



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2024 – 06:41 PM JST

PDB ID : 5H74
Title : Crystal structure of T2R-TTL-14b complex
Authors : Wang, Y.; Yu, Y.; Chen, Q.; Yang, J.
Deposited on : 2016-11-17
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 4.02b-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

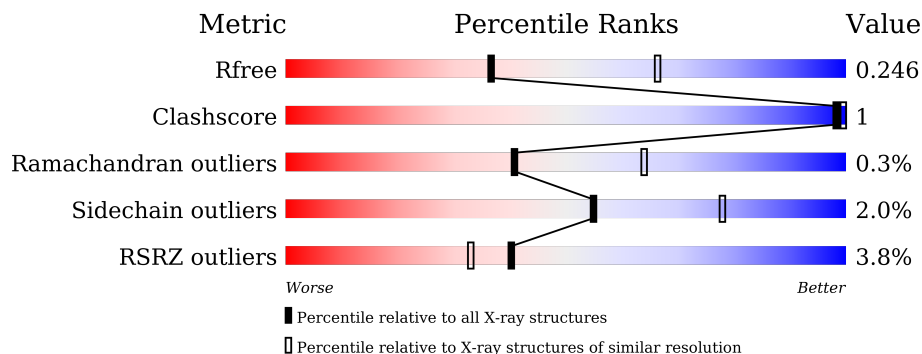
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	 2% (poor fit), 94% (0-3 outliers), 5% (4+ outliers), 1% (not modelled)
1	C	450	 94% (0-3 outliers), 5% (4+ outliers), 1% (not modelled)
2	B	445	 % (poor fit), 94% (0-3 outliers), 5% (4+ outliers), 1% (not modelled)
2	D	445	 4% (poor fit), 91% (0-3 outliers), 5% (4+ outliers), 1% (not modelled)
3	E	143	 3% (poor fit), 82% (0-3 outliers), 15% (4+ outliers), 1% (not modelled)
4	F	384	 12% (poor fit), 84% (0-3 outliers), 13% (4+ outliers), 1% (not modelled)

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
9	MES	C	504	-	-	-	X

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 17862 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	437	Total	C	N	O	S	0	0	0
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	428	Total	C	N	O	S	0	0	0
			3369	2115	577	650	27			
2	D	424	Total	C	N	O	S	0	0	0
			3333	2093	568	645	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	121	Total	C	N	O	S	0	0	0
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

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

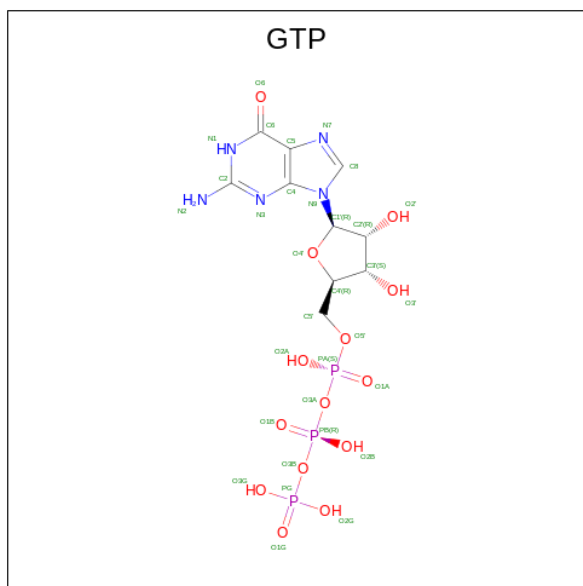
- Molecule 4 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	334	Total	C	N	O	S	0	0	0
			2744	1761	470	499	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 (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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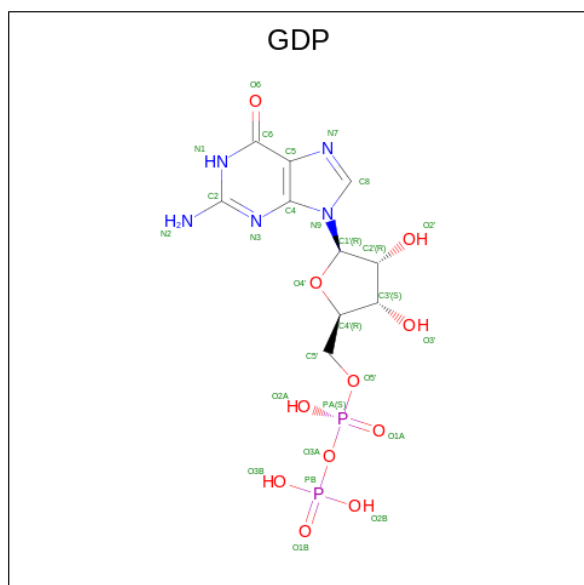
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		

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

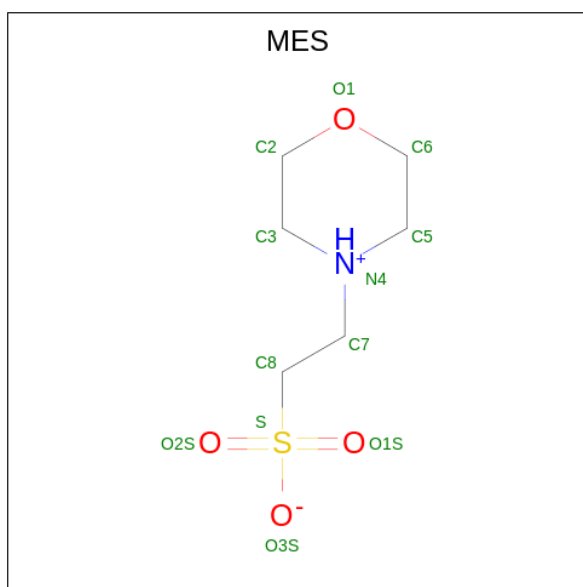
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	0	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



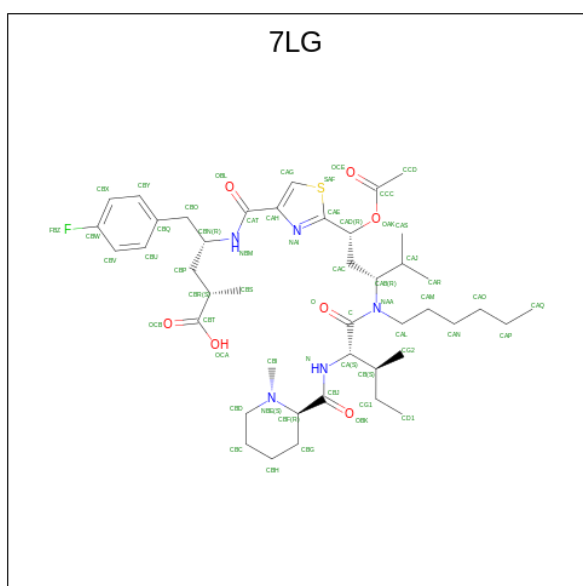
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



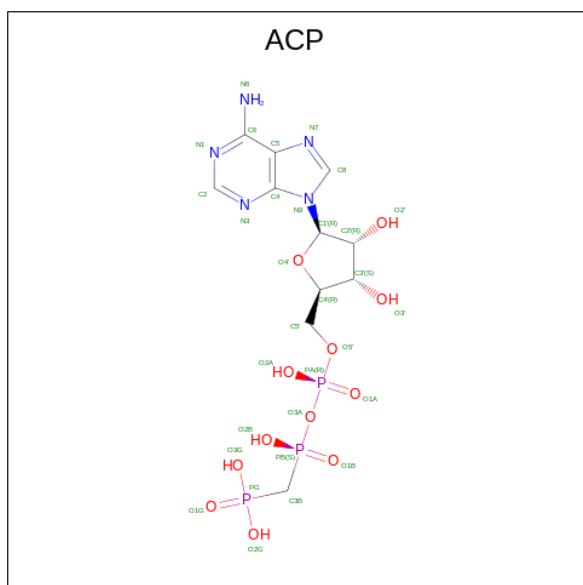
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
9	B	1	Total	12	6	1	4	1	0	0
9	B	1	Total	12	6	1	4	1	0	0
9	C	1	Total	12	6	1	4	1	0	0

- Molecule 10 is (2 {S},4 {R})-4-[[2-[(1 {R},3 {R})-1-acetyloxy-3-[hexyl-(2 {S},3 {S})-3-methyl-2-[[[(2 {R})-1-methylpiperidin-2-yl]carbonylamino]pentanoyl]amino]-4-methyl-pentyl]-1,3-thiazol-4-yl]carbonylamino]-5-(4-fluorophenyl)-2-methyl-pentanoic acid (three-letter code: 7LG) (formula: C₄₃H₆₆FN₅O₇S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
10	B	1	Total	C	F	N	O	S	0	0
			57	43	1	5	7	1		
10	D	1	Total	C	F	N	O	S	0	0
			57	43	1	5	7	1		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	F	1	Total	C <td>N <td>O <td>P <td>0</td> <td>0</td> </td></td></td>	N <td>O <td>P <td>0</td> <td>0</td> </td></td>	O <td>P <td>0</td> <td>0</td> </td>	P <td>0</td> <td>0</td>	0	0
			31	11	5	12	3		

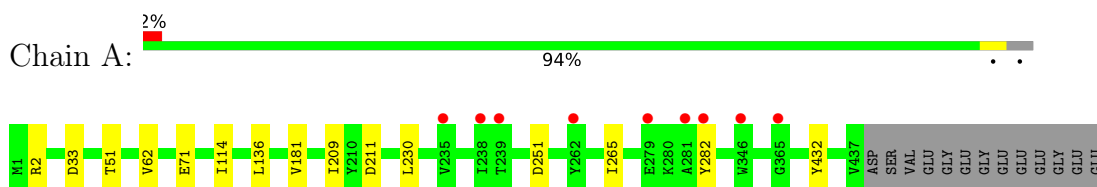
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	64	Total 64 O	0	0
12	B	67	Total 67 O	0	0
12	C	87	Total 87 O	0	0
12	D	12	Total 12 O	0	0
12	E	6	Total 6 O	0	0
12	F	16	Total 16 O	0	0

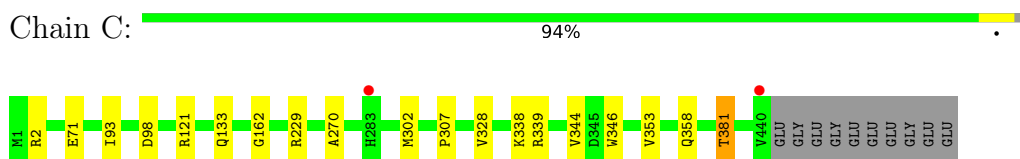
3 Residue-property plots [i](#)

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

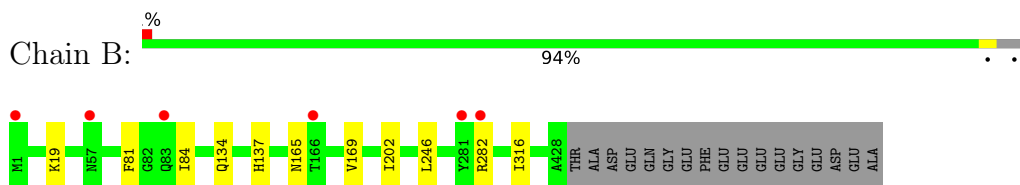
- Molecule 1: Tubulin alpha-1B chain



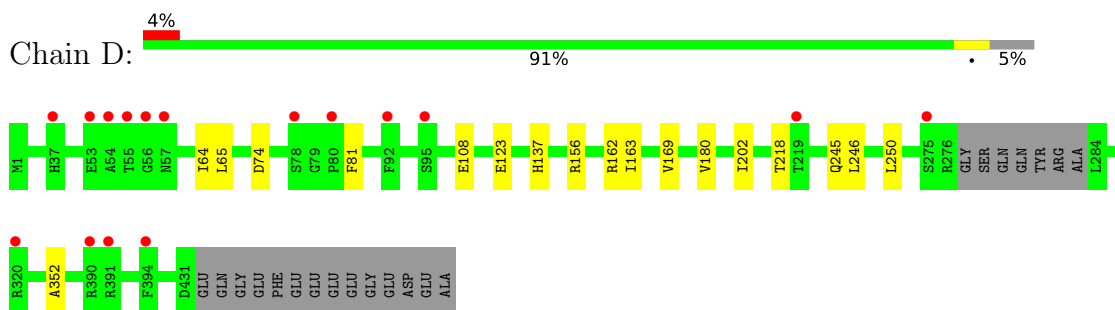
- Molecule 1: Tubulin alpha-1B chain



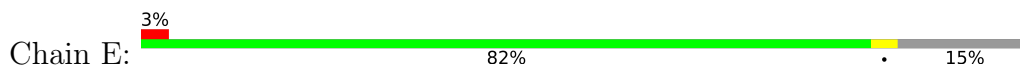
- Molecule 2: Tubulin beta-2B chain

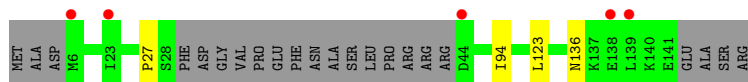


- Molecule 2: Tubulin beta-2B chain

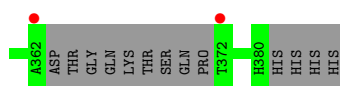
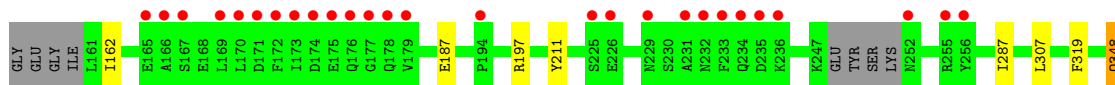
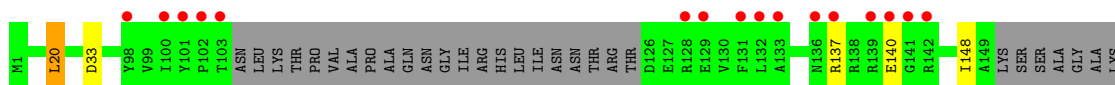
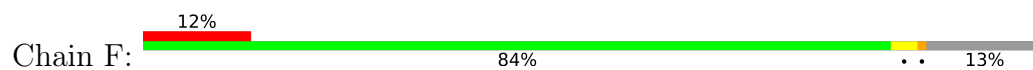


- Molecule 3: Stathmin-4





- Molecule 4: Uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.41Å 154.03Å 185.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 35.46 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.60) 99.8 (35.46-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.201 , 0.248 0.202 , 0.246	Depositor DCC
R_{free} test set	4591 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtrriage
Anisotropy	0.386	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17862	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: 7LG, GTP, GDP, MES, ACP, MG, CA

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	0.40	0/3494	0.61	0/4743
1	C	0.40	0/3515	0.63	0/4772
2	B	0.40	0/3444	0.61	0/4664
2	D	0.40	0/3406	0.60	0/4613
3	E	0.41	0/1008	0.59	0/1337
4	F	0.40	0/2806	0.59	0/3791
All	All	0.40	0/17673	0.61	0/23920

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	3416	0	3331	3	0
1	C	3437	0	3348	8	0
2	B	3369	0	3250	3	0
2	D	3333	0	3214	4	0
3	E	1000	0	1018	1	0
4	F	2744	0	2709	3	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
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
9	B	24	0	26	0	0
9	C	12	0	13	0	0
10	B	57	0	0	0	0
10	D	57	0	0	0	0
11	F	31	0	14	0	0
12	A	64	0	0	0	0
12	B	67	0	0	0	0
12	C	87	0	0	0	0
12	D	12	0	0	0	0
12	E	6	0	0	0	0
12	F	16	0	0	0	0
All	All	17862	0	16971	21	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 1.

All (21) 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)
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.37	0.59
2:D:246:LEU:HD12	2:D:352:ALA:HB2	1.91	0.52
2:D:64:ILE:HD11	2:D:123:GLU:HG3	1.91	0.51
2:B:134:GLN:HA	2:B:165:ASN:O	2.09	0.51
2:D:163:ILE:HG21	2:D:250:LEU:HB3	1.92	0.51
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.93	0.51
1:C:307:PRO:HB3	1:C:381:THR:HG21	1.92	0.51
2:B:169:VAL:HA	2:B:202:ILE:O	2.15	0.46
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.50	0.46
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.51	0.45
4:F:20:LEU:HD11	4:F:348:GLN:HG2	1.98	0.44
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.99	0.44
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:VAL:HA	2:D:202:ILE:O	2.19	0.42
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.00	0.42
1:A:2:ARG:O	1:A:51:THR:HG23	2.20	0.41
1:C:270:ALA:HB3	1:C:302:MET:CE	2.50	0.41
2:B:81:PHE:O	2:B:84:ILE:HG22	2.21	0.41
4:F:148:ILE:HD13	4:F:162:ILE:HG12	2.02	0.41
1:C:328:VAL:HG11	1:C:353:VAL:HG11	2.03	0.41
1:C:270:ALA:HB3	1:C:302:MET:HE2	2.03	0.41

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	435/450 (97%)	427 (98%)	7 (2%)	1 (0%)	47 71
1	C	438/450 (97%)	425 (97%)	11 (2%)	2 (0%)	29 52
2	B	426/445 (96%)	417 (98%)	9 (2%)	0	100 100
2	D	420/445 (94%)	407 (97%)	12 (3%)	1 (0%)	47 71
3	E	117/143 (82%)	115 (98%)	0	2 (2%)	9 18
4	F	324/384 (84%)	309 (95%)	15 (5%)	0	100 100
All	All	2160/2317 (93%)	2100 (97%)	54 (2%)	6 (0%)	41 64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	338	LYS
3	E	136	ASN
1	A	282	TYR
1	C	339	ARG

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Mol	Chain	Res	Type
3	E	27	PRO
2	D	81	PHE

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	368/378 (97%)	360 (98%)	8 (2%)	52	76
1	C	371/378 (98%)	366 (99%)	5 (1%)	69	86
2	B	370/383 (97%)	365 (99%)	5 (1%)	67	85
2	D	367/383 (96%)	358 (98%)	9 (2%)	47	73
3	E	109/127 (86%)	108 (99%)	1 (1%)	78	91
4	F	301/342 (88%)	292 (97%)	9 (3%)	41	67
All	All	1886/1991 (95%)	1849 (98%)	37 (2%)	55	78

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	62	VAL
1	A	71	GLU
1	A	114	ILE
1	A	136	LEU
1	A	181	VAL
1	A	211	ASP
1	A	251	ASP
2	B	19	LYS
2	B	137	HIS
2	B	246	LEU
2	B	282	ARG
2	B	316	ILE
1	C	2	ARG
1	C	133	GLN
1	C	229	ARG

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Mol	Chain	Res	Type
1	C	358	GLN
1	C	381	THR
2	D	65	LEU
2	D	74	ASP
2	D	108	GLU
2	D	137	HIS
2	D	156	ARG
2	D	162	ARG
2	D	180	VAL
2	D	218	THR
2	D	245	GLN
3	E	123	LEU
4	F	20	LEU
4	F	33	ASP
4	F	137	ARG
4	F	140	GLU
4	F	187	GLU
4	F	197	ARG
4	F	211	TYR
4	F	307	LEU
4	F	348	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	406	HIS
2	B	15	GLN
2	B	245	GLN
2	D	8	GLN
4	F	252	ASN

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 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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	501	-	24,30,30	0.90	0	30,47,47	1.02	2 (6%)
9	MES	B	503	-	12,12,12	1.96	1 (8%)	14,16,16	6.54	6 (42%)
9	MES	C	504	-	12,12,12	2.18	1 (8%)	14,16,16	1.33	2 (14%)
5	GTP	A	501	6	26,34,34	1.00	2 (7%)	32,54,54	1.11	3 (9%)
10	7LG	B	505	-	57,59,59	1.44	5 (8%)	66,80,80	1.95	9 (13%)
9	MES	B	504	-	12,12,12	2.39	1 (8%)	14,16,16	1.49	1 (7%)
11	ACP	F	401	-	27,33,33	1.79	7 (25%)	32,52,52	1.32	4 (12%)
5	GTP	D	501	6	26,34,34	0.91	0	32,54,54	1.15	4 (12%)
5	GTP	C	501	6	26,34,34	0.87	1 (3%)	32,54,54	1.03	1 (3%)
10	7LG	D	503	-	57,59,59	1.54	6 (10%)	66,80,80	1.51	13 (19%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GDP	B	501	-	-	3/12/32/32	0/3/3/3
9	MES	B	503	-	-	1/6/14/14	0/1/1/1
9	MES	C	504	-	-	3/6/14/14	0/1/1/1
5	GTP	A	501	6	-	4/18/38/38	0/3/3/3
10	7LG	B	505	-	-	3/60/79/79	1/3/3/3
9	MES	B	504	-	-	3/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ACP	F	401	-	-	1/15/38/38	0/3/3/3
5	GTP	D	501	6	-	3/18/38/38	0/3/3/3
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3
10	7LG	D	503	-	-	3/60/79/79	1/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.98	1.66	1.77
9	C	504	MES	C8-S	-7.21	1.67	1.77
9	B	503	MES	C8-S	-6.31	1.68	1.77
10	D	503	7LG	CAH-CAT	-6.03	1.36	1.50
10	B	505	7LG	CAH-CAT	-5.85	1.36	1.50
11	F	401	ACP	PG-O1G	5.52	1.61	1.50
10	D	503	7LG	CBO-CBQ	-4.17	1.41	1.51
10	B	505	7LG	CBO-CBQ	-4.04	1.41	1.51
10	D	503	7LG	CAE-SAF	-3.30	1.63	1.73
11	F	401	ACP	PB-O3A	2.96	1.61	1.58
11	F	401	ACP	PG-O3G	2.95	1.61	1.54
11	F	401	ACP	PG-O2G	-2.76	1.48	1.54
5	A	501	GTP	C6-N1	-2.71	1.33	1.37
11	F	401	ACP	C5-C4	2.62	1.47	1.40
10	B	505	7LG	CBG-CBF	2.60	1.58	1.53
10	D	503	7LG	CAC-CAD	2.58	1.55	1.52
10	D	503	7LG	CBG-CBF	2.37	1.58	1.53
11	F	401	ACP	C2-N3	2.35	1.35	1.32
10	B	505	7LG	CAC-CAD	2.35	1.55	1.52
11	F	401	ACP	PB-O2B	2.24	1.61	1.56
10	B	505	7LG	CAE-SAF	-2.22	1.66	1.73
10	D	503	7LG	CAC-CAB	2.15	1.56	1.53
5	C	501	GTP	C6-N1	-2.13	1.34	1.37
5	A	501	GTP	O4'-C1'	2.12	1.44	1.41

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	MES	O2S-S-C8	-14.89	88.98	106.92
9	B	503	MES	O3S-S-O2S	-12.02	81.91	111.27
10	B	505	7LG	CAD-OAK-CCC	11.72	127.58	117.37
9	B	503	MES	O2S-S-O1S	-9.19	82.14	113.95
9	B	503	MES	O1S-S-C8	9.15	117.94	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	503	MES	O3S-S-O1S	5.48	124.65	111.27
9	B	503	MES	O3S-S-C8	5.31	114.36	105.77
10	B	505	7LG	CAM-CAL-NAA	-4.39	106.53	113.31
9	B	504	MES	O3S-S-C8	4.12	112.43	105.77
10	B	505	7LG	OAK-CCC-CCD	4.03	118.50	111.09
10	D	503	7LG	CAM-CAL-NAA	-3.91	107.27	113.31
11	F	401	ACP	N3-C2-N1	-3.69	122.90	128.68
10	D	503	7LG	CBP-CBN-CBO	-3.58	107.91	112.42
10	D	503	7LG	CBP-CBN-NBM	3.43	118.71	110.49
10	D	503	7LG	CAH-CAG-SAF	-3.38	107.63	111.79
10	B	505	7LG	CAO-CAN-CAM	-3.32	97.59	114.42
10	D	503	7LG	OAK-CCC-CCD	3.14	116.86	111.09
10	D	503	7LG	CAD-OAK-CCC	3.04	120.02	117.37
11	F	401	ACP	PB-O3A-PA	-2.98	123.12	132.56
5	D	501	GTP	PB-O3B-PG	-2.72	123.49	132.83
10	D	503	7LG	CAH-CAT-NBM	2.68	120.17	115.20
11	F	401	ACP	C3'-C2'-C1'	2.64	104.95	100.98
9	C	504	MES	O2S-S-C8	2.63	110.08	106.92
10	B	505	7LG	CBX-CBW-CBV	-2.54	119.45	122.83
11	F	401	ACP	C4-C5-N7	-2.53	106.76	109.40
9	C	504	MES	O1S-S-C8	2.46	109.87	106.92
10	D	503	7LG	CBX-CBW-CBV	-2.42	119.61	122.83
5	A	501	GTP	C5-C6-N1	2.40	118.19	113.95
10	D	503	7LG	CBC-CBH-CBG	-2.38	106.56	111.42
5	C	501	GTP	C5-C6-N1	2.37	118.14	113.95
10	B	505	7LG	CAH-CAG-SAF	-2.36	108.89	111.79
5	D	501	GTP	C8-N7-C5	2.34	107.45	102.99
5	D	501	GTP	PA-O3A-PB	-2.29	124.97	132.83
5	A	501	GTP	C8-N7-C5	2.27	107.31	102.99
8	B	501	GDP	PA-O3A-PB	-2.25	125.11	132.83
10	D	503	7LG	CAO-CAN-CAM	-2.19	103.33	114.42
10	B	505	7LG	CBY-CBX-CBW	2.17	120.60	118.36
5	D	501	GTP	C5-C6-N1	2.13	117.72	113.95
10	B	505	7LG	CBD-NBE-CBF	-2.05	108.37	112.39
10	D	503	7LG	CBO-CBN-NBM	-2.04	106.47	110.39
8	B	501	GDP	C5-C6-N1	2.04	117.55	113.95
10	B	505	7LG	CAH-CAT-NBM	2.03	118.98	115.20
10	D	503	7LG	CBY-CBX-CBW	2.02	120.45	118.36
10	D	503	7LG	OAK-CAD-CAC	2.01	110.94	106.54
5	A	501	GTP	PA-O3A-PB	-2.01	125.92	132.83

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O1A
9	B	503	MES	C7-C8-S-O3S
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O3S
9	C	504	MES	N4-C7-C8-S
10	B	505	7LG	OCE-CCC-OAK-CAD
10	D	503	7LG	OCE-CCC-OAK-CAD
10	D	503	7LG	CCD-CCC-OAK-CAD
10	B	505	7LG	CCD-CCC-OAK-CAD
9	C	504	MES	C8-C7-N4-C5
10	D	503	7LG	CAM-CAN-CAO-CAP
5	A	501	GTP	PB-O3B-PG-O2G
8	B	501	GDP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
10	B	505	7LG	CAN-CAO-CAP-CAQ
9	B	504	MES	C7-C8-S-O2S
9	C	504	MES	C8-C7-N4-C3
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A

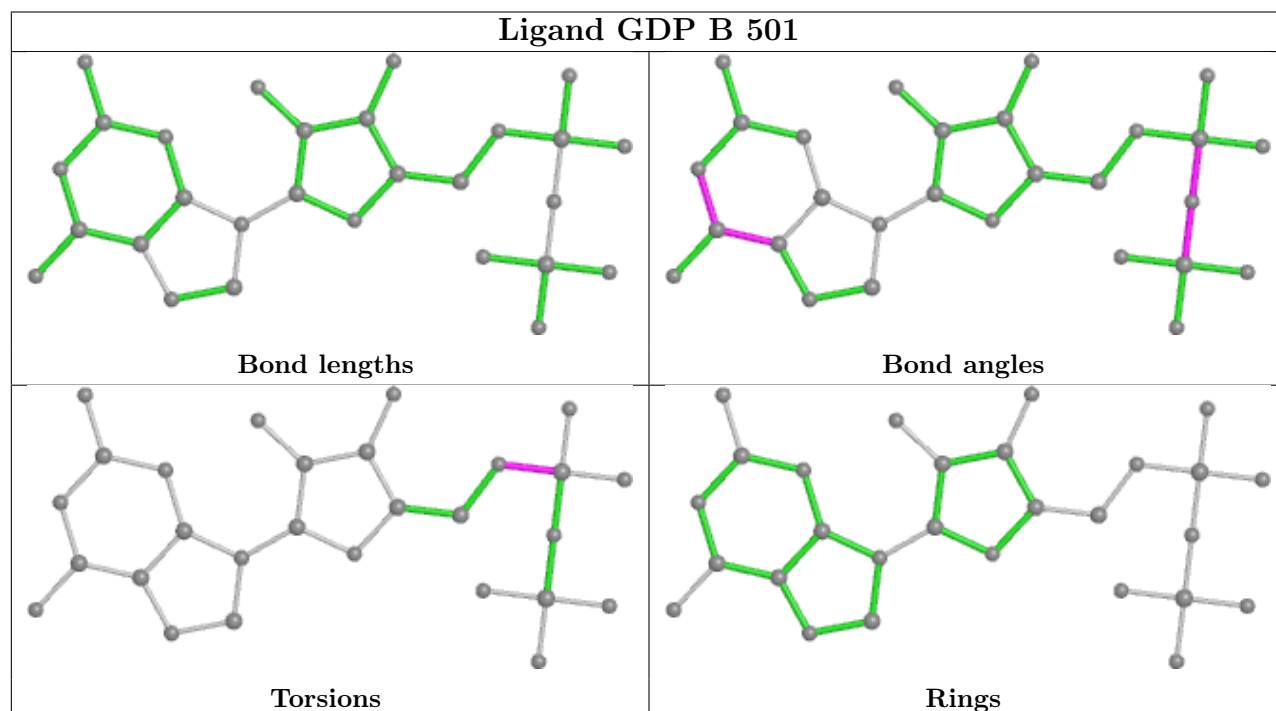
All (2) ring outliers are listed below:

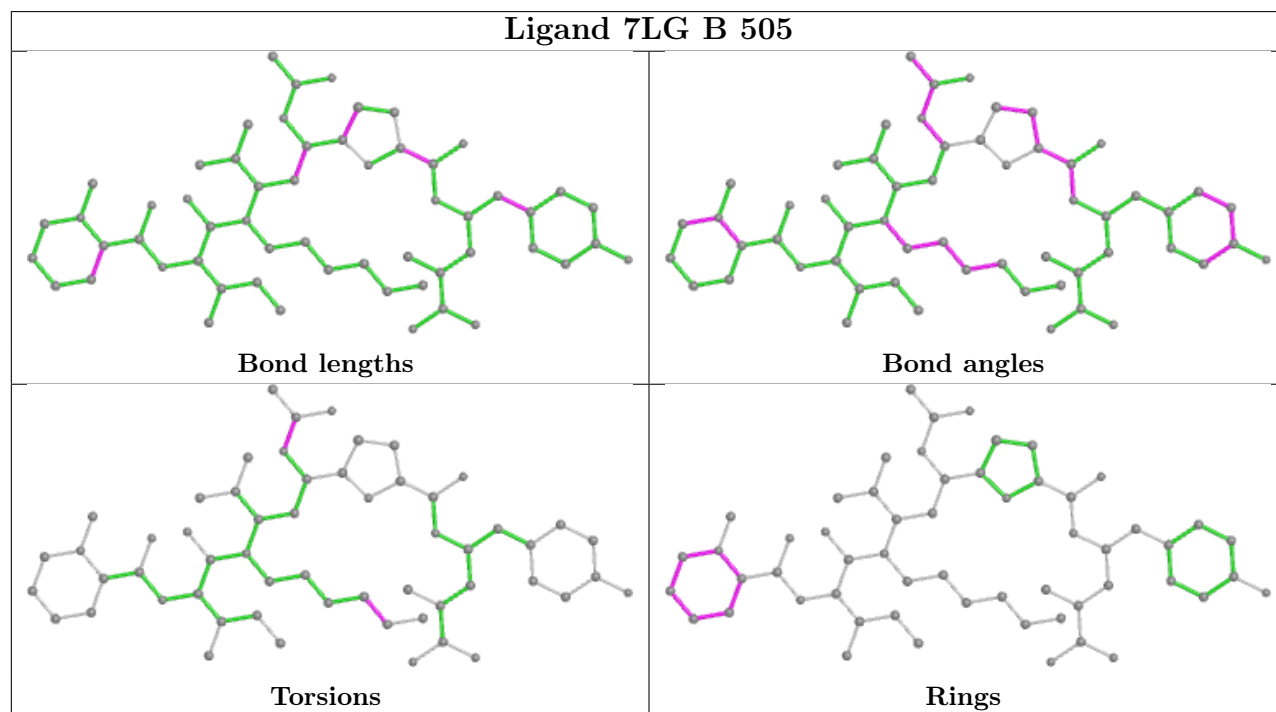
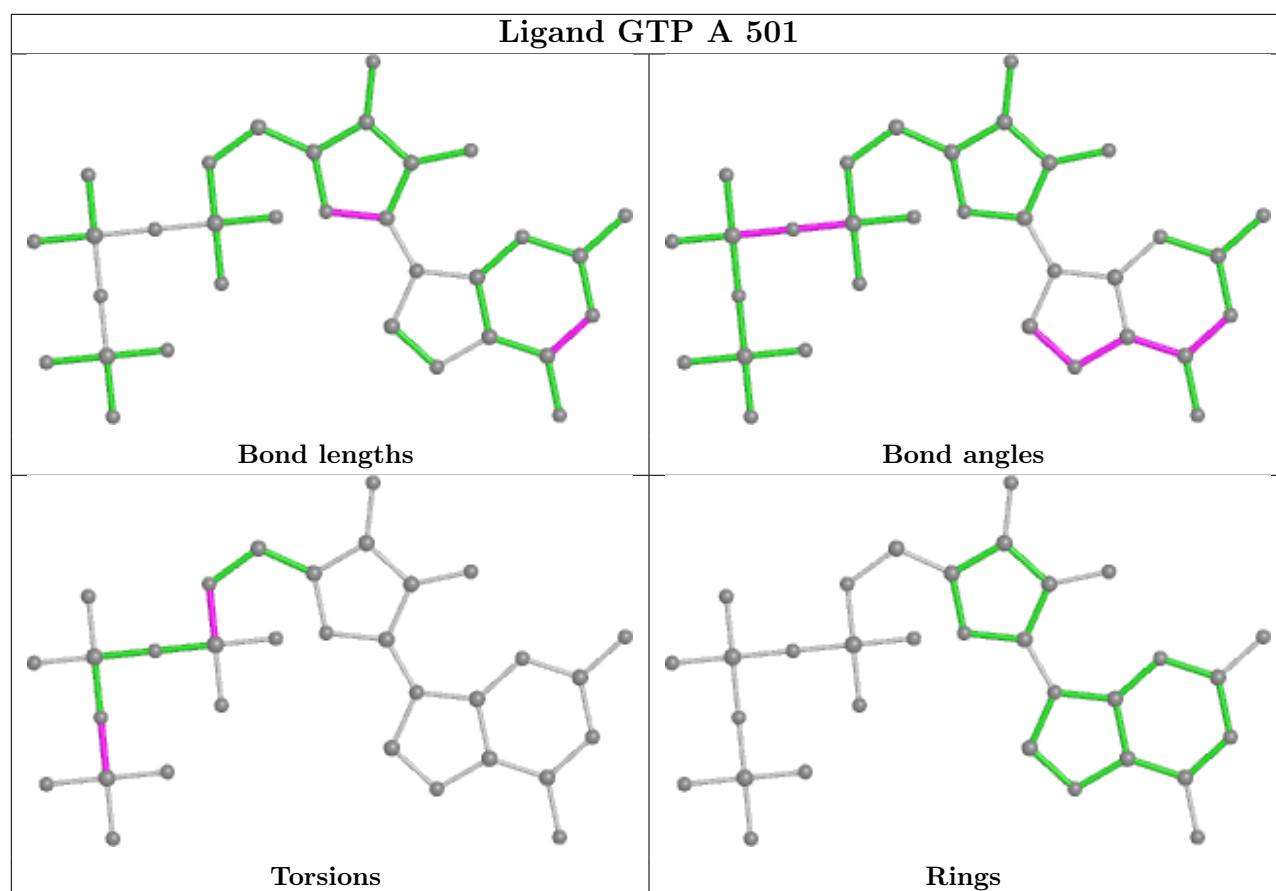
Mol	Chain	Res	Type	Atoms
10	B	505	7LG	CBC-CBD-CBF-CBG-CBH-NBE
10	D	503	7LG	CBC-CBD-CBF-CBG-CBH-NBE

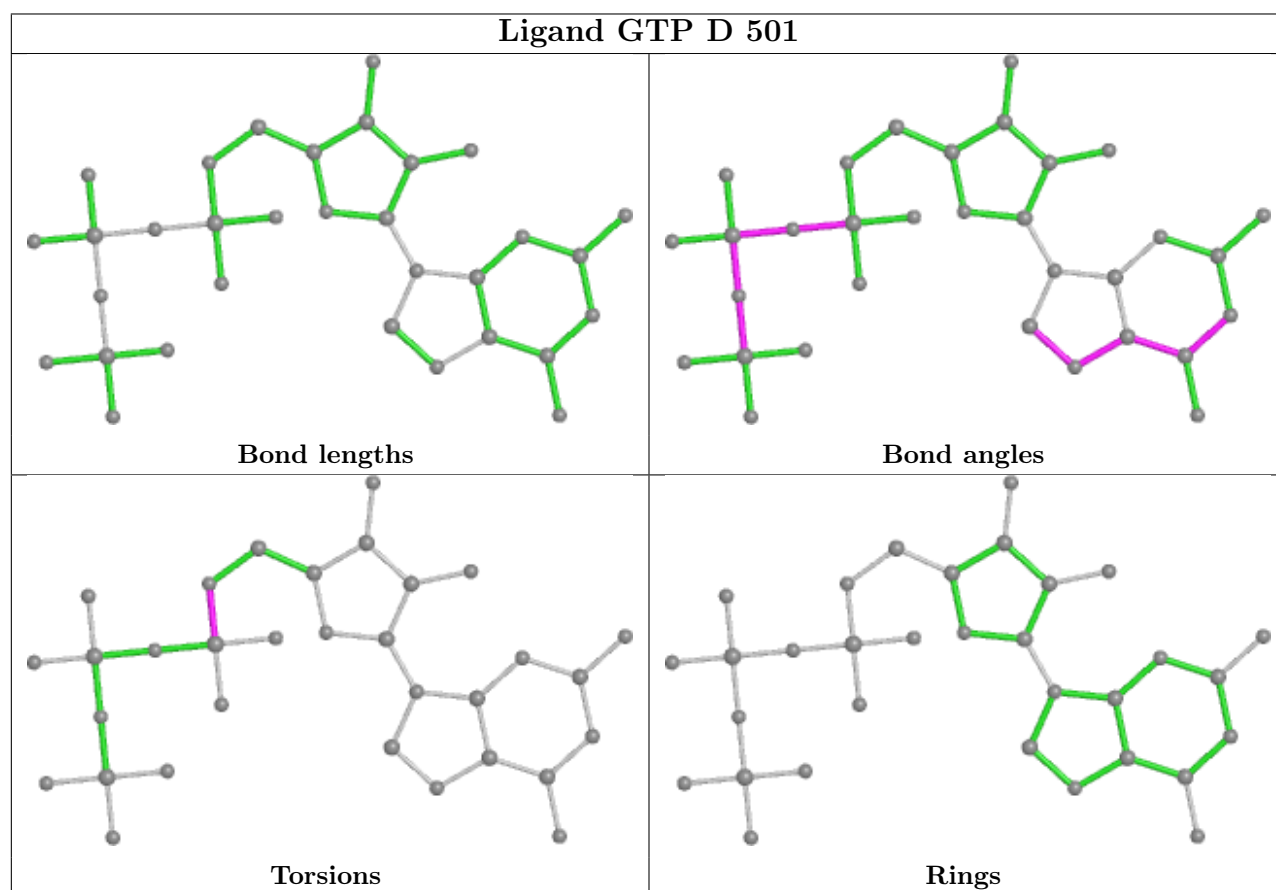
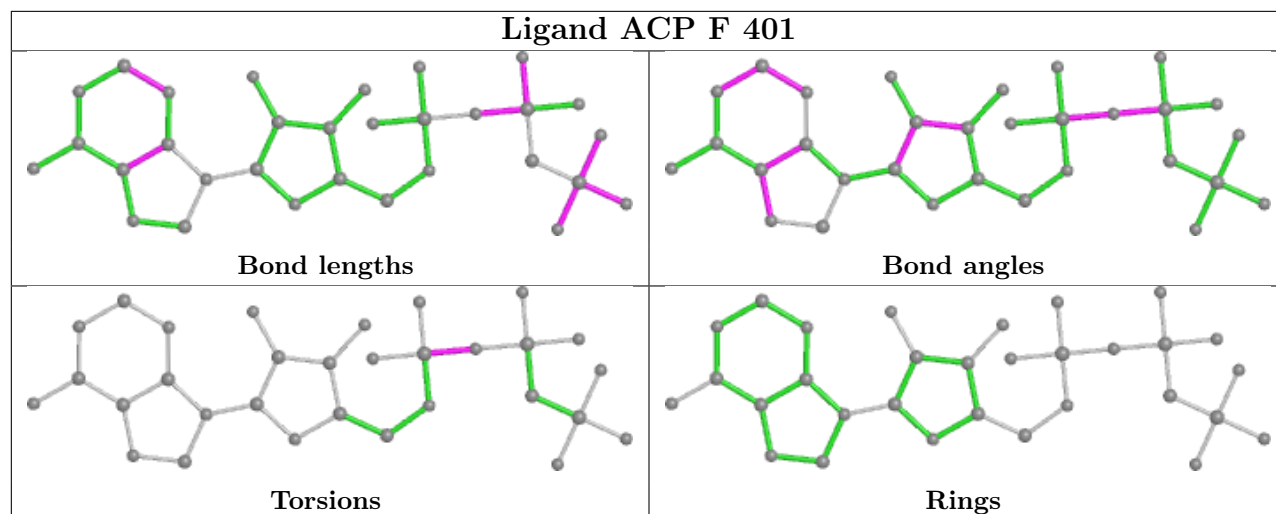
No monomer is involved in short contacts.

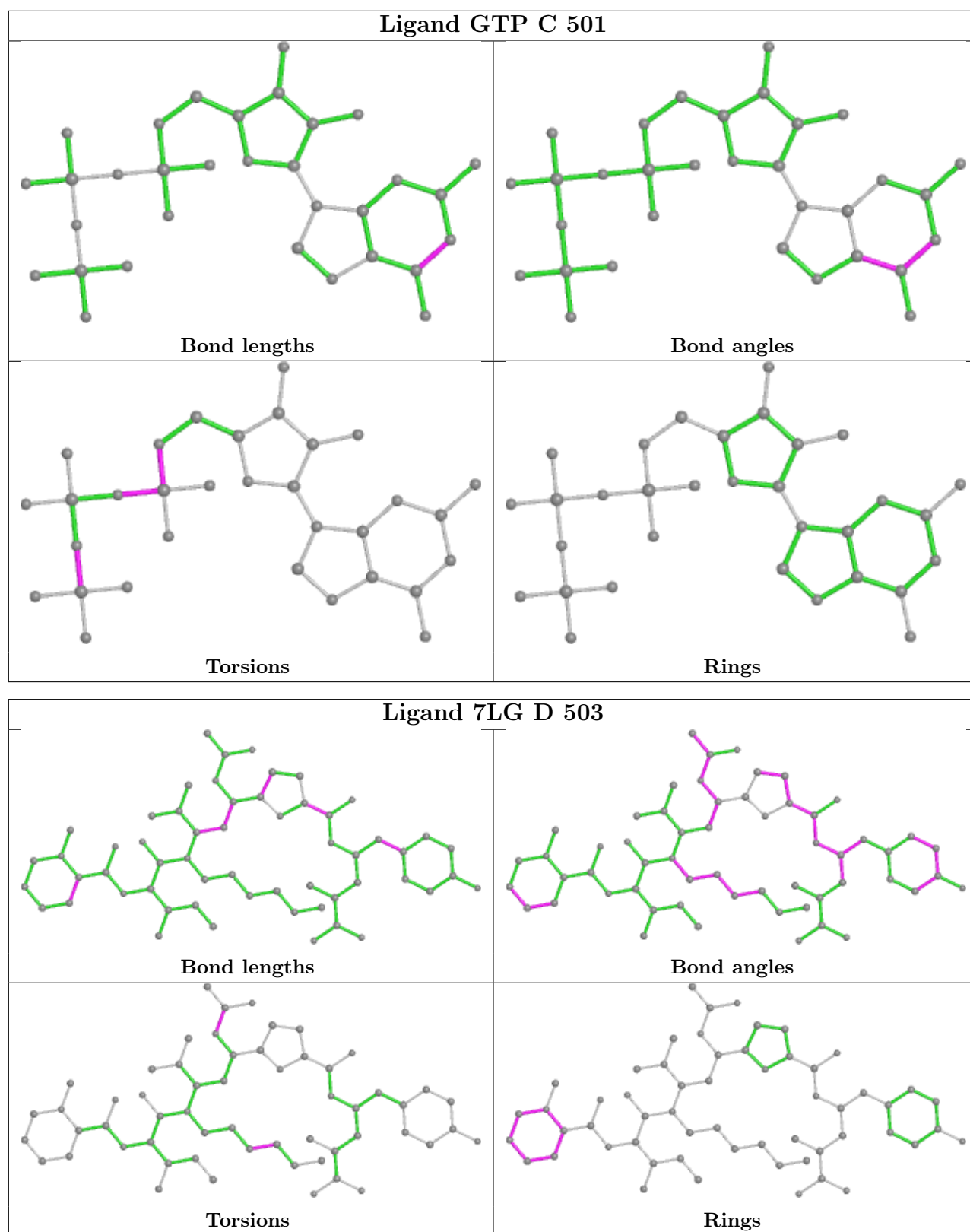
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	437/450 (97%)	-0.17	9 (2%) 63 58	26, 42, 65, 114	0
1	C	440/450 (97%)	-0.42	2 (0%) 91 89	23, 36, 57, 89	0
2	B	428/445 (96%)	-0.29	6 (1%) 75 71	24, 37, 67, 95	0
2	D	424/445 (95%)	0.18	16 (3%) 40 33	33, 56, 86, 112	0
3	E	121/143 (84%)	0.25	5 (4%) 37 30	36, 57, 84, 101	0
4	F	334/384 (86%)	0.40	45 (13%) 3 1	34, 65, 118, 141	0
All	All	2184/2317 (94%)	-0.07	83 (3%) 40 33	23, 46, 87, 141	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	372	THR	6.4
4	F	137	ARG	5.8
1	A	282	TYR	5.6
4	F	177	GLY	5.0
4	F	175	GLU	5.0
2	D	55	THR	5.0
4	F	140	GLU	4.6
4	F	255	ARG	4.5
2	D	80	PRO	4.4
4	F	234	GLN	4.3
2	D	391	ARG	4.2
4	F	178	GLN	4.1
4	F	232	ASN	3.9
2	D	57	ASN	3.8
4	F	103	THR	3.7
4	F	236	LYS	3.7
2	D	320	ARG	3.6
4	F	142	ARG	3.5
4	F	141	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	56	GLY	3.5
3	E	6	MET	3.5
4	F	171	ASP	3.5
4	F	170	LEU	3.4
4	F	101	TYR	3.4
2	D	390	ARG	3.4
4	F	166	ALA	3.4
4	F	169	LEU	3.4
4	F	256	TYR	3.3
2	B	1	MET	3.3
1	C	440	VAL	3.3
4	F	167	SER	3.3
4	F	133	ALA	3.3
4	F	174	ASP	3.2
2	D	92	PHE	3.2
2	D	95	SER	3.1
1	A	235	VAL	3.1
1	A	281	ALA	3.1
2	D	53	GLU	3.1
1	A	279	GLU	3.0
4	F	176	GLN	3.0
4	F	173	ILE	2.9
4	F	235	ASP	2.9
4	F	136	ASN	2.9
4	F	179	VAL	2.8
4	F	128	ARG	2.8
2	D	54	ALA	2.8
4	F	233	PHE	2.8
3	E	138	GLU	2.7
4	F	165	GLU	2.7
3	E	44	ASP	2.6
1	A	346	TRP	2.6
4	F	139	ARG	2.6
4	F	194	PRO	2.5
1	A	262	TYR	2.5
2	D	219	THR	2.5
4	F	98	TYR	2.5
4	F	102	PRO	2.5
4	F	231	ALA	2.4
2	B	83	GLN	2.4
2	D	78	SER	2.4
2	D	37	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	365	GLY	2.3
2	D	394	PHE	2.3
1	A	238	ILE	2.3
4	F	131	PHE	2.3
4	F	132	LEU	2.3
4	F	172	PHE	2.3
1	A	239	THR	2.2
2	D	275	SER	2.2
3	E	139	LEU	2.2
4	F	252	ASN	2.2
4	F	362	ALA	2.1
4	F	226	GLU	2.1
4	F	225	SER	2.1
2	B	57	ASN	2.1
2	B	282	ARG	2.1
4	F	100	ILE	2.1
4	F	129	GLU	2.1
1	C	283	HIS	2.1
4	F	229	ASN	2.1
3	E	23	ILE	2.0
2	B	166	THR	2.0
2	B	281	TYR	2.0

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 [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

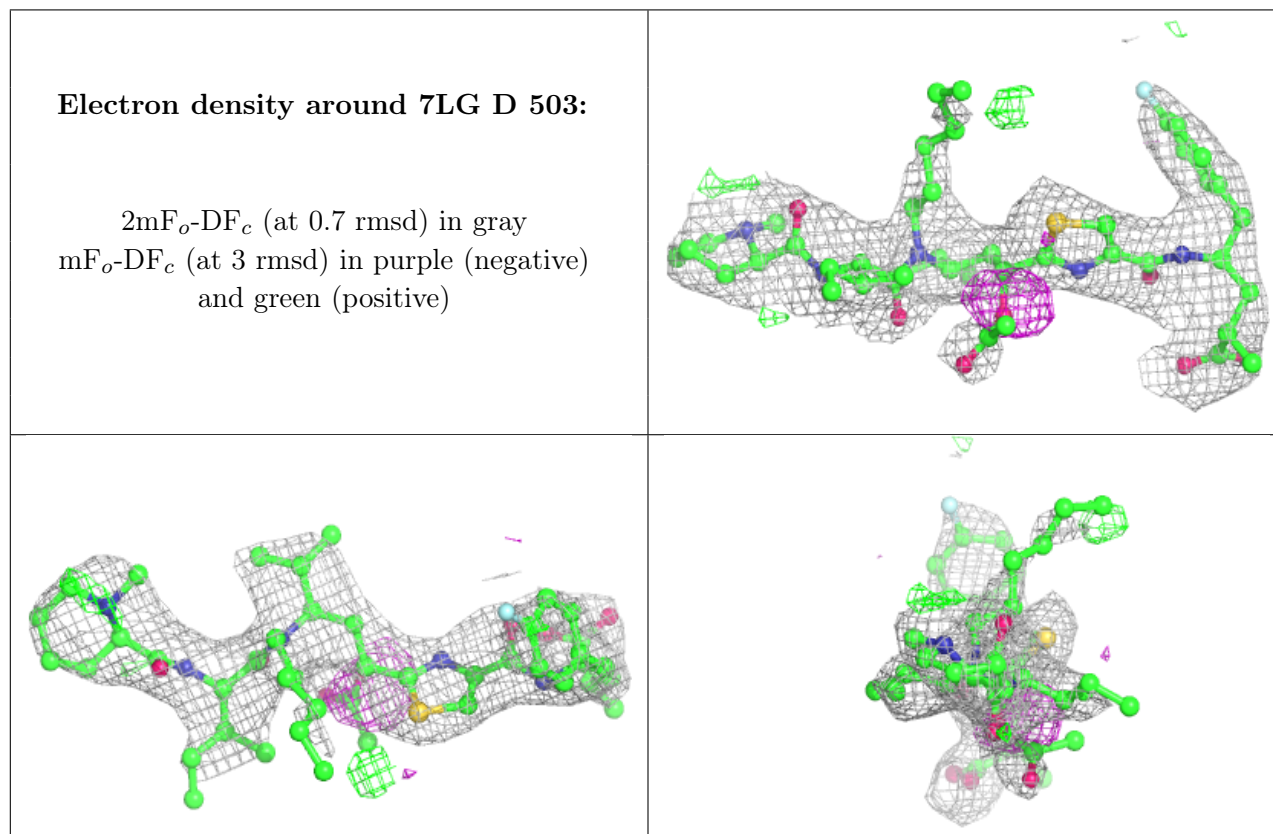
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	MES	C	504	12/12	0.70	0.49	104,108,127,129	0

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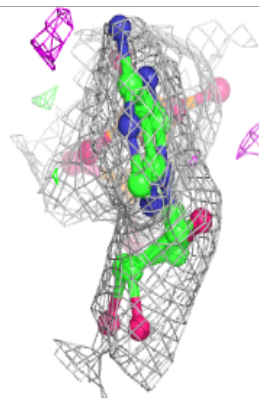
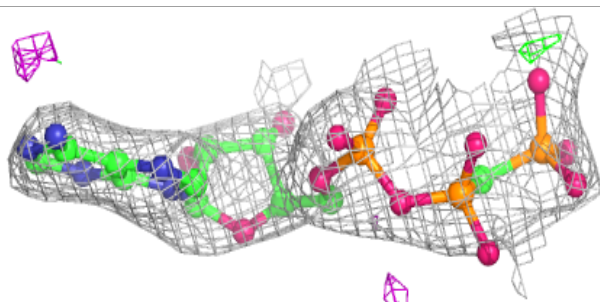
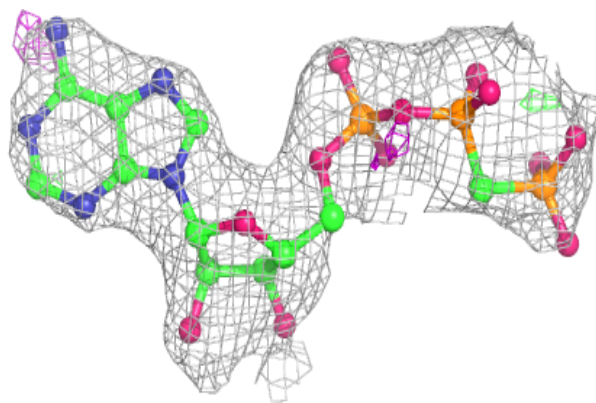
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	7LG	D	503	57/57	0.86	0.38	70,74,87,91	0
6	MG	C	502	1/1	0.87	0.12	36,36,36,36	0
11	ACP	F	401	31/31	0.87	0.17	77,86,112,116	0
6	MG	D	502	1/1	0.88	0.21	71,71,71,71	0
9	MES	B	504	12/12	0.91	0.17	61,65,74,74	0
5	GTP	D	501	32/32	0.92	0.18	44,49,80,86	0
7	CA	C	503	1/1	0.93	0.07	46,46,46,46	0
9	MES	B	503	12/12	0.94	0.17	68,69,70,71	0
10	7LG	B	505	57/57	0.94	0.17	31,36,44,47	0
7	CA	A	503	1/1	0.97	0.06	58,58,58,58	0
6	MG	B	502	1/1	0.97	0.22	38,38,38,38	0
5	GTP	A	501	32/32	0.98	0.12	27,29,32,32	0
8	GDP	B	501	28/28	0.98	0.17	25,28,30,31	0
6	MG	A	502	1/1	0.98	0.06	34,34,34,34	0
5	GTP	C	501	32/32	0.98	0.11	25,26,29,29	0

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

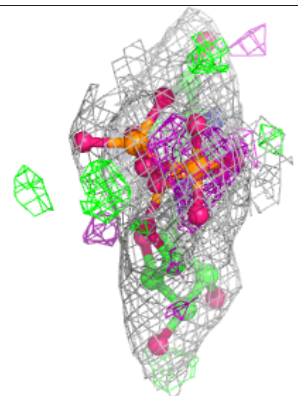
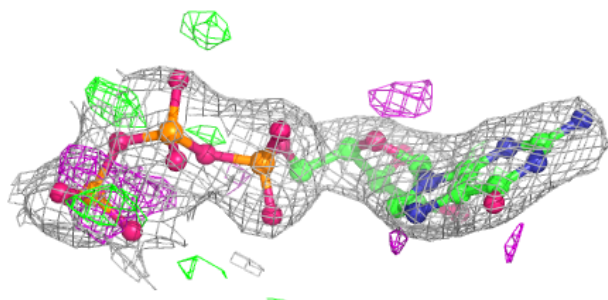
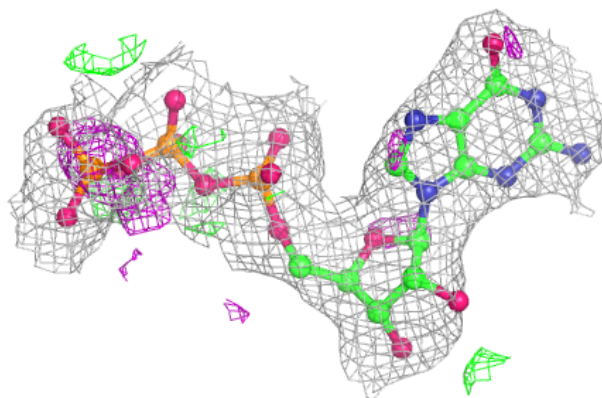


Electron density around ACP F 401:

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

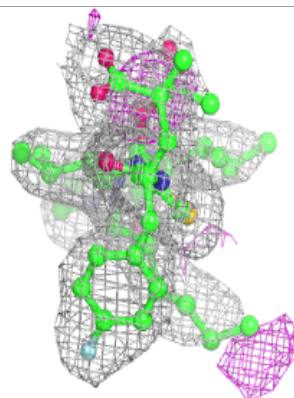
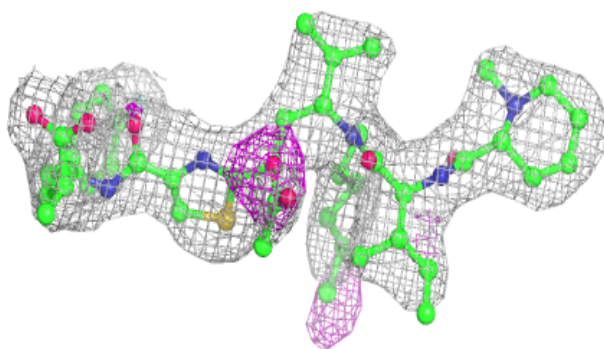
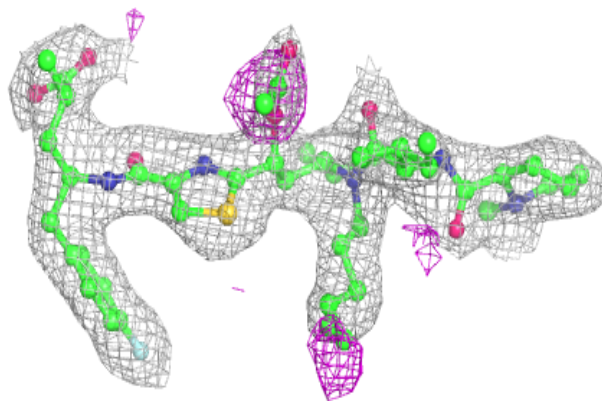
**Electron density around GTP D 501:**

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

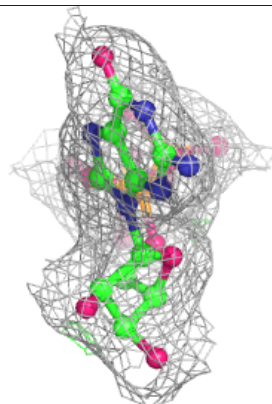
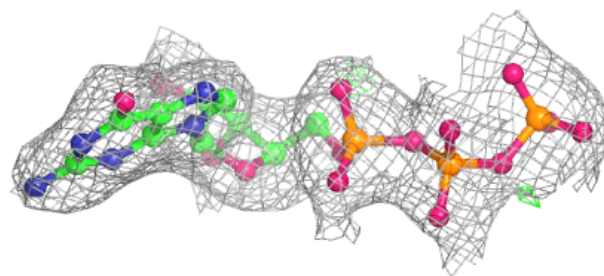
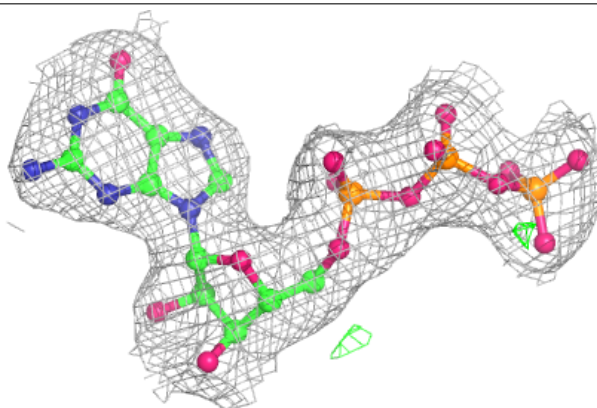


Electron density around 7LG B 505:

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

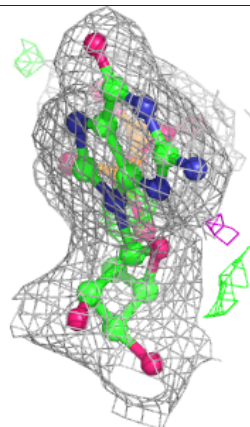
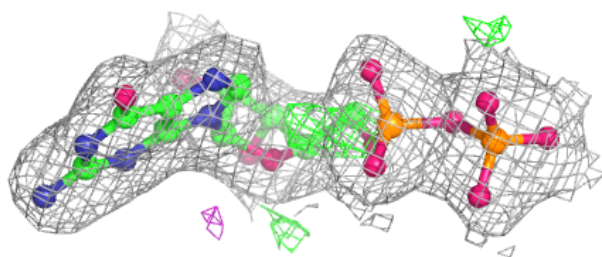
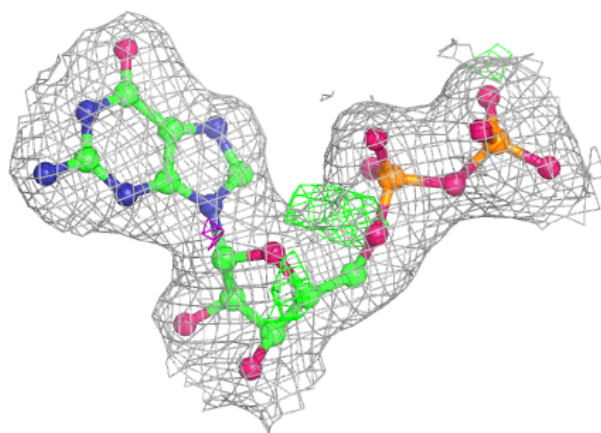
**Electron density around GTP A 501:**

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

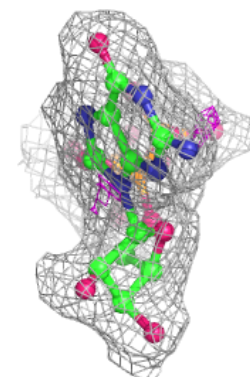
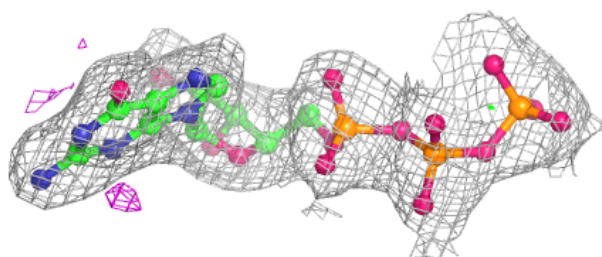
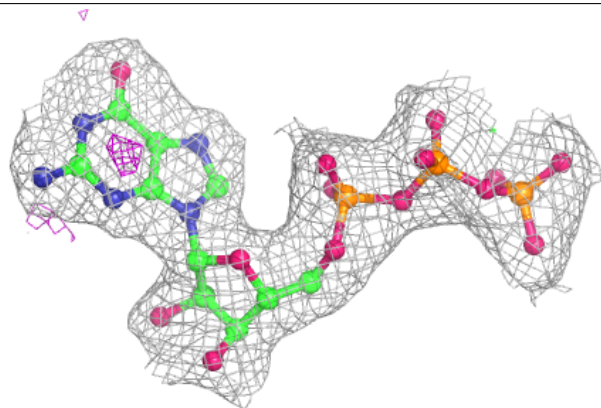


Electron density around GDP B 501:

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

**Electron density around GTP C 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.