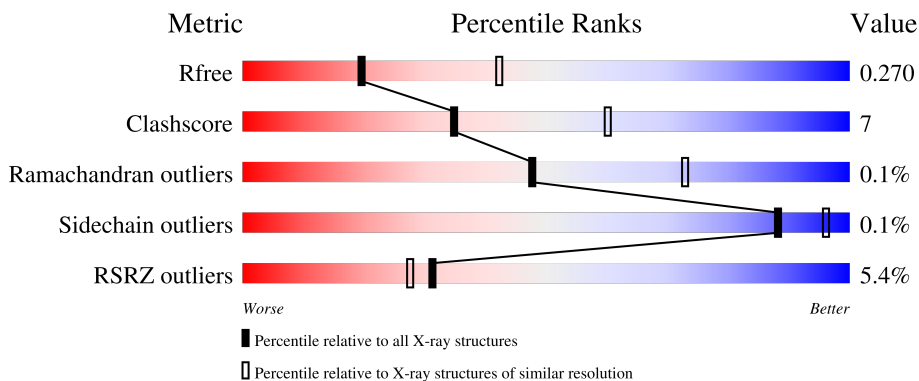
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	450	
1	C	450	
2	B	445	
2	D	445	
3	E	143	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	

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
11	CL	D	505	-	-	-	X

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	Total	C	H	N	O	S	0	2	0
			6768	2173	3334	583	655	23			
1	C	440	Total	C	H	N	O	S	0	6	0
			6839	2196	3373	587	660	23			

- 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	Total	C	H	N	O	S	0	3	0
			6593	2111	3234	574	647	27			
2	D	423	Total	C	H	N	O	S	0	1	0
			6520	2089	3195	564	644	28			

- Molecule 3 is a protein called Stathmin-4.

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

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

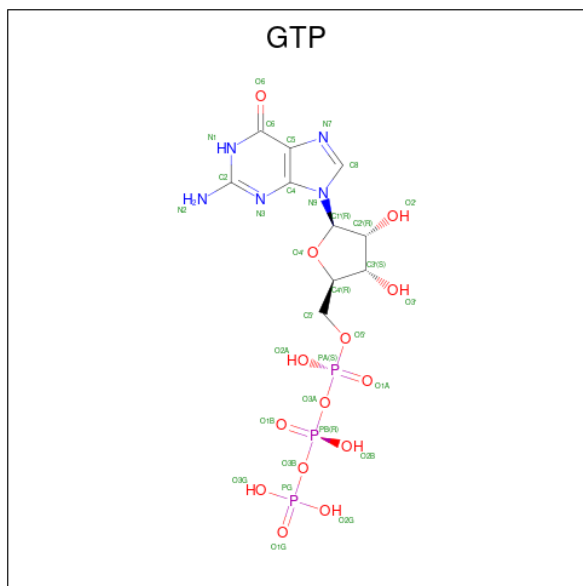
- Molecule 4 is a protein called Tubulin tyrosine ligase.

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

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 (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



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 (CCD ID: 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		

Continued on next page...

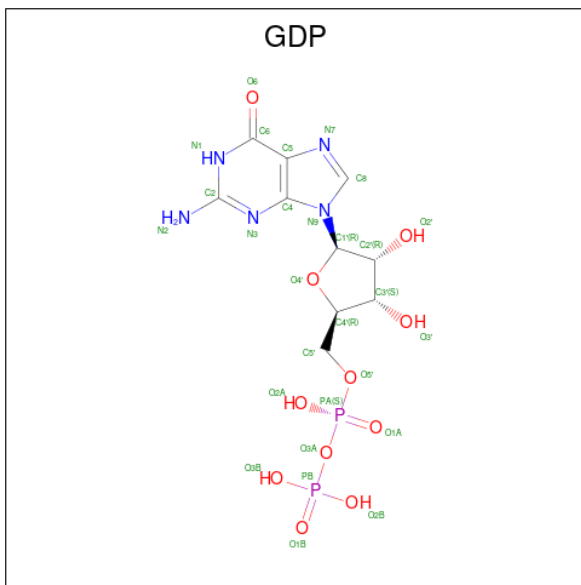
Continued from previous page...

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 (CCD ID: 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

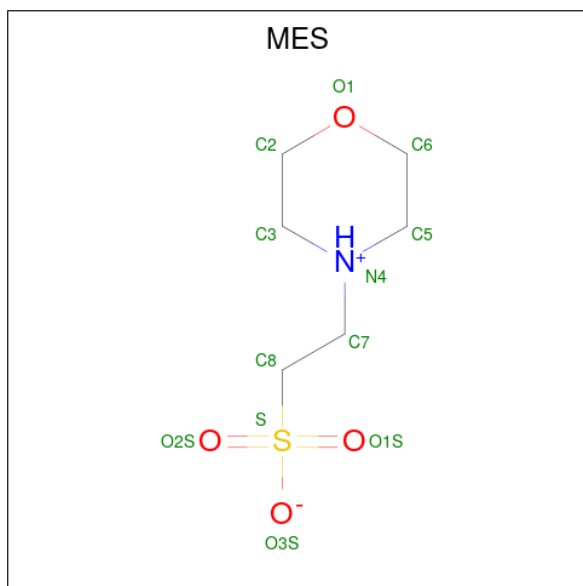
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

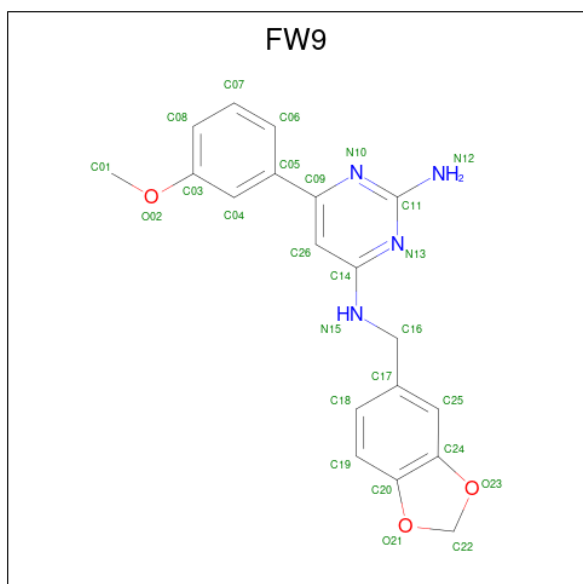
- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula:

C₆H₁₃NO₄S).



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 (CCD ID: FW9) (formula: C₁₉H₁₈N₄O₃) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

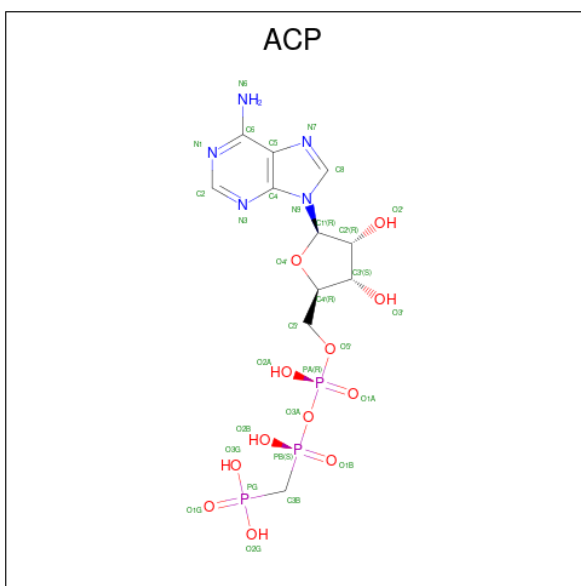
Continued from previous page...

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

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

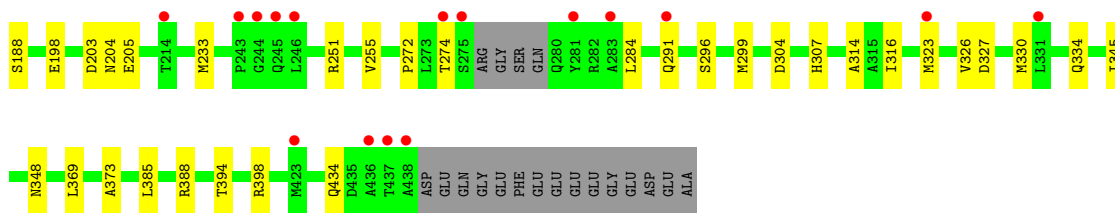
- Molecule 13 is water.

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

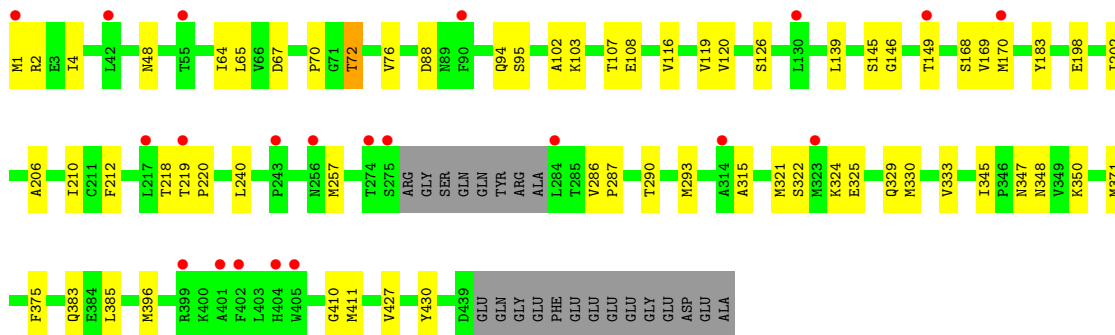
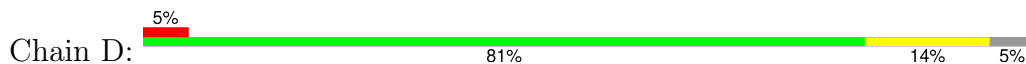
Continued on next page...

Continued from previous page...

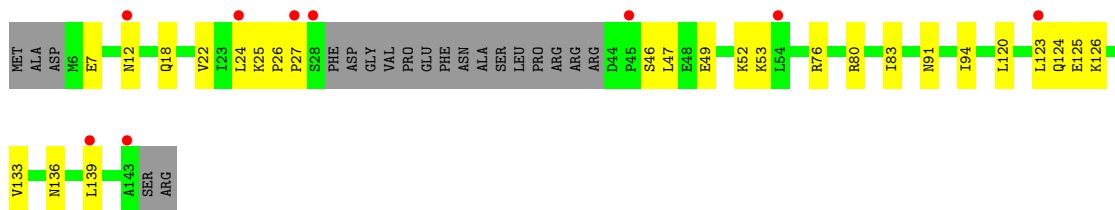
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	D	15	Total 15	O 15	0	0
13	E	1	Total 1	O 1	0	0
13	F	9	Total 9	O 9	0	0



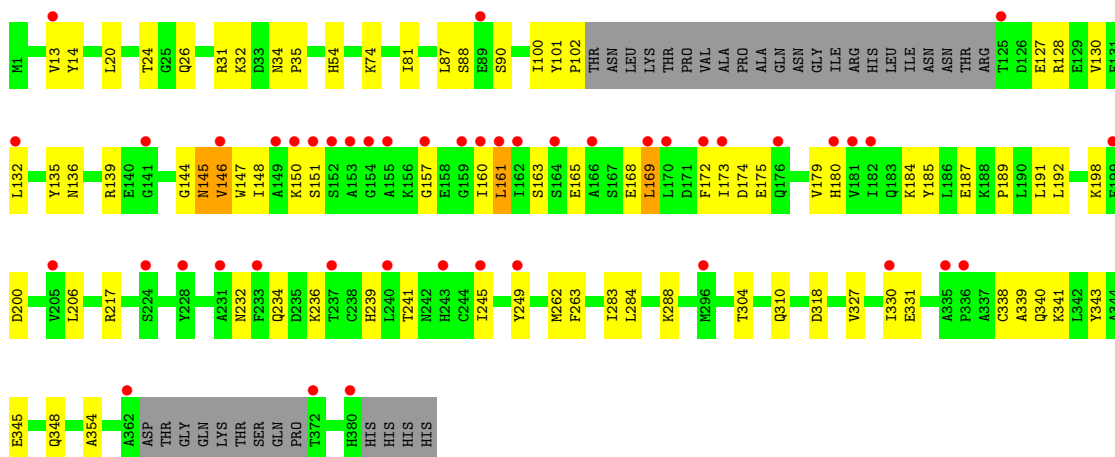
- Molecule 2: Tubulin beta chain



- 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, α , β , γ	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) 99.6 (48.26-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.69Å)	Xtrriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.228 , 0.271 0.229 , 0.270	Depositor DCC
R_{free} test set	1008 reflections (1.20%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtrriage
Anisotropy	0.285	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, CL, GDP, CA, FW9, ACP, MG, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.23	0/3515	0.39	0/4772
1	C	0.30	2/3560 (0.1%)	0.40	0/4835
2	B	0.22	0/3442	0.37	0/4662
2	D	0.23	0/3401	0.43	0/4607
3	E	0.23	0/1036	0.38	0/1375
4	F	0.30	1/2914 (0.0%)	0.54	2/3936 (0.1%)
All	All	0.26	3/17868 (0.0%)	0.42	2/24187 (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	-8.09	1.37	1.53
4	F	161	LEU	CG-CD2	7.75	1.78	1.52
1	C	342	GLN	CB-CG	-6.25	1.33	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	169	LEU	CD1-CG-CD2	13.56	140.63	110.80
4	F	161	LEU	CD1-CG-CD2	8.09	128.59	110.80

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	36	0
1	C	3466	3373	3386	48	1
2	B	3359	3234	3244	41	0
2	D	3325	3195	3206	54	0
3	E	1025	1036	1039	21	1
4	F	2849	2801	2816	73	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	260	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 260 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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	420/445 (94%)	399 (95%)	19 (4%)	2 (0%)	24	48
3	E	121/143 (85%)	115 (95%)	6 (5%)	0	100	100
4	F	343/384 (89%)	326 (95%)	16 (5%)	1 (0%)	36	60
All	All	2190/2317 (94%)	2095 (96%)	92 (4%)	3 (0%)	48	73

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%)	371 (100%)	0	100	100
1	C	377/378 (100%)	375 (100%)	2 (0%)	81	92
2	B	370/383 (97%)	370 (100%)	0	100	100
2	D	367/383 (96%)	367 (100%)	0	100	100
3	E	112/127 (88%)	112 (100%)	0	100	100
4	F	311/342 (91%)	311 (100%)	0	100	100
All	All	1908/1991 (96%)	1906 (100%)	2 (0%)	88	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	151[A]	SER
1	C	151[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	347	ASN
4	F	209	HIS
1	C	11	GLN
4	F	252	ASN
2	D	105	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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
9	MES	B	503	-	12,12,12	2.15	1 (8%)	15,16,16	1.71	1 (6%)
12	ACP	F	402	6	31,33,33	2.60	9 (29%)	47,52,52	2.49	15 (31%)
5	GTP	D	504	6	33,34,34	0.96	2 (6%)	50,54,54	1.68	9 (18%)
5	GTP	A	501	6	33,34,34	1.02	2 (6%)	50,54,54	1.61	8 (16%)
8	GDP	B	501	6	29,30,30	1.22	3 (10%)	45,47,47	1.99	14 (31%)
10	FW9	B	506	-	29,29,29	1.32	3 (10%)	39,40,40	0.99	3 (7%)
10	FW9	D	503	-	29,29,29	1.42	4 (13%)	39,40,40	1.12	5 (12%)
5	GTP	C	501	6	33,34,34	0.98	3 (9%)	50,54,54	1.56	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
12	ACP	F	402	6	-	6/19/38/38	0/3/3/3
5	GTP	D	504	6	-	5/22/38/38	0/3/3/3
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3
8	GDP	B	501	6	-	4/16/32/32	0/3/3/3
10	FW9	B	506	-	-	0/11/17/17	0/4/4/4
10	FW9	D	503	-	-	2/11/17/17	0/4/4/4
5	GTP	C	501	6	-	4/22/38/38	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-7.01	1.67	1.77
12	F	402	ACP	PB-O3A	6.61	1.65	1.58
12	F	402	ACP	PA-O3A	5.97	1.65	1.59
12	F	402	ACP	O4'-C1'	4.68	1.52	1.42
12	F	402	ACP	C6-N6	4.49	1.45	1.34

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	402	ACP	C4-N9-C8	8.93	115.11	105.74
12	F	402	ACP	N3-C4-N9	5.93	137.26	127.17
12	F	402	ACP	C5-C4-N3	-5.63	118.97	126.72
8	B	501	GDP	C5-C4-N3	-5.60	119.48	128.39
5	D	504	GTP	C5-C4-N3	-5.09	120.28	128.39

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

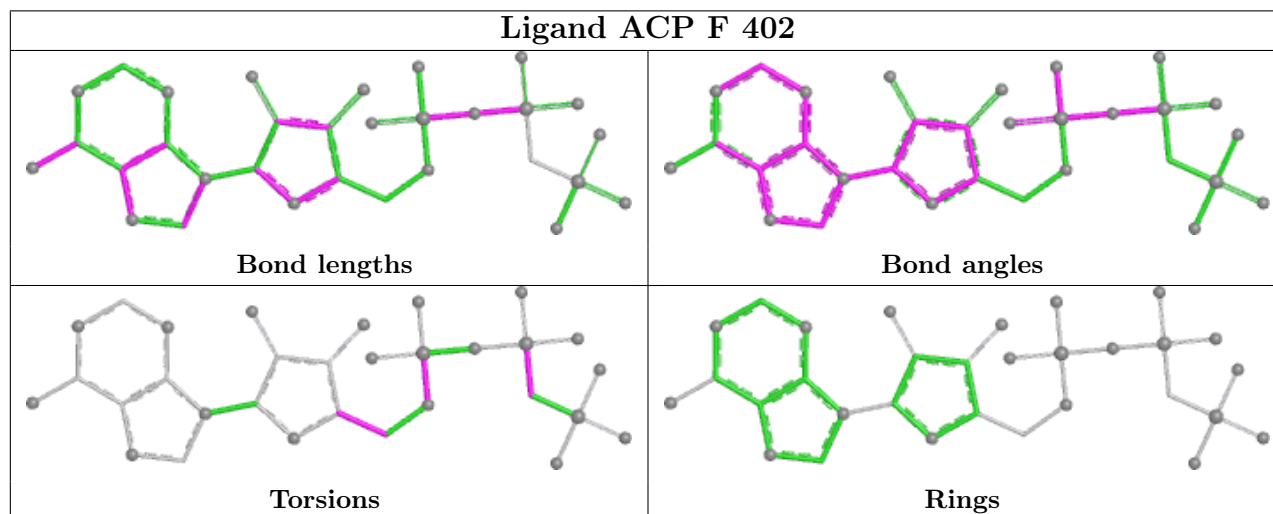
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A

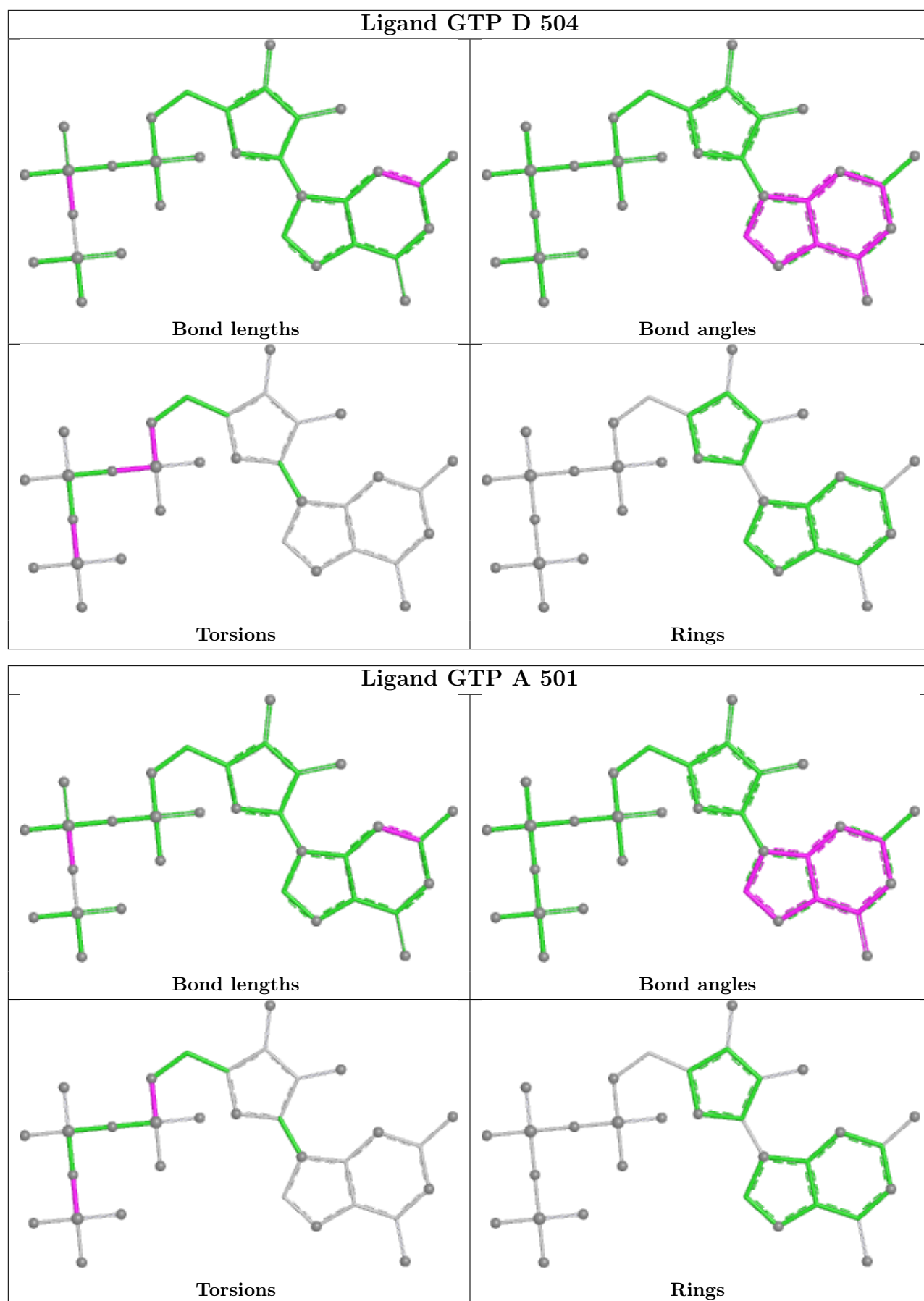
There are no ring outliers.

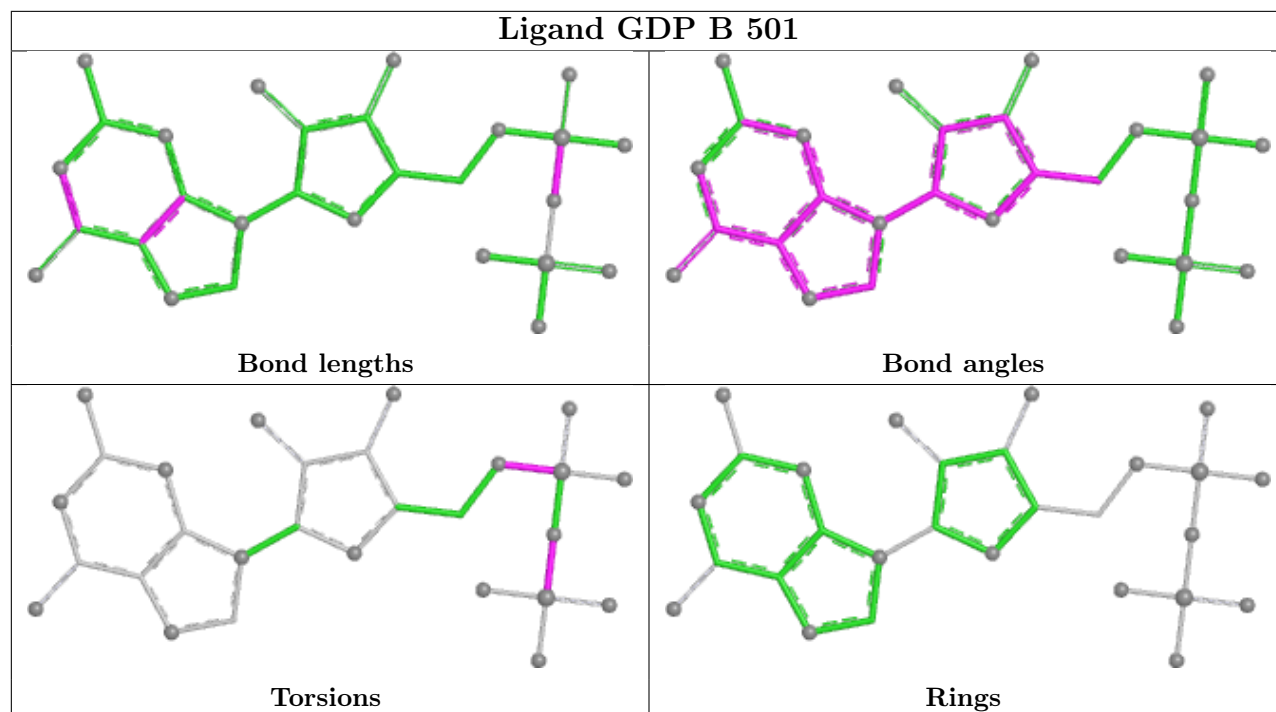
3 monomers are involved in 6 short contacts:

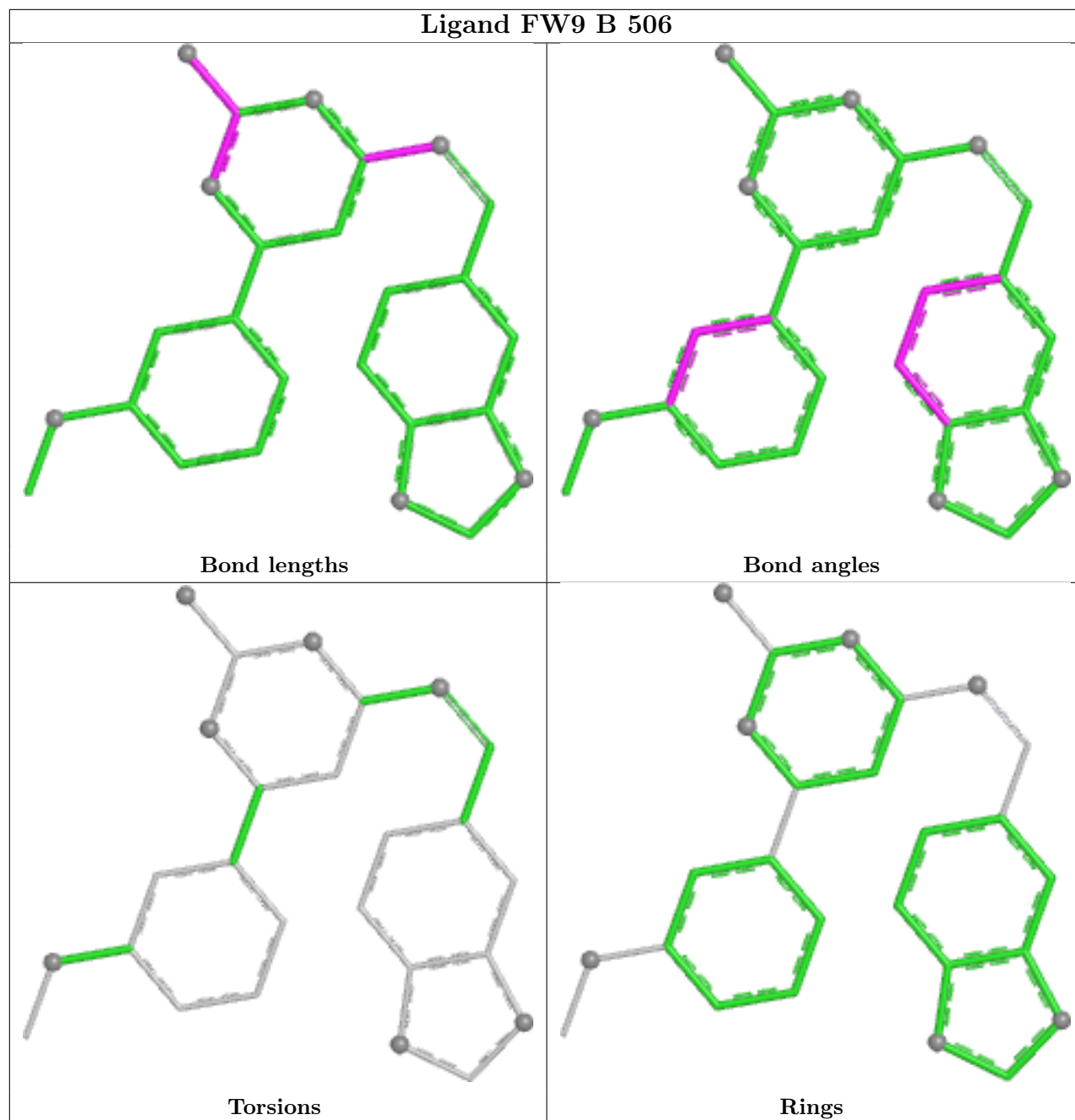
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	F	402	ACP	2	0
8	B	501	GDP	3	0
10	B	506	FW9	1	0

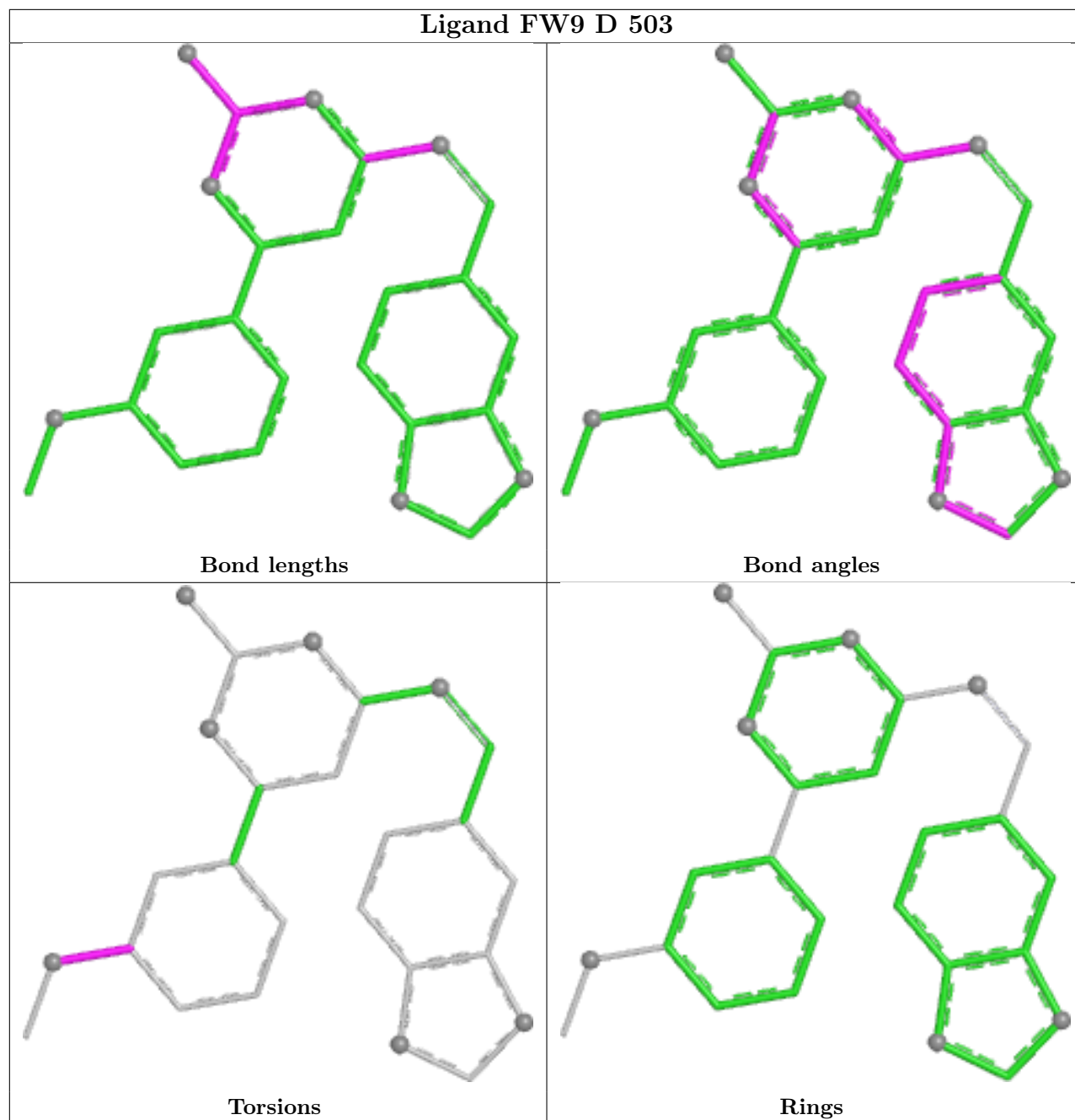
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

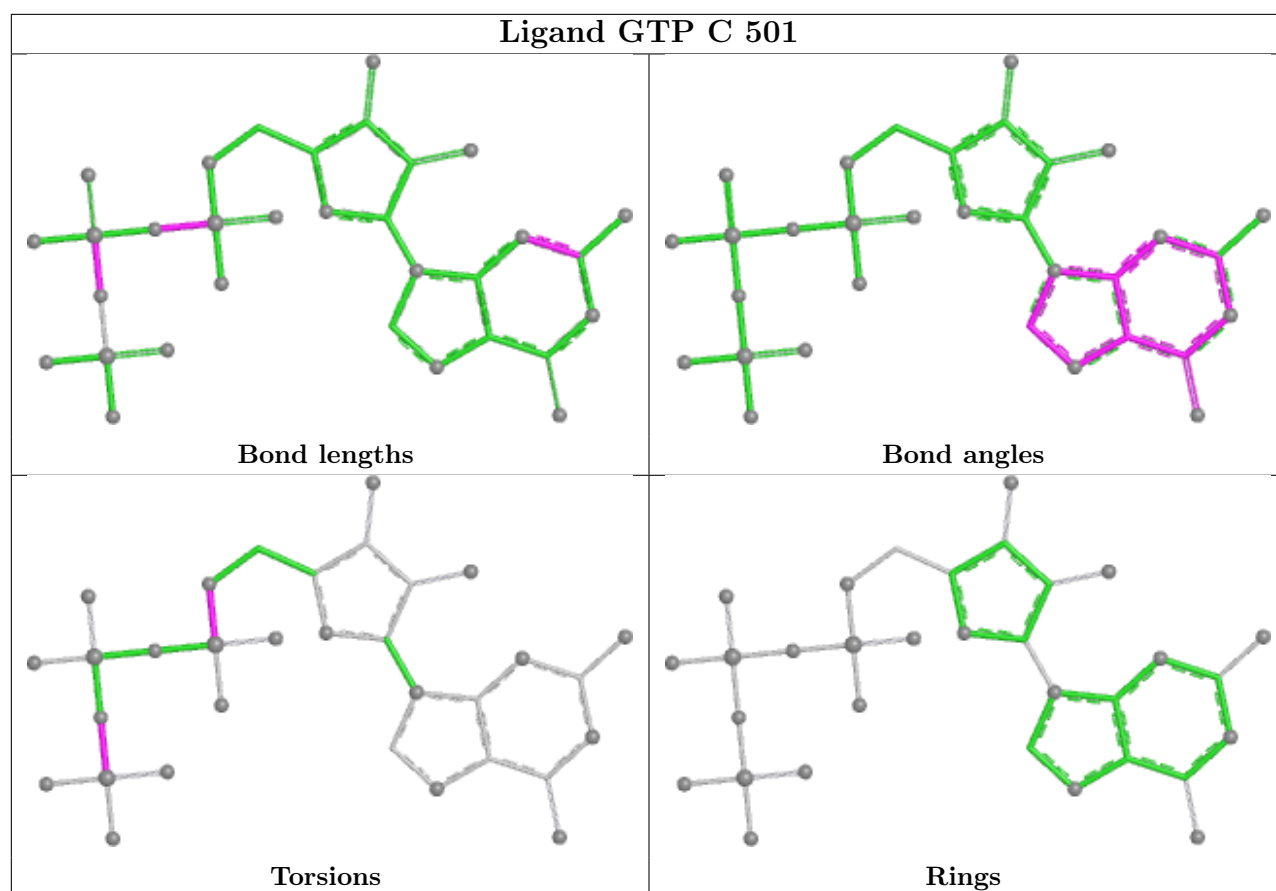












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	438/450 (97%)	0.37	12 (2%) 56 53	31, 67, 85, 119	2 (0%)
1	C	440/450 (97%)	0.19	11 (2%) 58 55	27, 58, 75, 87	6 (1%)
2	B	425/445 (95%)	0.47	19 (4%) 38 34	35, 67, 93, 109	3 (0%)
2	D	423/445 (95%)	0.73	21 (4%) 34 30	44, 79, 98, 109	1 (0%)
3	E	123/143 (86%)	0.74	9 (7%) 21 18	34, 76, 102, 121	2 (1%)
4	F	349/384 (90%)	1.00	46 (13%) 7 6	63, 90, 143, 151	0
All	All	2198/2317 (94%)	0.54	118 (5%) 31 27	27, 71, 111, 151	14 (0%)

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	159	GLY	5.7
2	D	275	SER	5.4
1	C	178	SER	4.7
1	C	179	THR	4.6
4	F	161	LEU	4.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

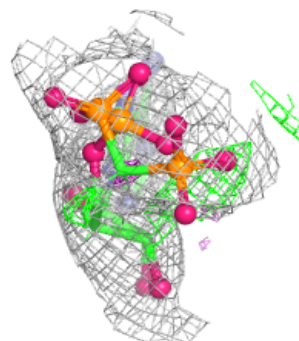
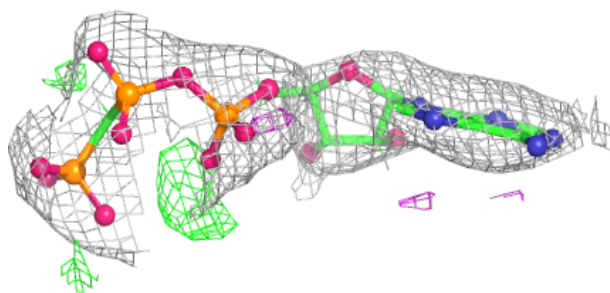
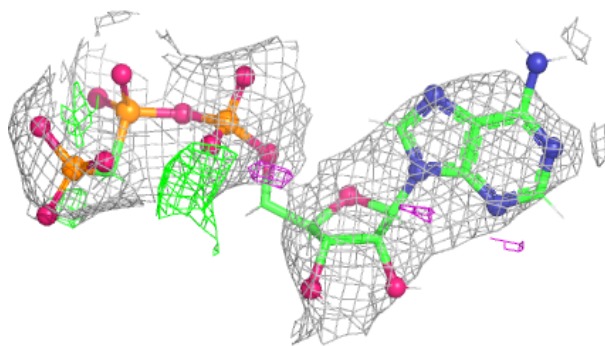
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	F	401	1/1	0.55	0.18	106,106,106,106	0
11	CL	D	505	1/1	0.71	0.52	118,118,118,118	0
7	CA	D	502	1/1	0.77	0.18	98,98,98,98	0
12	ACP	F	402	31/31	0.77	0.13	99,108,133,133	0
7	CA	B	505	1/1	0.81	0.12	88,88,88,88	0
7	CA	E	201	1/1	0.82	0.13	95,95,95,95	0
7	CA	B	504	1/1	0.86	0.12	97,97,97,97	0
10	FW9	B	506	26/26	0.86	0.16	55,67,81,89	0
10	FW9	D	503	26/26	0.88	0.14	58,66,80,82	0
5	GTP	D	504	32/32	0.91	0.10	66,73,86,94	0
9	MES	B	503	12/12	0.91	0.11	55,67,75,76	0
6	MG	D	501	1/1	0.91	0.13	79,79,79,79	0
8	GDP	B	501	28/28	0.93	0.12	46,55,66,77	0
7	CA	A	503	1/1	0.95	0.05	79,79,79,79	0
5	GTP	A	501	32/32	0.96	0.08	47,55,67,73	0
5	GTP	C	501	32/32	0.96	0.08	38,49,61,71	0
7	CA	C	503	1/1	0.99	0.03	66,66,66,66	0
6	MG	B	502	1/1	0.99	0.06	55,55,55,55	0
6	MG	A	502	1/1	0.99	0.06	53,53,53,53	0
6	MG	C	502	1/1	1.00	0.07	44,44,44,44	0

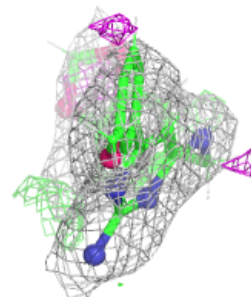
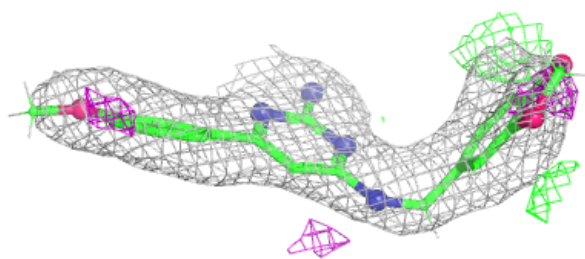
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

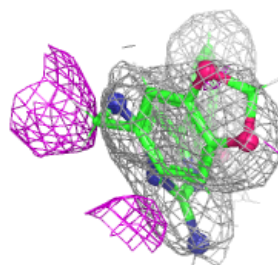
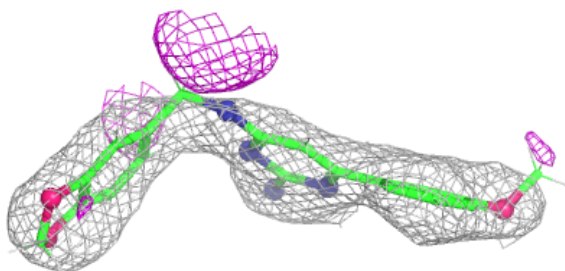
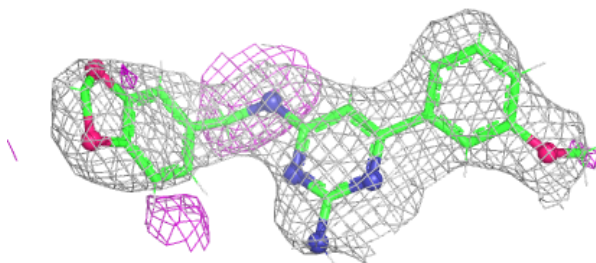
**Electron density around FW9 B 506:**

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

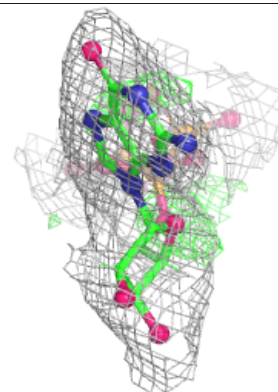
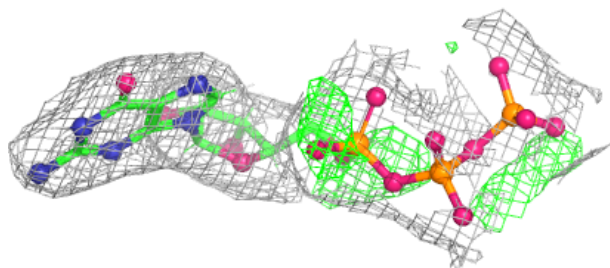
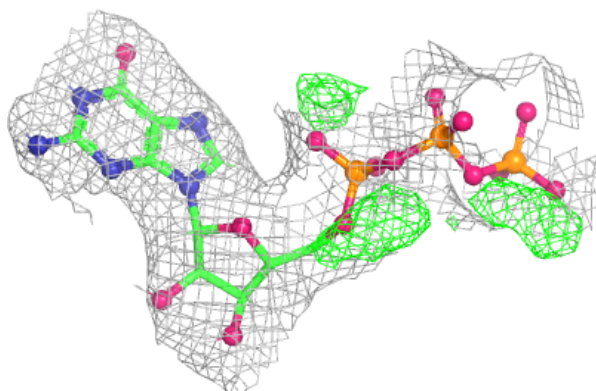


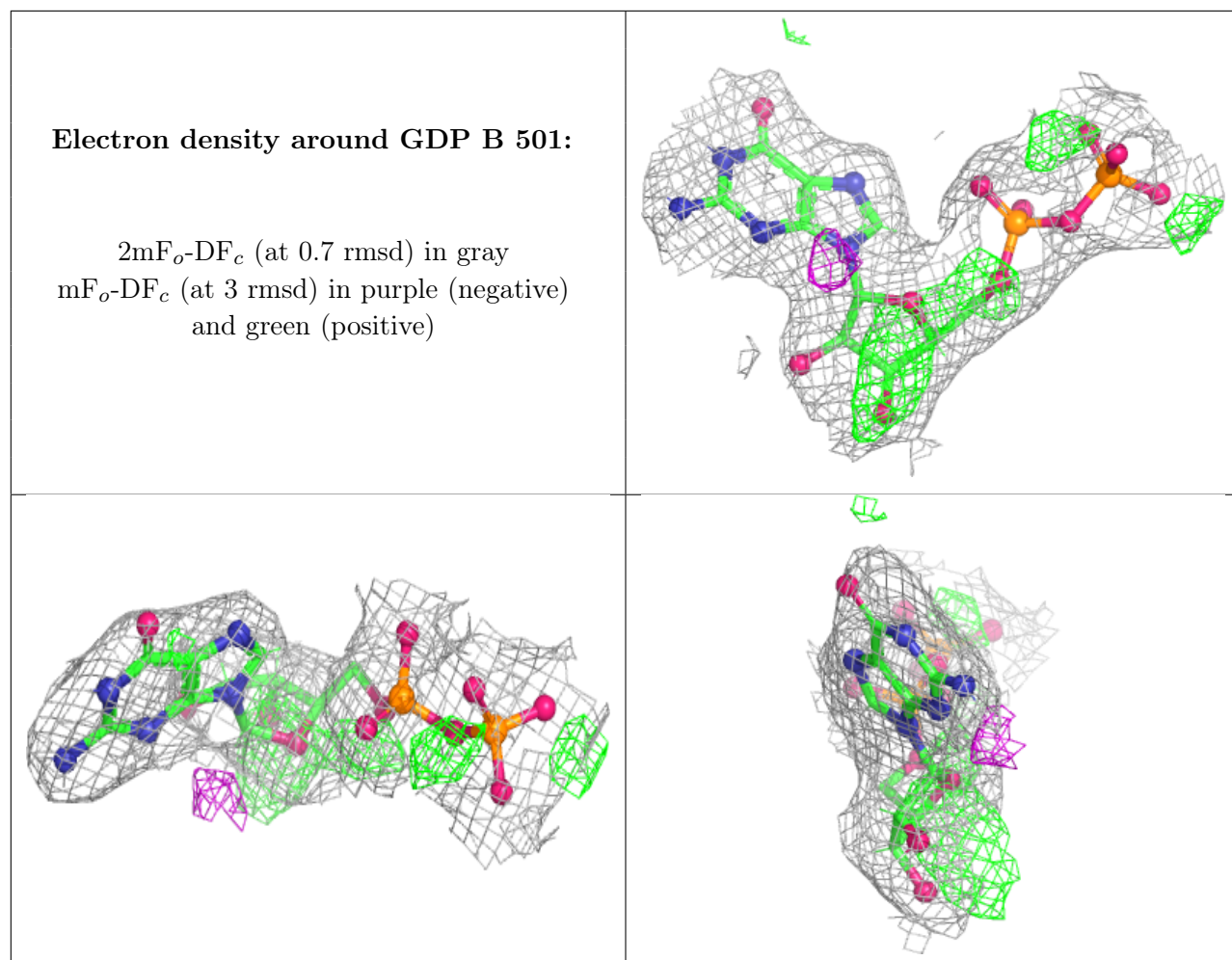
Electron density around FW9 D 503:

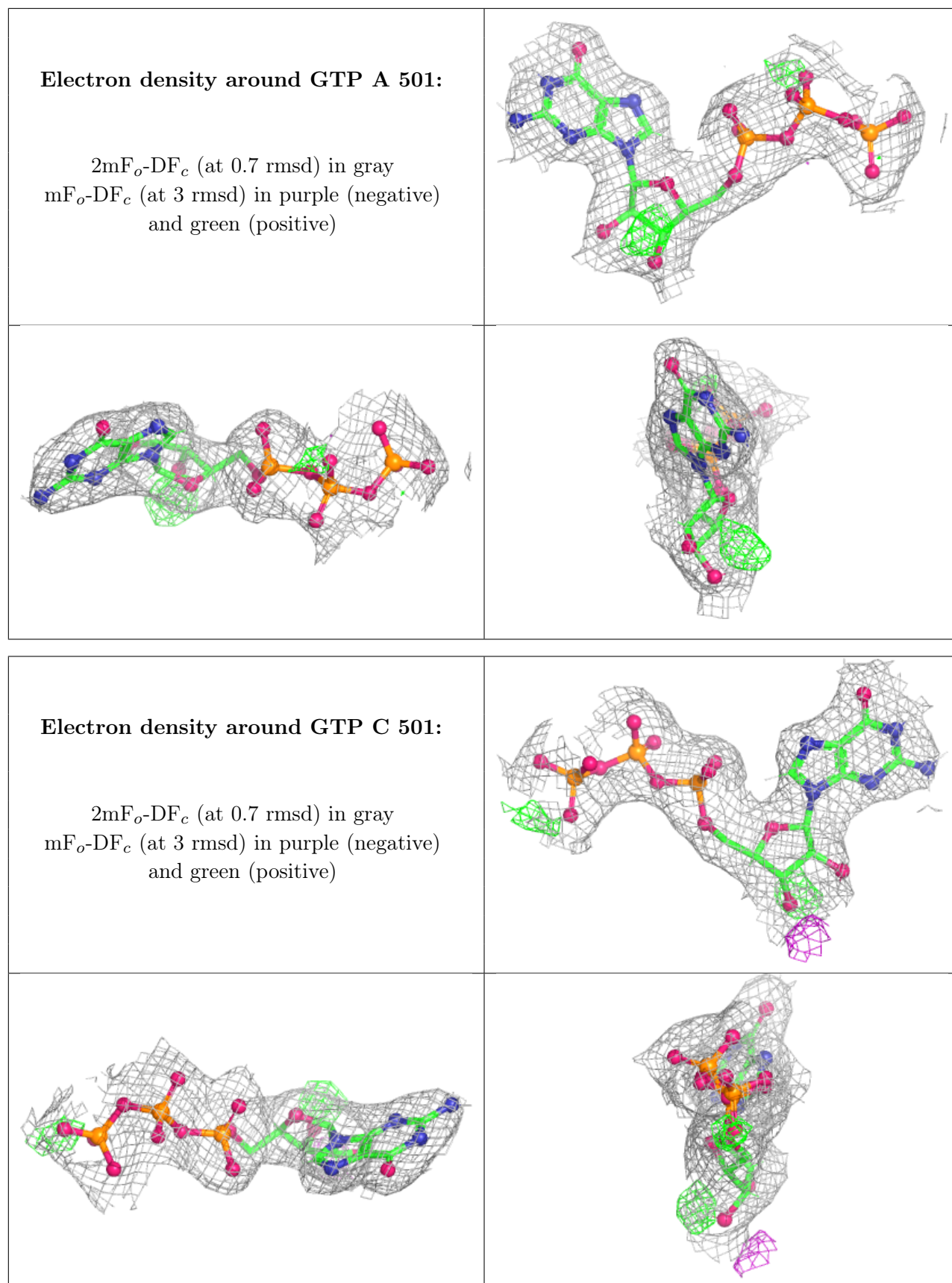
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**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)







6.5 Other polymers [i](#)

There are no such residues in this entry.