



wwPDB EM Validation Summary Report ⓘ

Nov 27, 2022 – 07:33 PM EST

PDB ID : 7KZO
EMDB ID : EMD-23084
Title : Outer dynein arm docking complex bound to doublet microtubules from *C. reinhardtii*
Authors : Walton, T.; Wu, H.; Brown, A.B.
Deposited on : 2020-12-10
Resolution : 3.30 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

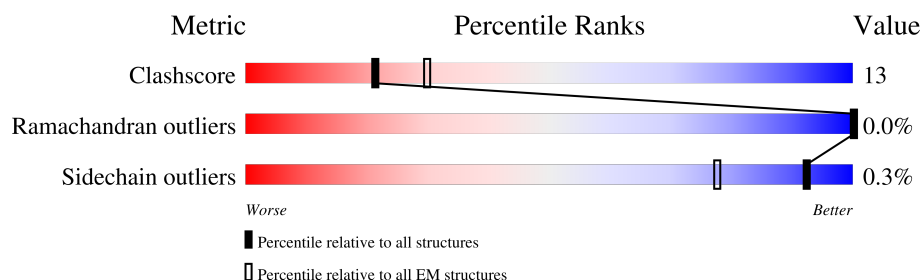
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.









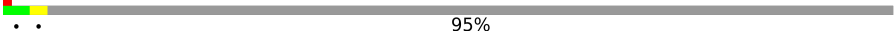





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A1	443	
1	A3	443	
1	A5	443	
1	A7	443	
1	B1	443	
1	B3	443	
1	B5	443	
1	B7	443	

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Mol	Chain	Length	Quality of chain
2	A2	451	 65%30%5%
2	A4	451	 67%28%5%
2	A6	451	 64%31%5%
2	B2	451	 66%25%9%
2	B4	451	 63%27%9%
2	B6	451	 71%24%5%
3	C	4485	 95%
4	X	749	 5%18%79%
4	X1	749	 14%5%81%
5	Y	552	 7%17%5%78%
5	Y1	552	 19%7%73%
6	Z	184	 10%61%30%8%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 54110 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A3	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A5	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	A7	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	B1	419	Total	C	N	O	S	0	0
			3298	2077	563	628	30		
1	B3	410	Total	C	N	O	S	0	0
			3227	2030	553	614	30		
1	B5	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
1	B7	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		

- Molecule 2 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	430	Total	C	N	O	S	0	0
			3339	2114	568	636	21		
2	A4	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
2	A6	429	Total	C	N	O	S	0	0
			3335	2112	567	635	21		
2	B2	411	Total	C	N	O	S	0	0
			3204	2035	544	605	20		
2	B4	409	Total	C	N	O	S	0	0
			3193	2028	542	603	20		
2	B6	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

- Molecule 3 is a protein called Dynein gamma chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	218	Total	C	N	O	S	0	0
			1771	1123	302	335	11		

- Molecule 4 is a protein called Outer dynein arm-docking complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	157	Total	C	N	O	S	0	0
			985	594	198	190	3		
4	X1	142	Total	C	N	O	S	0	0
			1178	715	223	235	5		

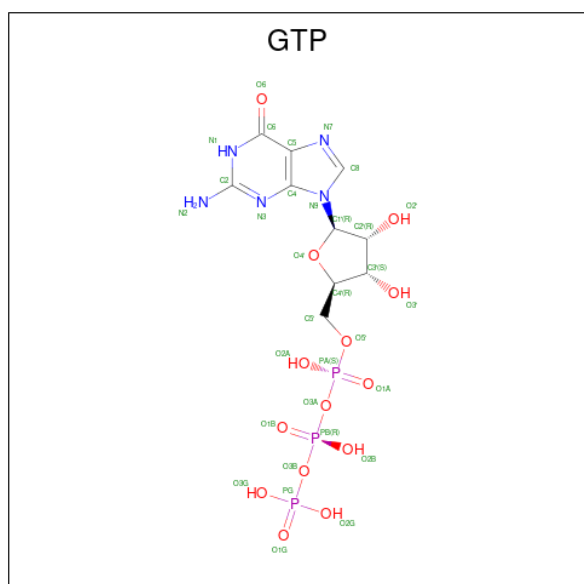
- Molecule 5 is a protein called Outer dynein arm protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	121	Total	C	N	O	S	0	0
			844	508	162	171	3		
5	Y1	147	Total	C	N	O	S	0	0
			1185	729	223	224	9		

- Molecule 6 is a protein called Outer dynein arm-docking complex protein DC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	170	Total	C	N	O	S	0	0
			1384	863	242	270	9		

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

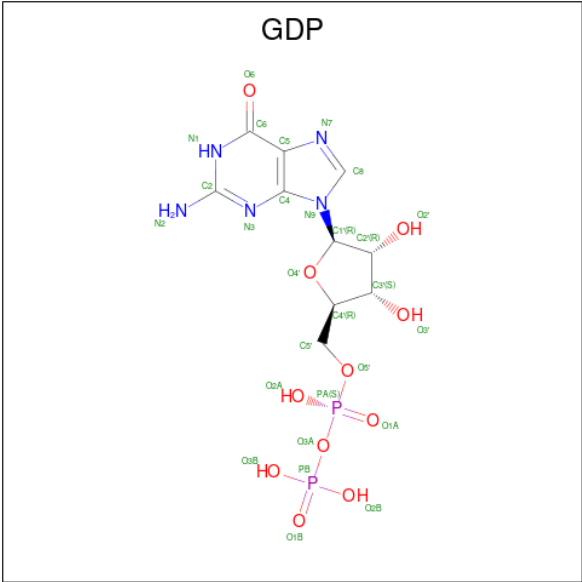


Mol	Chain	Residues	Atoms					AltConf
7	A1	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	A3	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	A5	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	A7	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	B2	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	B5	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	B7	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	A1	1	Total	Mg	0
			1	1	
8	A2	1	Total	Mg	0
			1	1	
8	A4	1	Total	Mg	0
			1	1	
8	A6	1	Total	Mg	0
			1	1	
8	B3	1	Total	Mg	0
			1	1	
8	B4	1	Total	Mg	0
			1	1	
8	B6	1	Total	Mg	0
			1	1	

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

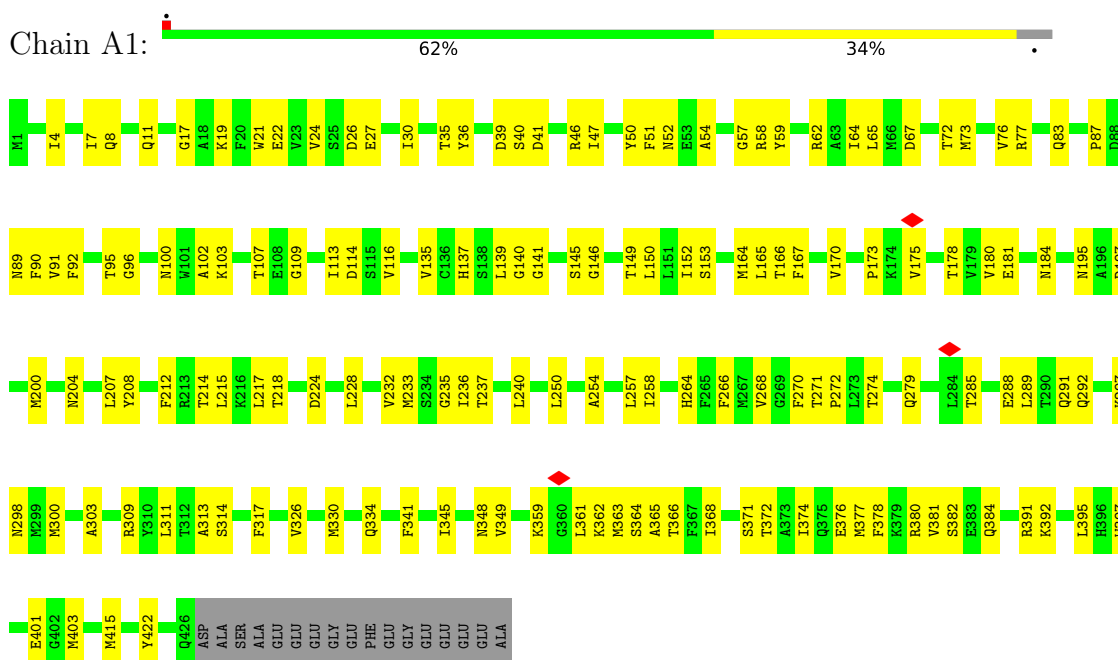


Mol	Chain	Residues	Atoms					AltConf
9	A1	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A3	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A5	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A7	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B1	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B3	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B5	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B7	1	Total	C	N	O	P	0
			28	10	5	11	2	

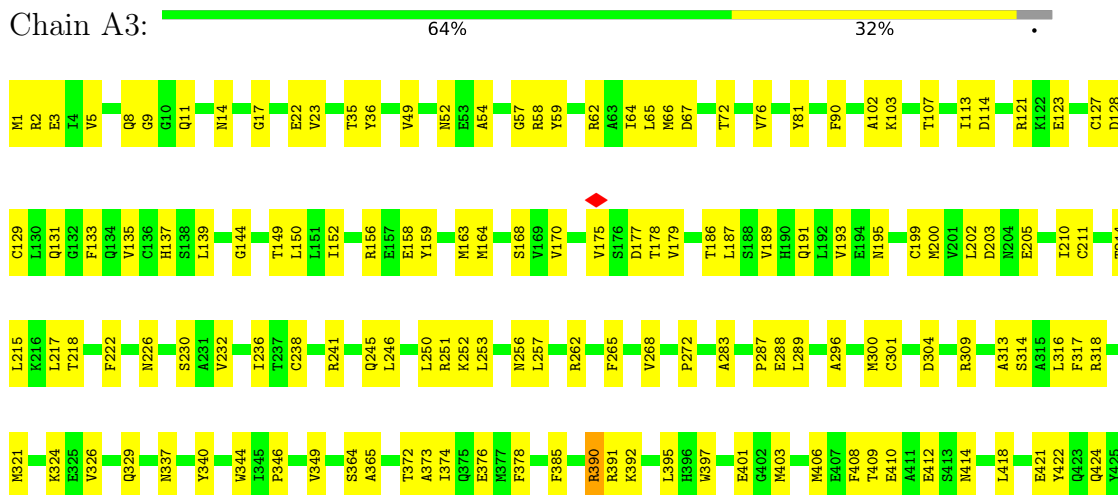
3 Residue-property plots

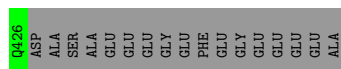
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 beta



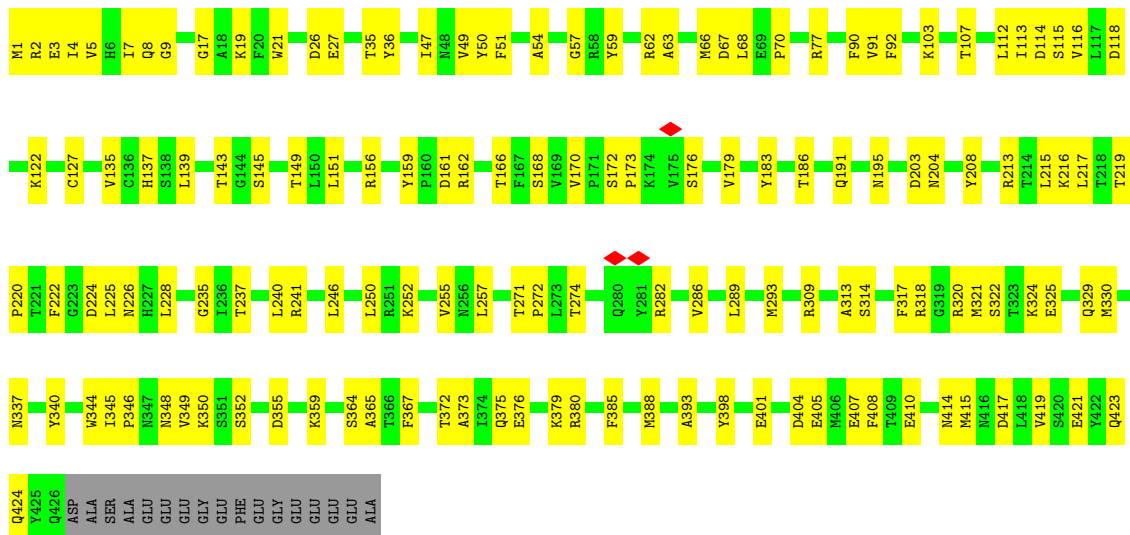
• Molecule 1: Tubulin beta





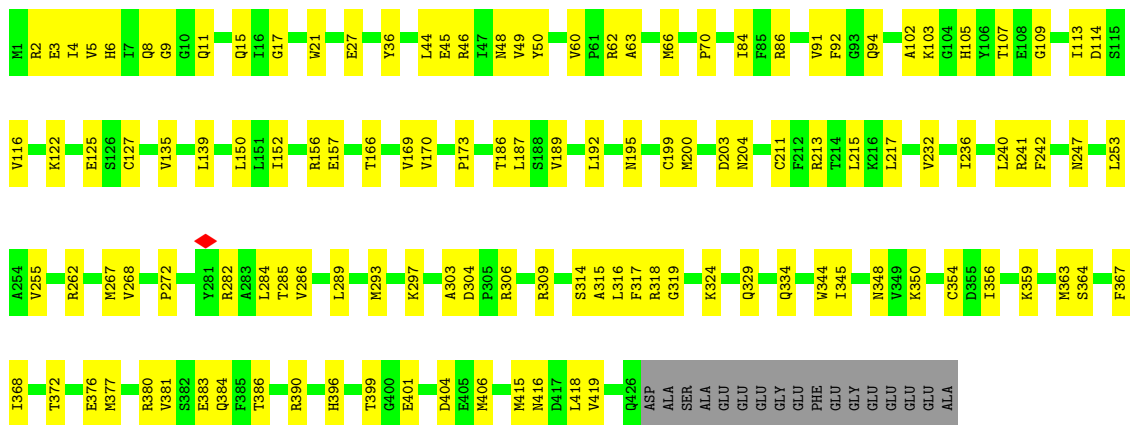
• Molecule 1: Tubulin beta

Chain A5:  64% 32%



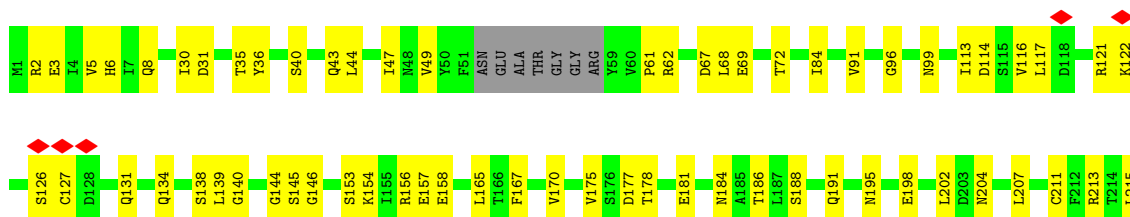
• Molecule 1: Tubulin beta

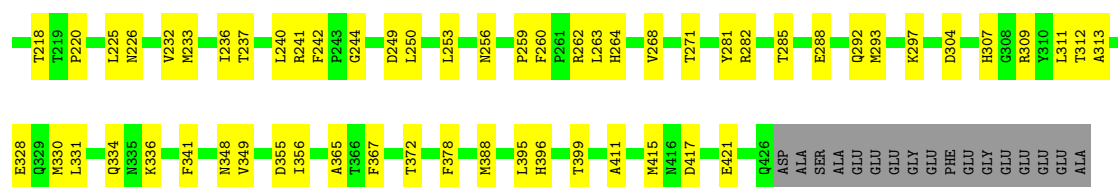
Chain A7:  68% 28%



• Molecule 1: Tubulin beta

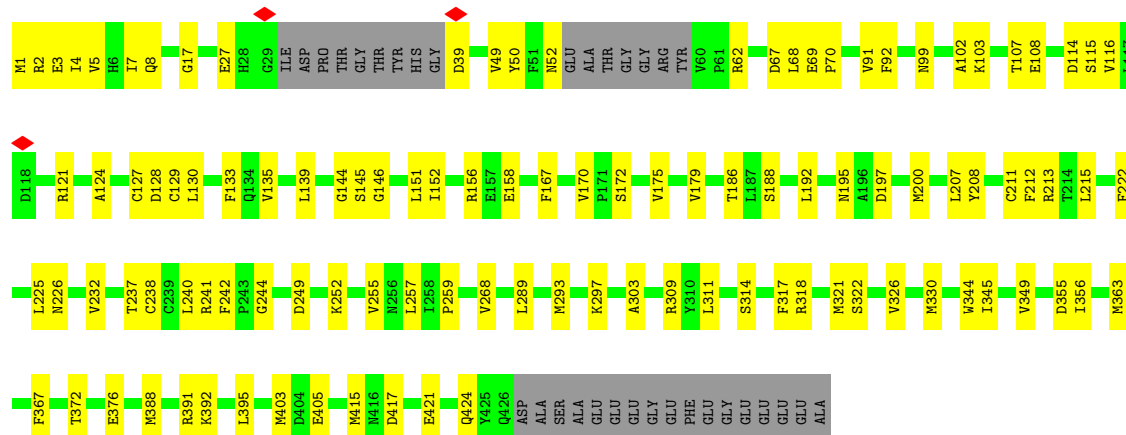
Chain B1:  67% 28% 5%





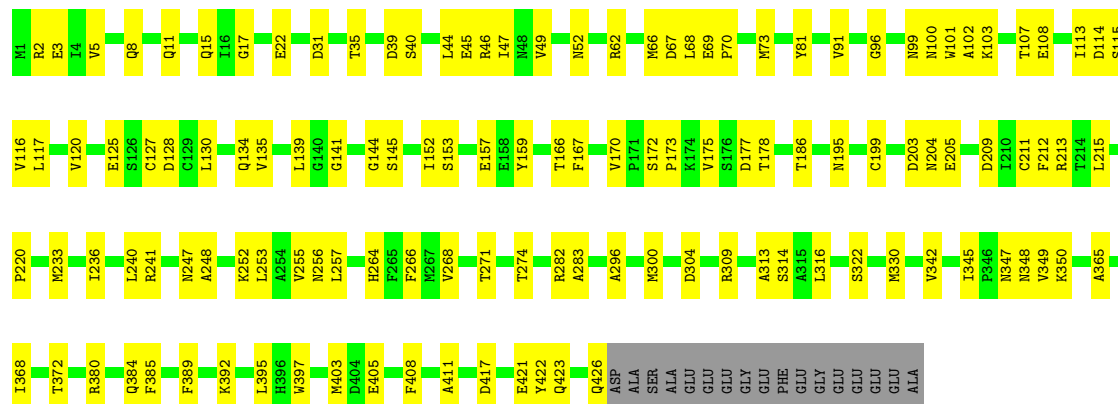
• Molecule 1: Tubulin beta

Chain B3: 68% 25% 7%



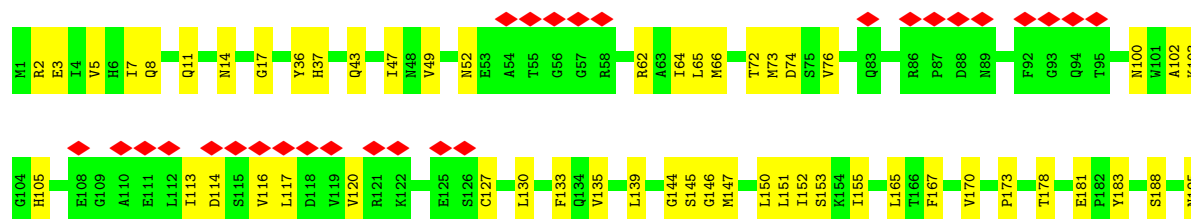
• Molecule 1: Tubulin beta

Chain B5: 67% 29%



• Molecule 1: Tubulin beta

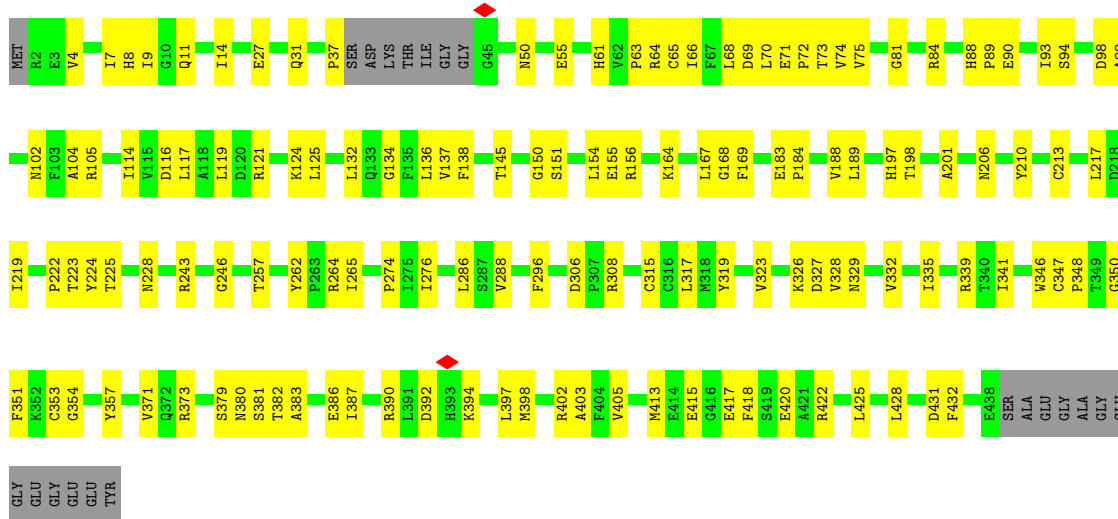
Chain B7: 8% 69% 27%





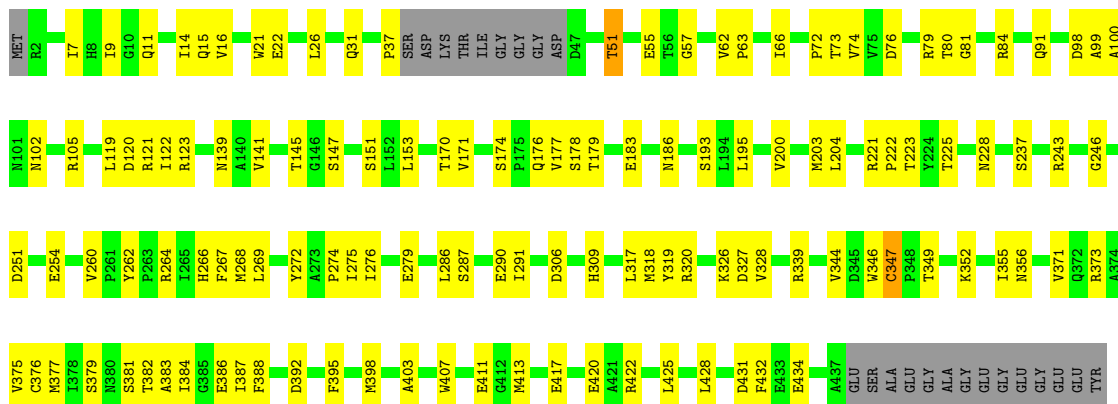
- Molecule 2: Tubulin alpha

Chain A2: 65% 30% 5%



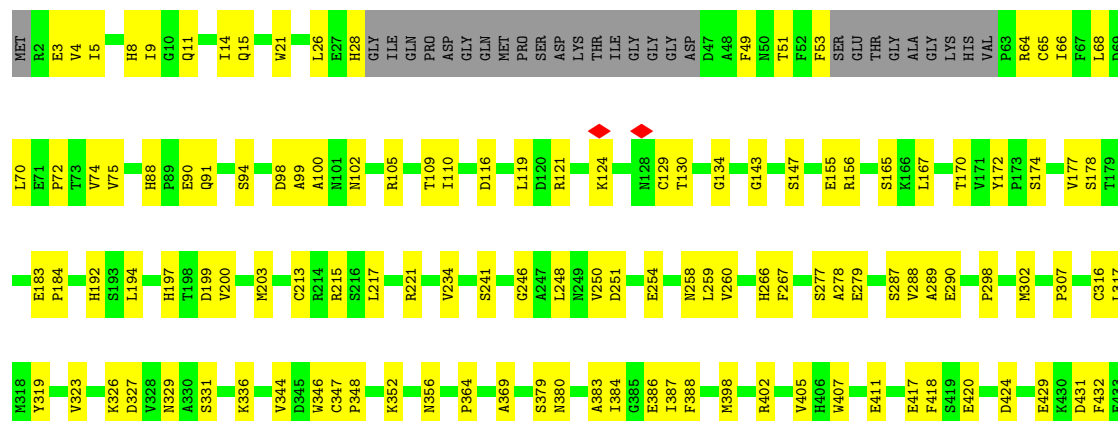
- Molecule 2: Tubulin alpha

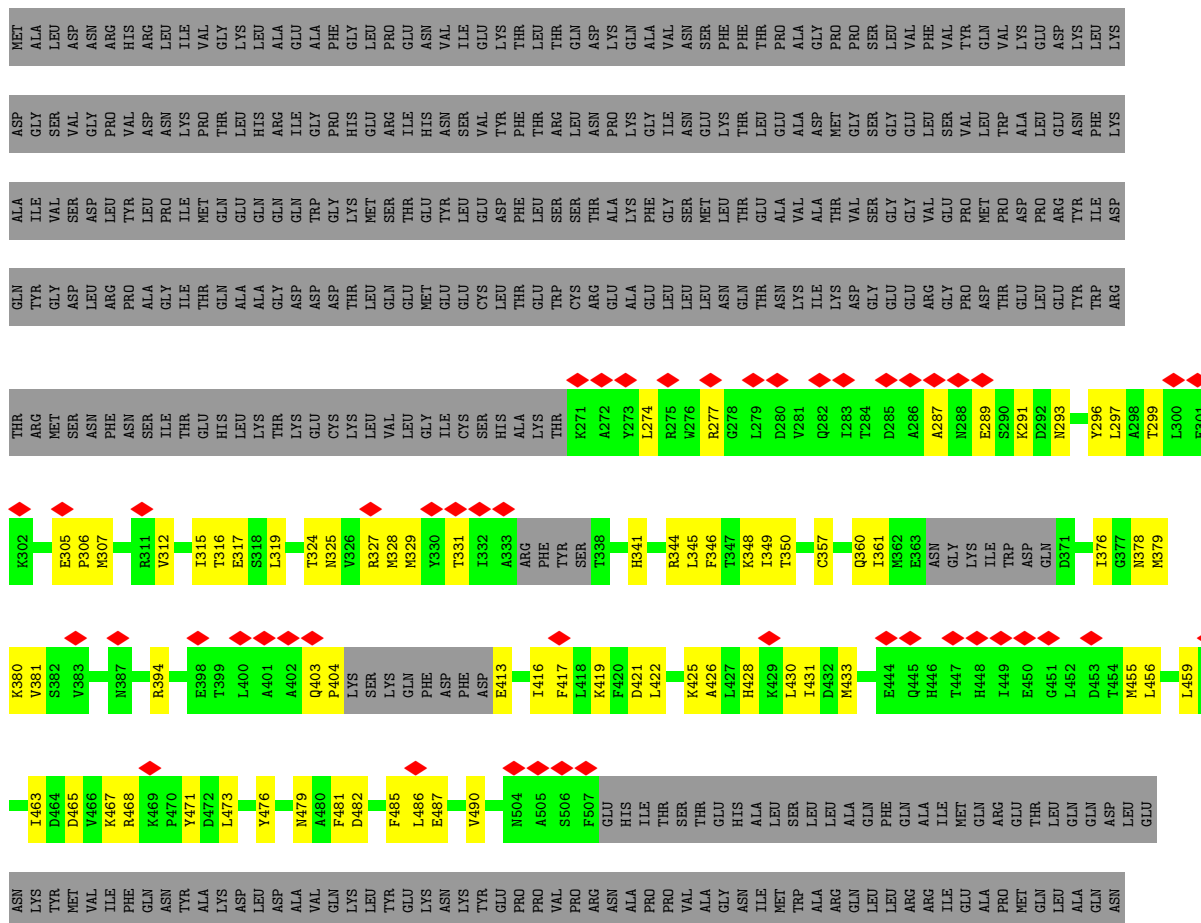
Chain A4: 67% 28% 5%



- Molecule 2: Tubulin alpha

Chain A6: 64% 31% 5%





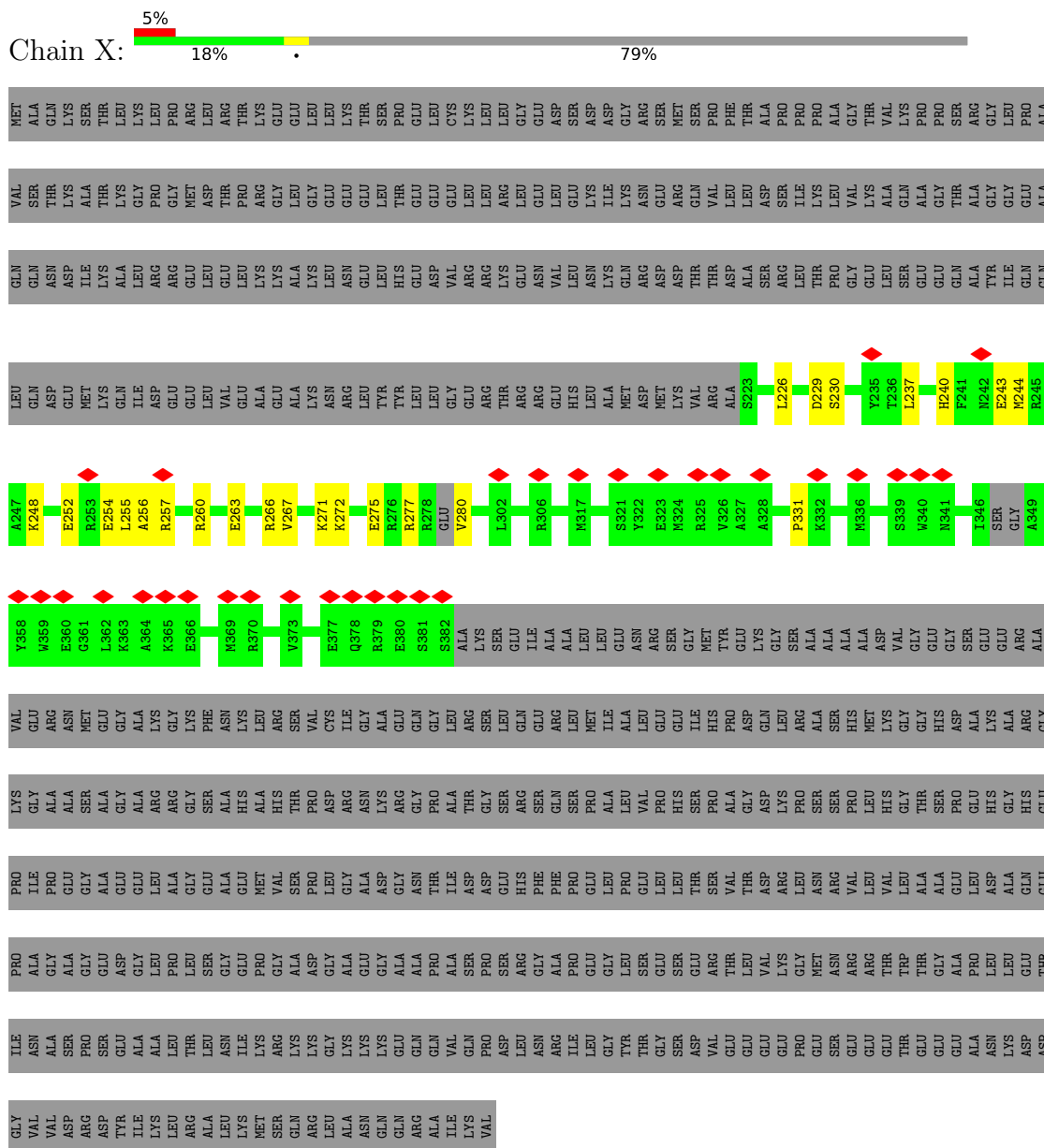






[illegible]

- Molecule 4: Outer dynein arm-docking complex subunit 1



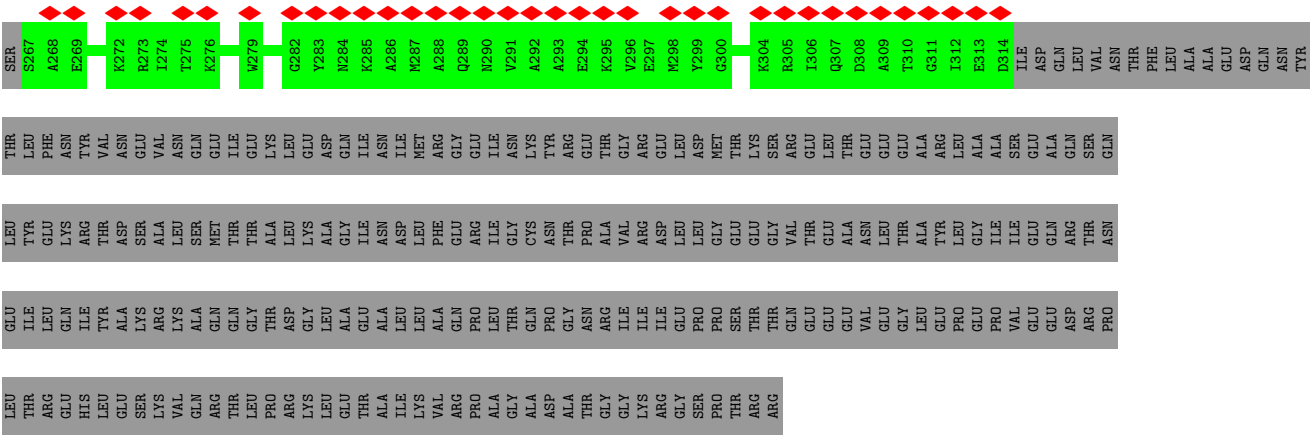
- Molecule 4: Outer dynein arm-docking complex subunit 1

Response	Percentage
Yes	14%
No	5%
Don't know	81%

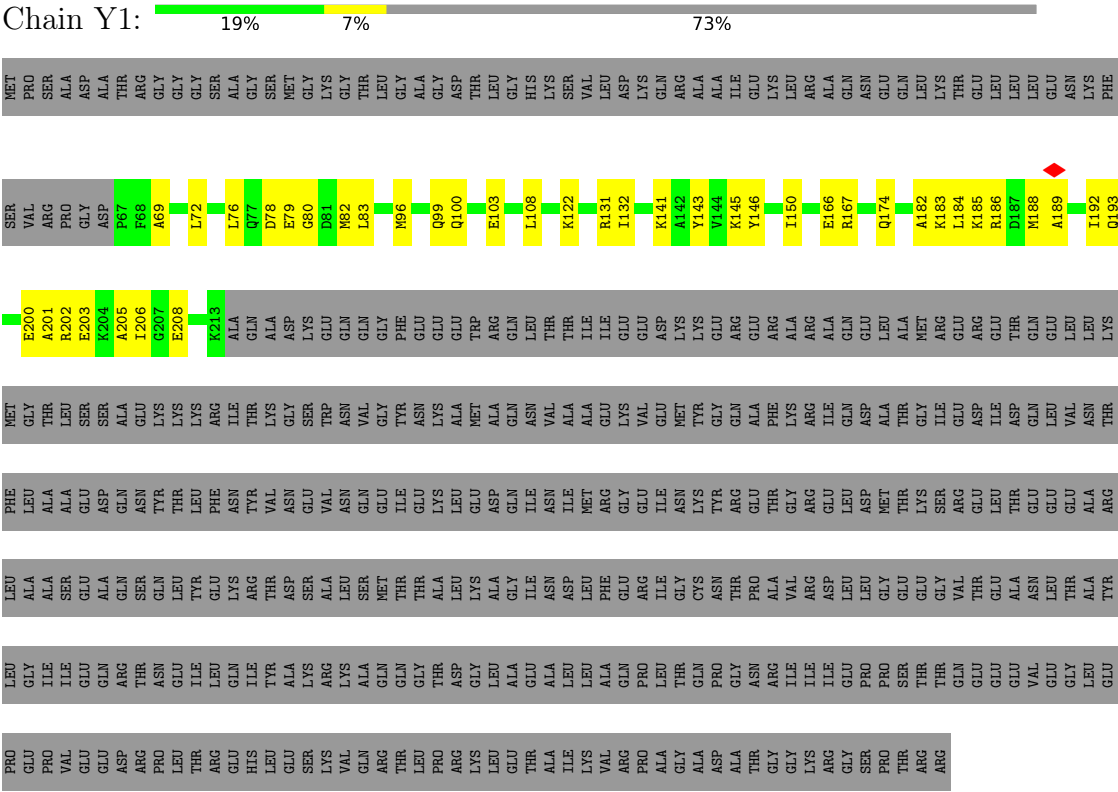


Category	Percentage
Very bad	7%
Bad	17%
Average	5%
Good	78%

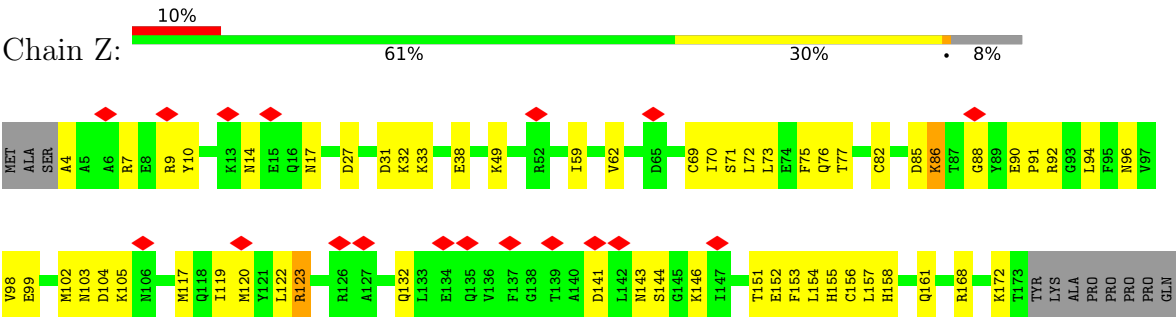




• Molecule 5: Outer dynein arm protein 1



• Molecule 6: Outer dynein arm-docking complex protein DC3



LYS
ARG
LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=0°, rise=82 Å, axial sym=C1	Depositor
Number of segments used	485694	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61.48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	394.4, 394.4, 394.4	wwPDB
Map dimensions	290, 290, 290	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

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, GDP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A1	0.28	0/3420	0.53	0/4628
1	A3	0.31	0/3420	0.54	0/4628
1	A5	0.30	0/3420	0.52	0/4628
1	A7	0.28	0/3420	0.51	0/4628
1	B1	0.29	0/3371	0.49	0/4561
1	B3	0.32	0/3295	0.49	0/4454
1	B5	0.31	0/3420	0.51	0/4628
1	B7	0.28	0/3420	0.50	0/4628
2	A2	0.31	0/3410	0.53	0/4623
2	A4	0.34	0/3389	0.58	0/4595
2	A6	0.31	0/3406	0.54	0/4618
2	B2	0.31	0/3271	0.52	0/4434
2	B4	0.32	0/3260	0.52	0/4418
2	B6	0.29	0/3389	0.50	0/4595
3	C	0.26	0/1796	0.50	0/2418
4	X	0.27	0/987	0.50	2/1341 (0.1%)
4	X1	0.31	0/1186	0.51	0/1582
5	Y	0.29	0/846	0.48	0/1132
5	Y1	0.29	0/1192	0.52	0/1585
6	Z	0.34	0/1403	0.67	0/1885
All	All	0.30	0/54721	0.52	2/74009 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	331	PRO	N-CA-CB	5.82	110.28	103.30
4	X	352	PRO	N-CA-CB	5.73	110.17	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	3346	0	3238	107	0
1	A3	3346	0	3238	108	0
1	A5	3346	0	3238	103	0
1	A7	3346	0	3238	89	0
1	B1	3298	0	3196	82	0
1	B3	3227	0	3134	82	0
1	B5	3346	0	3238	106	0
1	B7	3346	0	3238	92	0
2	A2	3339	0	3272	104	0
2	A4	3318	0	3259	93	0
2	A6	3335	0	3269	105	0
2	B2	3204	0	3152	84	0
2	B4	3193	0	3141	106	0
2	B6	3318	0	3259	82	0
3	C	1771	0	1781	45	0
4	X	985	0	714	19	0
4	X1	1178	0	1179	28	0
5	Y	844	0	735	22	0
5	Y1	1185	0	1230	36	0
6	Z	1384	0	1359	46	0
7	A1	32	0	12	0	0
7	A3	32	0	12	1	0
7	A5	32	0	12	1	0
7	A7	32	0	12	4	0
7	B2	32	0	12	1	0
7	B5	32	0	12	0	0
7	B7	32	0	12	0	0
8	A1	1	0	0	0	0
8	A2	1	0	0	0	0
8	A4	1	0	0	0	0
8	A6	1	0	0	0	0
8	B3	1	0	0	0	0
8	B4	1	0	0	0	0
8	B6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A1	28	0	12	0	0
9	A3	28	0	12	2	0
9	A5	28	0	12	0	0
9	A7	28	0	12	2	0
9	B1	28	0	12	3	0
9	B3	28	0	12	2	0
9	B5	28	0	12	1	0
9	B7	28	0	12	2	0
All	All	54110	0	52288	1396	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 13.

The worst 5 of 1396 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:A3:215:LEU:HB3	1:A3:217:LEU:HD13	1.54	0.90
1:B5:175:VAL:HG22	2:B6:329:ASN:HD21	1.35	0.87
1:B3:330:MET:HE2	1:B3:349:VAL:HG11	1.55	0.86
1:B7:113:ILE:HD13	1:B7:150:LEU:HD11	1.55	0.85
1:A1:215:LEU:HB3	1:A1:217:LEU:HD13	1.59	0.84

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 PDB entries followed by that with respect to all EM entries.

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	A1	424/443 (96%)	399 (94%)	25 (6%)	0	100	100
1	A3	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
1	A5	424/443 (96%)	407 (96%)	17 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A7	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
1	B1	415/443 (94%)	396 (95%)	19 (5%)	0	100	100
1	B3	404/443 (91%)	392 (97%)	12 (3%)	0	100	100
1	B5	424/443 (96%)	403 (95%)	21 (5%)	0	100	100
1	B7	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
2	A2	426/451 (94%)	402 (94%)	24 (6%)	0	100	100
2	A4	423/451 (94%)	409 (97%)	14 (3%)	0	100	100
2	A6	425/451 (94%)	408 (96%)	17 (4%)	0	100	100
2	B2	405/451 (90%)	391 (96%)	14 (4%)	0	100	100
2	B4	403/451 (89%)	385 (96%)	18 (4%)	0	100	100
2	B6	423/451 (94%)	407 (96%)	16 (4%)	0	100	100
3	C	210/4485 (5%)	204 (97%)	6 (3%)	0	100	100
4	X	151/749 (20%)	151 (100%)	0	0	100	100
4	X1	140/749 (19%)	140 (100%)	0	0	100	100
5	Y	117/552 (21%)	116 (99%)	1 (1%)	0	100	100
5	Y1	145/552 (26%)	145 (100%)	0	0	100	100
6	Z	168/184 (91%)	156 (93%)	10 (6%)	2 (1%)	13	42
All	All	6799/13521 (50%)	6526 (96%)	271 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	Z	86	LYS
6	Z	141	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	A1	367/379 (97%)	367 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A3	367/379 (97%)	366 (100%)	1 (0%)	92	96
1	A5	367/379 (97%)	367 (100%)	0	100	100
1	A7	367/379 (97%)	367 (100%)	0	100	100
1	B1	363/379 (96%)	363 (100%)	0	100	100
1	B3	356/379 (94%)	356 (100%)	0	100	100
1	B5	367/379 (97%)	367 (100%)	0	100	100
1	B7	367/379 (97%)	366 (100%)	1 (0%)	92	96
2	A2	361/374 (96%)	360 (100%)	1 (0%)	92	96
2	A4	359/374 (96%)	354 (99%)	5 (1%)	67	82
2	A6	361/374 (96%)	361 (100%)	0	100	100
2	B2	347/374 (93%)	347 (100%)	0	100	100
2	B4	346/374 (92%)	346 (100%)	0	100	100
2	B6	359/374 (96%)	359 (100%)	0	100	100
3	C	197/3945 (5%)	197 (100%)	0	100	100
4	X	50/618 (8%)	50 (100%)	0	100	100
4	X1	125/618 (20%)	121 (97%)	4 (3%)	39	67
5	Y	63/462 (14%)	63 (100%)	0	100	100
5	Y1	128/462 (28%)	127 (99%)	1 (1%)	81	89
6	Z	150/162 (93%)	146 (97%)	4 (3%)	44	71
All	All	5767/11543 (50%)	5750 (100%)	17 (0%)	92	96

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	Z	10	TYR
6	Z	123	ARG
1	B7	72	THR
4	X1	204	LEU
4	X1	208	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	B6	329	ASN

Continued on next page...

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Mol	Chain	Res	Type
1	B7	100	ASN
3	C	378	ASN
1	B1	6	HIS
1	A7	204	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 22 ligands modelled in this entry, 7 are monoatomic - leaving 15 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	GDP	A5	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	5 (16%)
9	GDP	B5	502	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
7	GTP	A7	501	8	26,34,34	1.20	2 (7%)	32,54,54	1.66	7 (21%)
7	GTP	A1	501	8	26,34,34	1.14	2 (7%)	32,54,54	1.64	7 (21%)
9	GDP	B7	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.41	5 (16%)
9	GDP	A1	503	-	24,30,30	0.96	1 (4%)	30,47,47	1.29	4 (13%)
7	GTP	B7	501	8	26,34,34	1.20	2 (7%)	32,54,54	1.58	7 (21%)
9	GDP	A3	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GDP	B1	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	4 (13%)
7	GTP	B5	501	8	26,34,34	1.21	2 (7%)	32,54,54	1.62	7 (21%)
9	GDP	B3	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
9	GDP	A7	502	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	5 (16%)
7	GTP	B2	501	8	26,34,34	1.19	2 (7%)	32,54,54	1.73	7 (21%)
7	GTP	A3	501	8	26,34,34	1.17	2 (7%)	32,54,54	1.72	7 (21%)
7	GTP	A5	501	8	26,34,34	1.22	2 (7%)	32,54,54	1.66	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
9	GDP	A5	502	-	-	1/12/32/32	0/3/3/3
9	GDP	B5	502	-	-	4/12/32/32	0/3/3/3
7	GTP	A7	501	8	-	7/18/38/38	0/3/3/3
7	GTP	A1	501	8	-	5/18/38/38	0/3/3/3
9	GDP	B7	502	-	-	6/12/32/32	0/3/3/3
9	GDP	A1	503	-	-	3/12/32/32	0/3/3/3
7	GTP	B7	501	8	-	6/18/38/38	0/3/3/3
9	GDP	A3	502	-	-	1/12/32/32	0/3/3/3
9	GDP	B1	501	-	-	2/12/32/32	0/3/3/3
7	GTP	B5	501	8	-	7/18/38/38	0/3/3/3
9	GDP	B3	502	-	-	3/12/32/32	0/3/3/3
9	GDP	A7	502	-	-	4/12/32/32	0/3/3/3
7	GTP	B2	501	8	-	4/18/38/38	0/3/3/3
7	GTP	A3	501	8	-	7/18/38/38	0/3/3/3
7	GTP	A5	501	8	-	6/18/38/38	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A7	501	GTP	C5-C6	-4.28	1.38	1.47
7	B5	501	GTP	C5-C6	-4.27	1.38	1.47
7	A5	501	GTP	C5-C6	-4.25	1.38	1.47
7	B7	501	GTP	C5-C6	-4.23	1.38	1.47
7	B2	501	GTP	C5-C6	-4.16	1.39	1.47

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B2	501	GTP	PB-O3B-PG	-4.99	115.69	132.83
7	A5	501	GTP	PA-O3A-PB	-4.67	116.80	132.83
7	A3	501	GTP	PB-O3B-PG	-4.46	117.50	132.83
7	A3	501	GTP	PA-O3A-PB	-4.46	117.53	132.83
7	A7	501	GTP	PA-O3A-PB	-4.45	117.54	132.83

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A1	501	GTP	C5'-O5'-PA-O1A
7	A3	501	GTP	C5'-O5'-PA-O1A
7	A3	501	GTP	C5'-O5'-PA-O2A
7	A5	501	GTP	C5'-O5'-PA-O1A
7	A7	501	GTP	C5'-O5'-PA-O1A

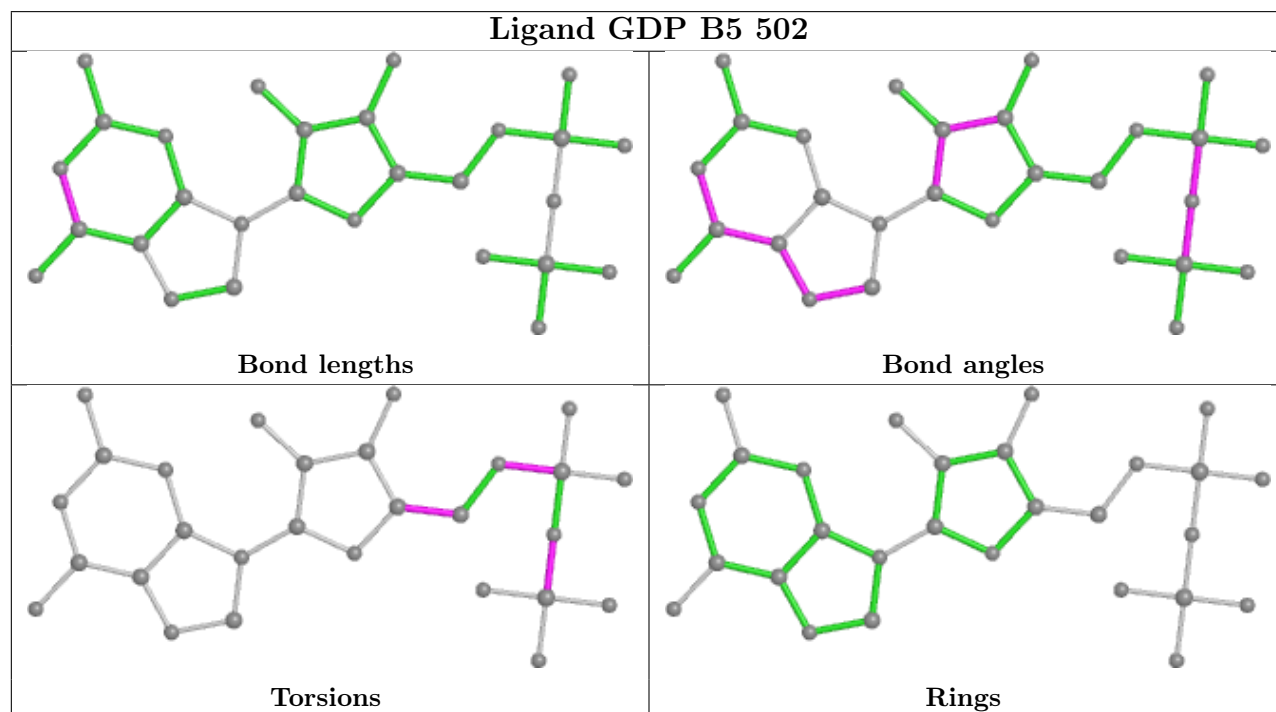
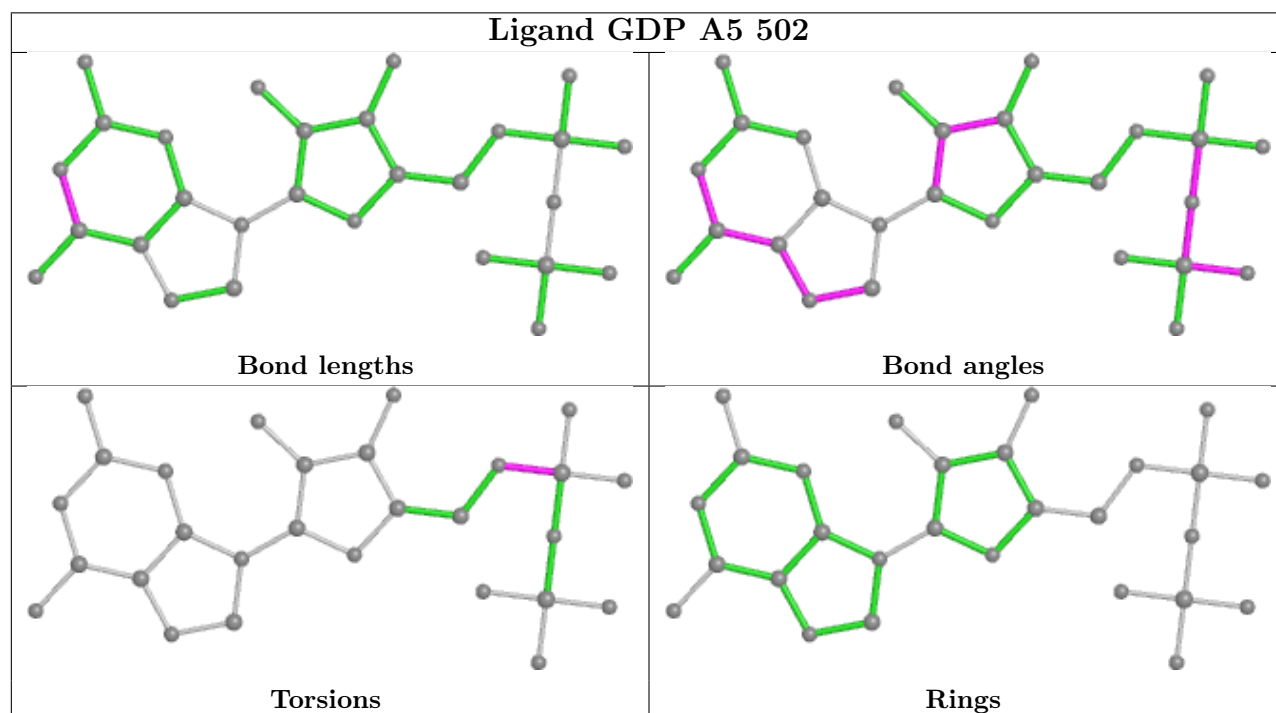
There are no ring outliers.

10 monomers are involved in 19 short contacts:

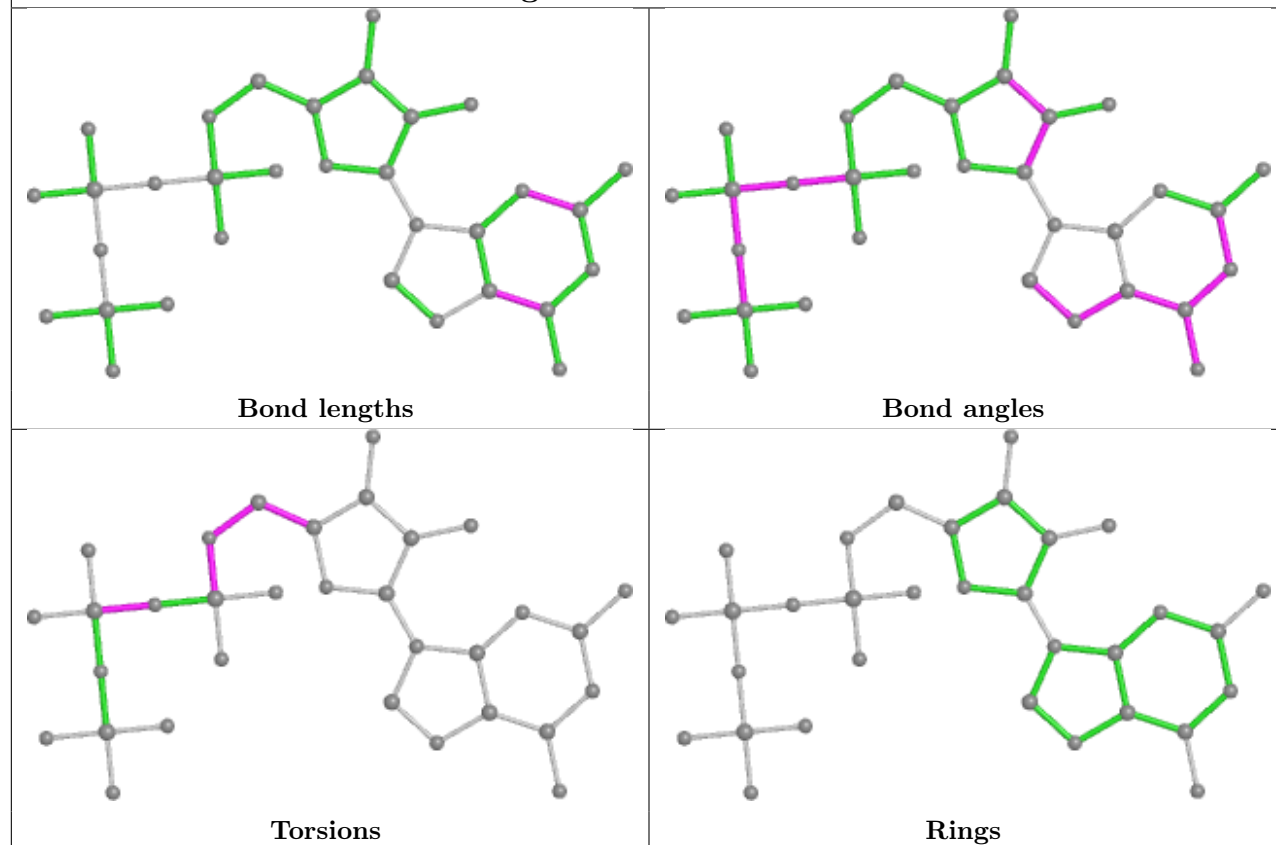
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B5	502	GDP	1	0
7	A7	501	GTP	4	0
9	B7	502	GDP	2	0
9	A3	502	GDP	2	0
9	B1	501	GDP	3	0
9	B3	502	GDP	2	0
9	A7	502	GDP	2	0
7	B2	501	GTP	1	0
7	A3	501	GTP	1	0
7	A5	501	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

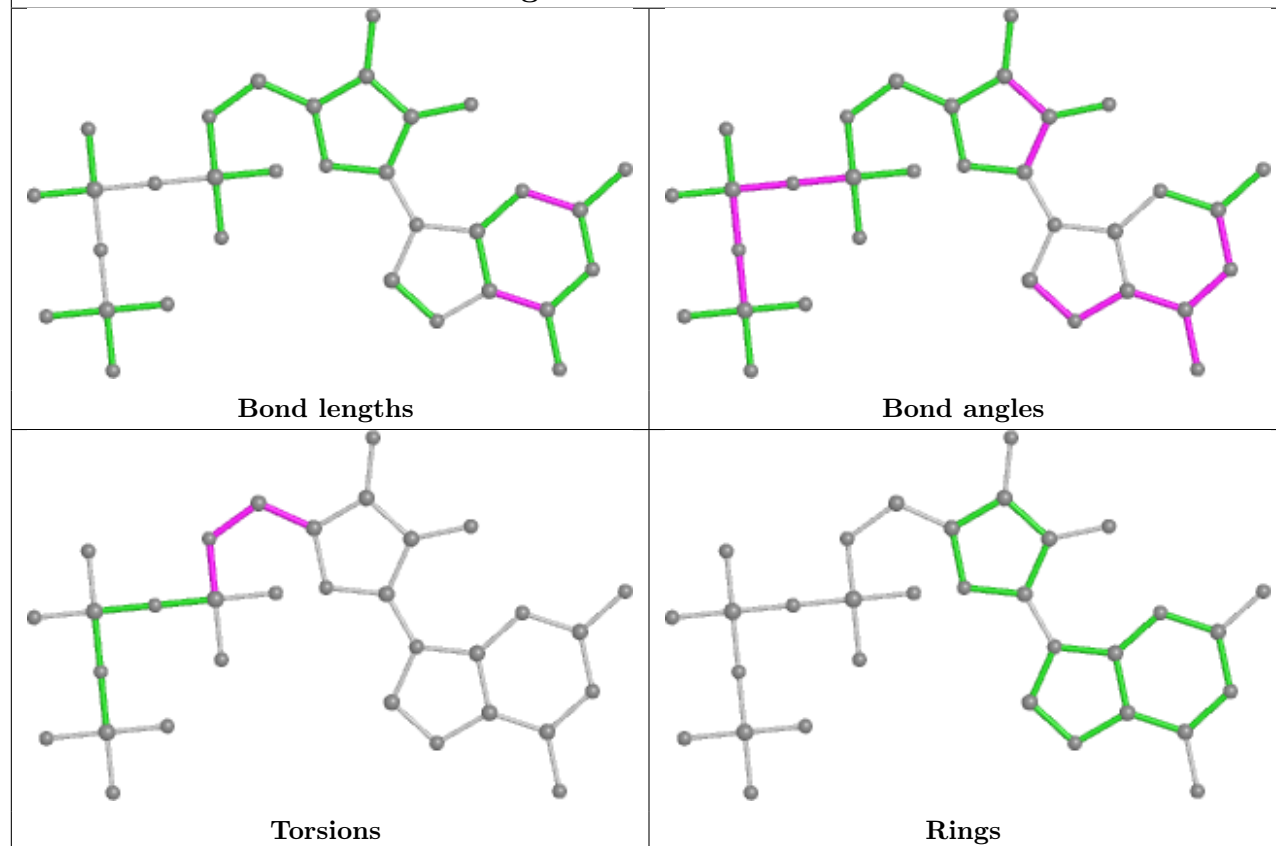
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

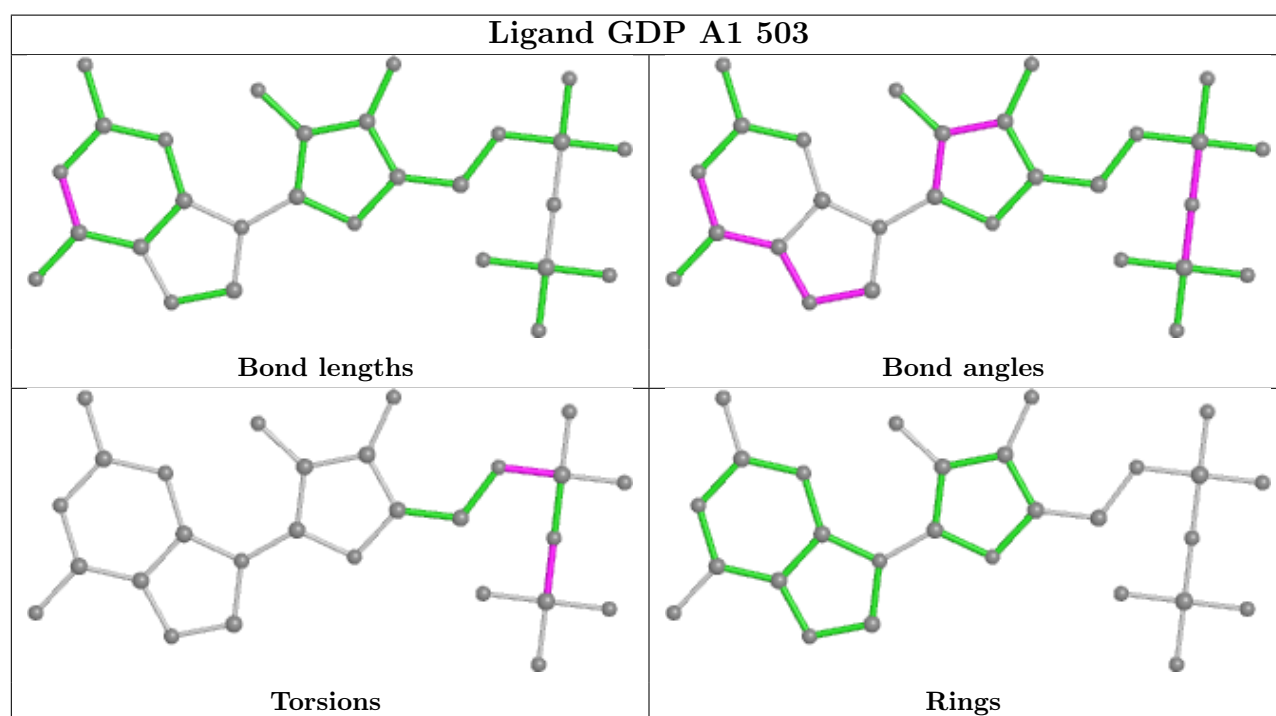
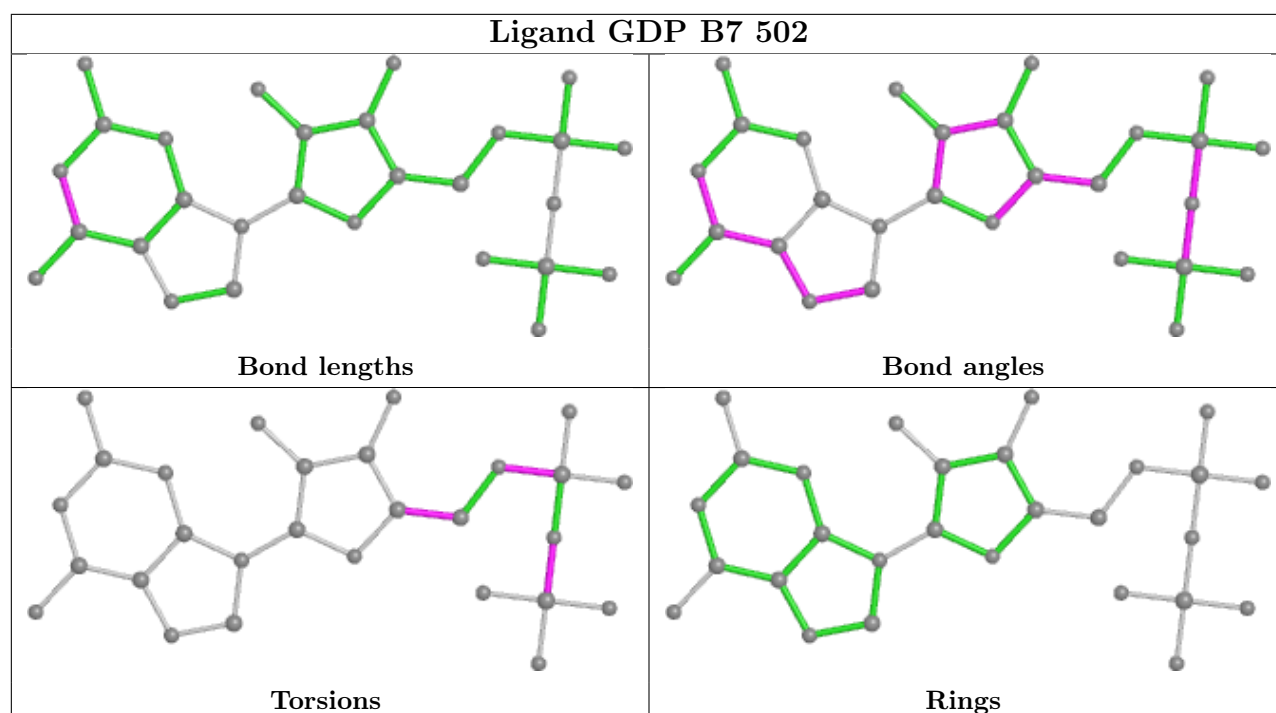


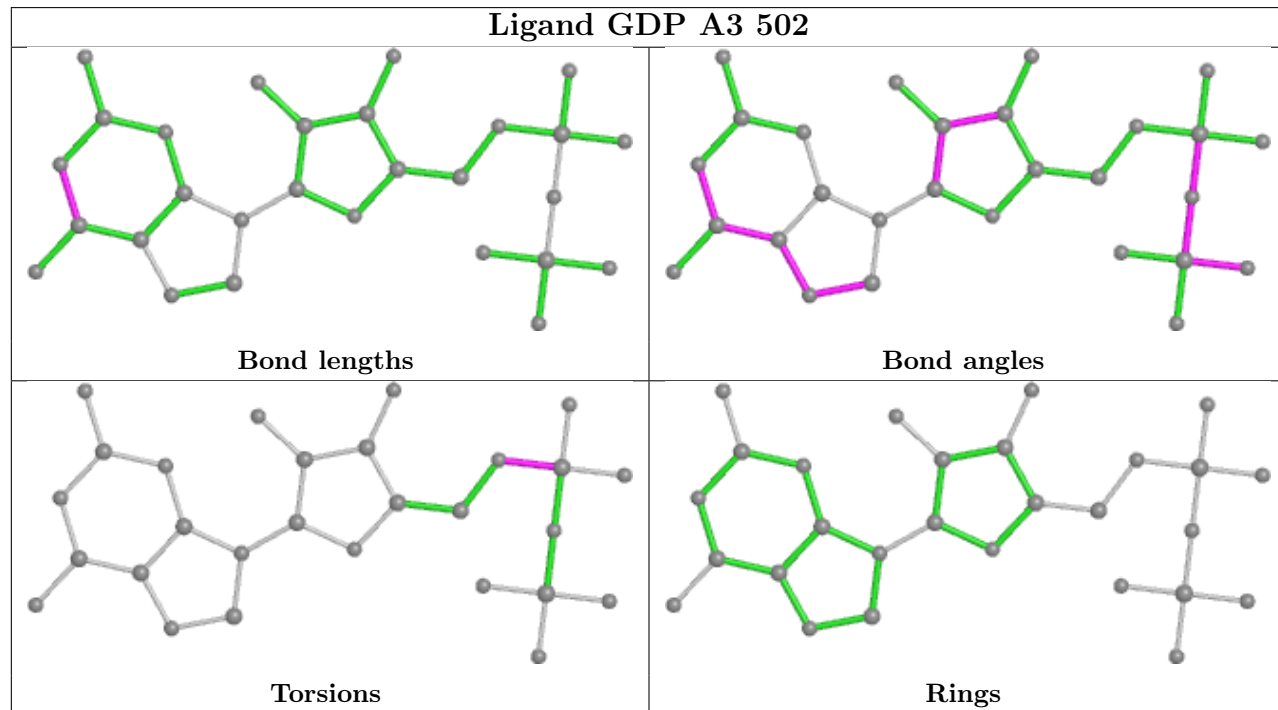
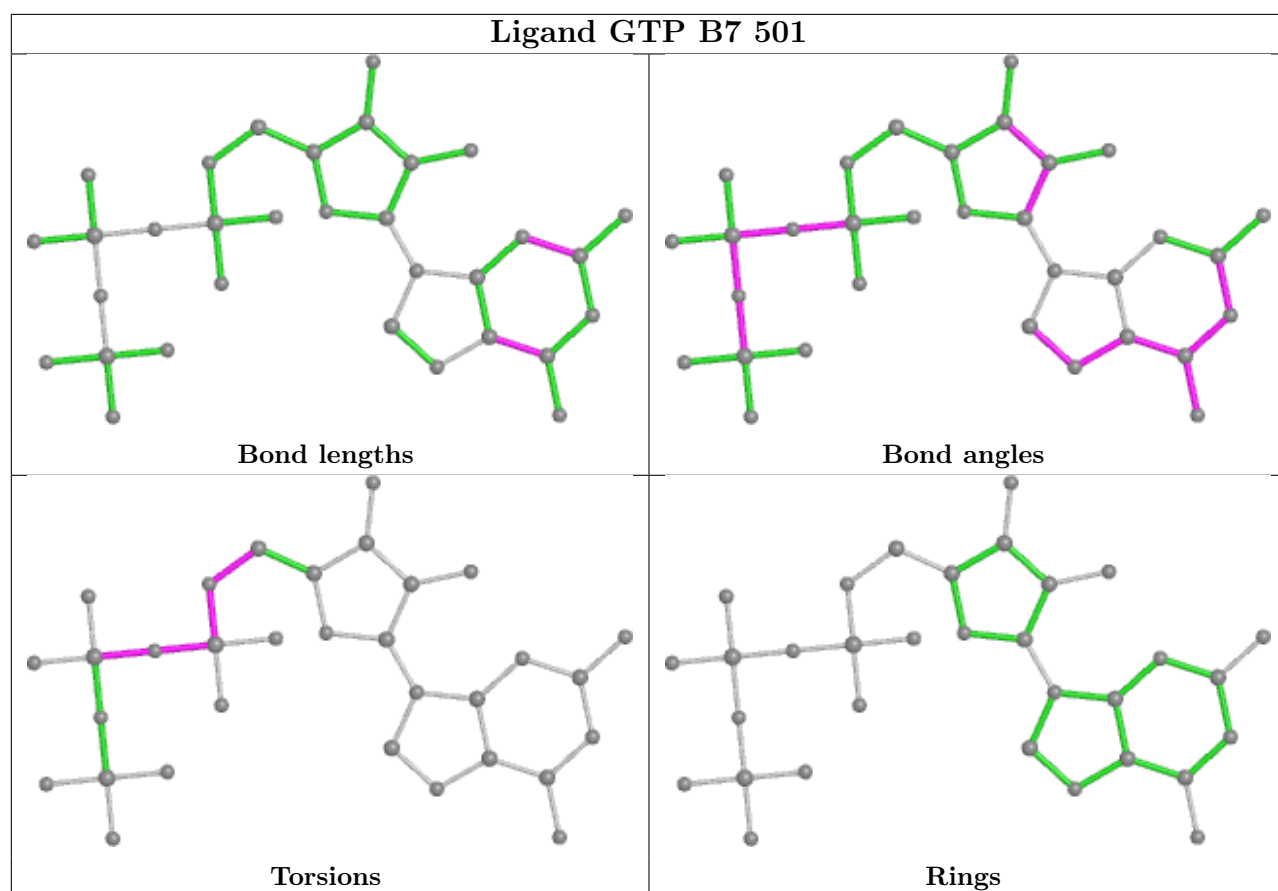
Ligand GTP A7 501

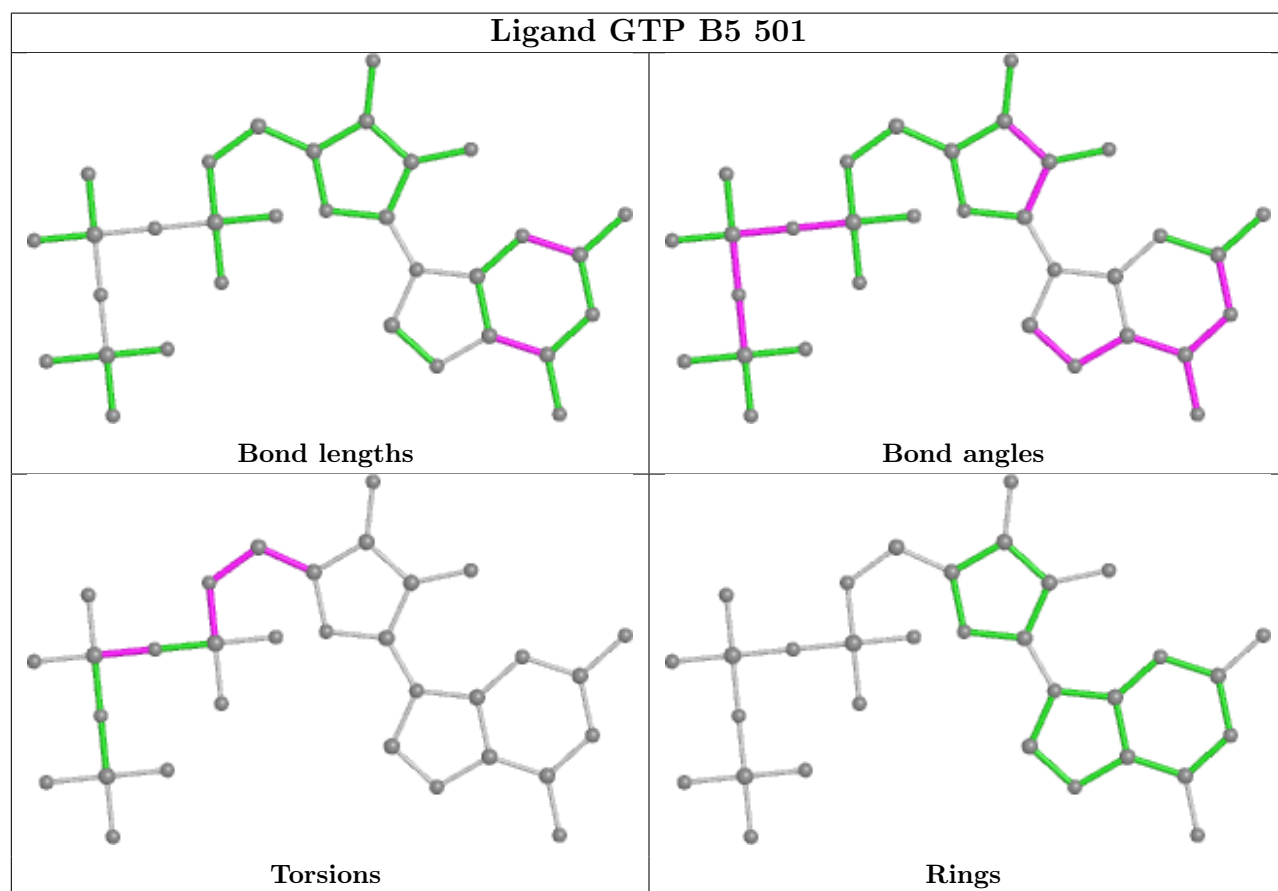
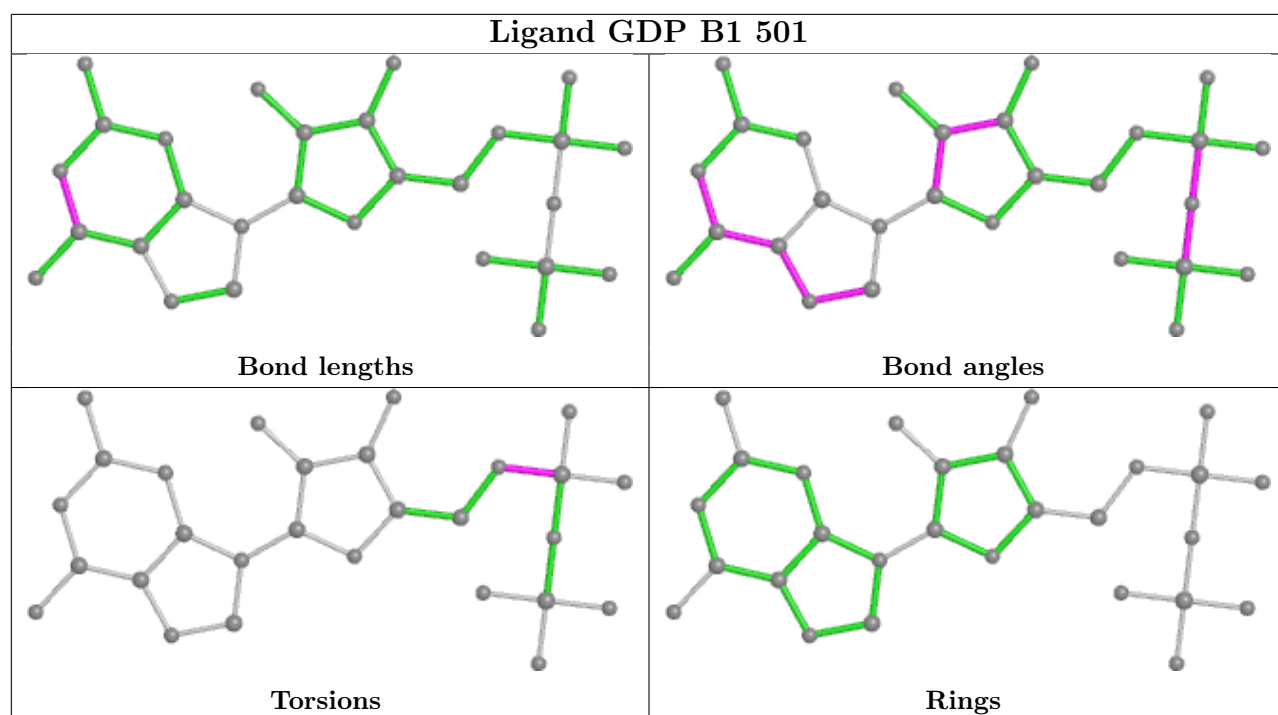


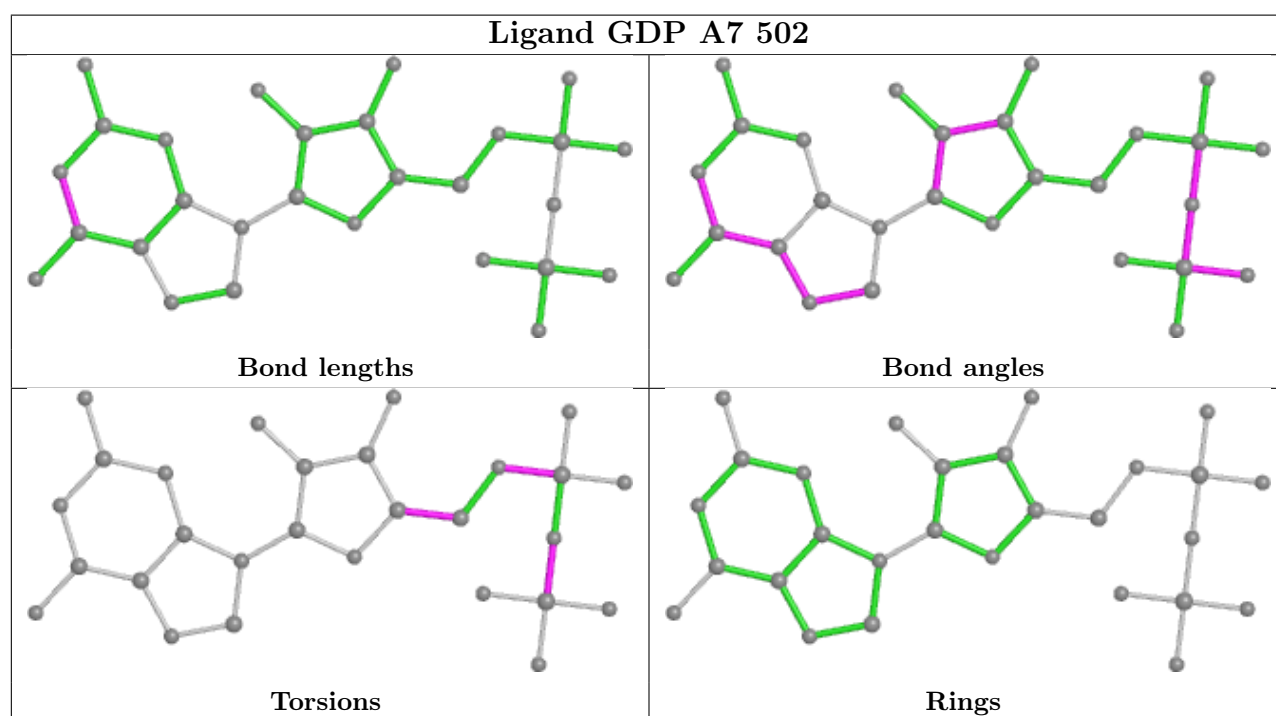
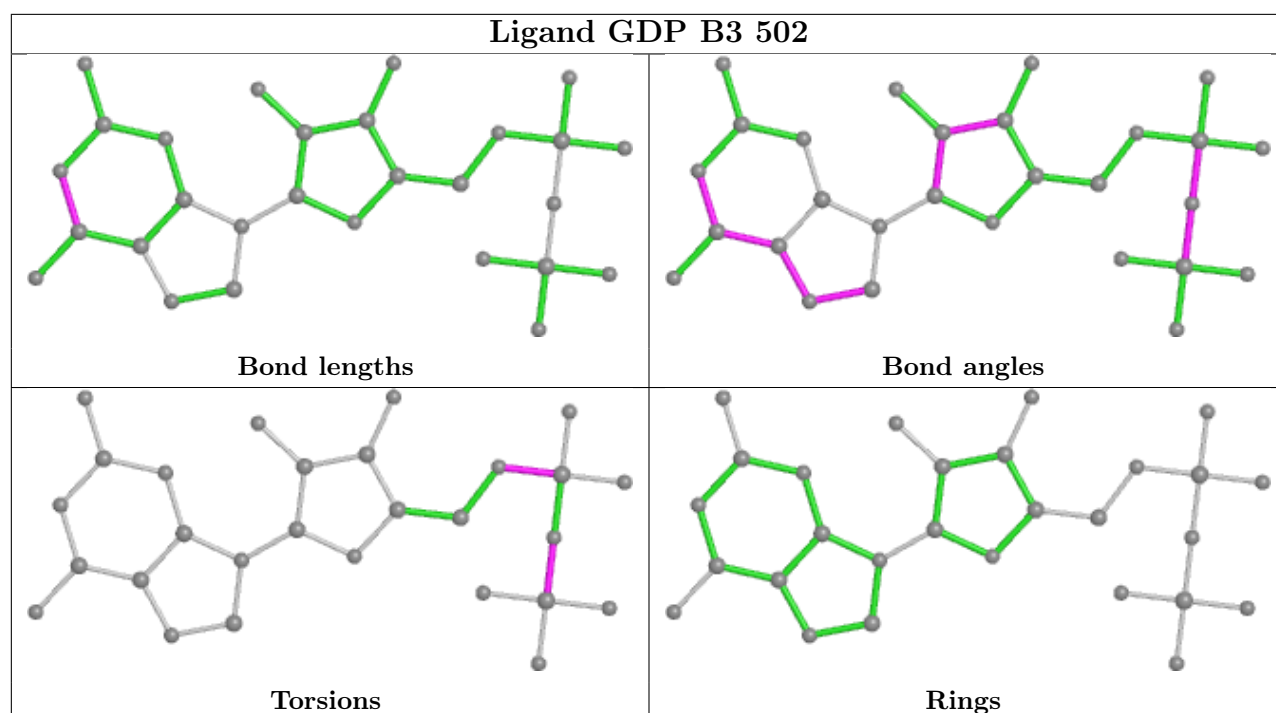
Ligand GTP A1 501



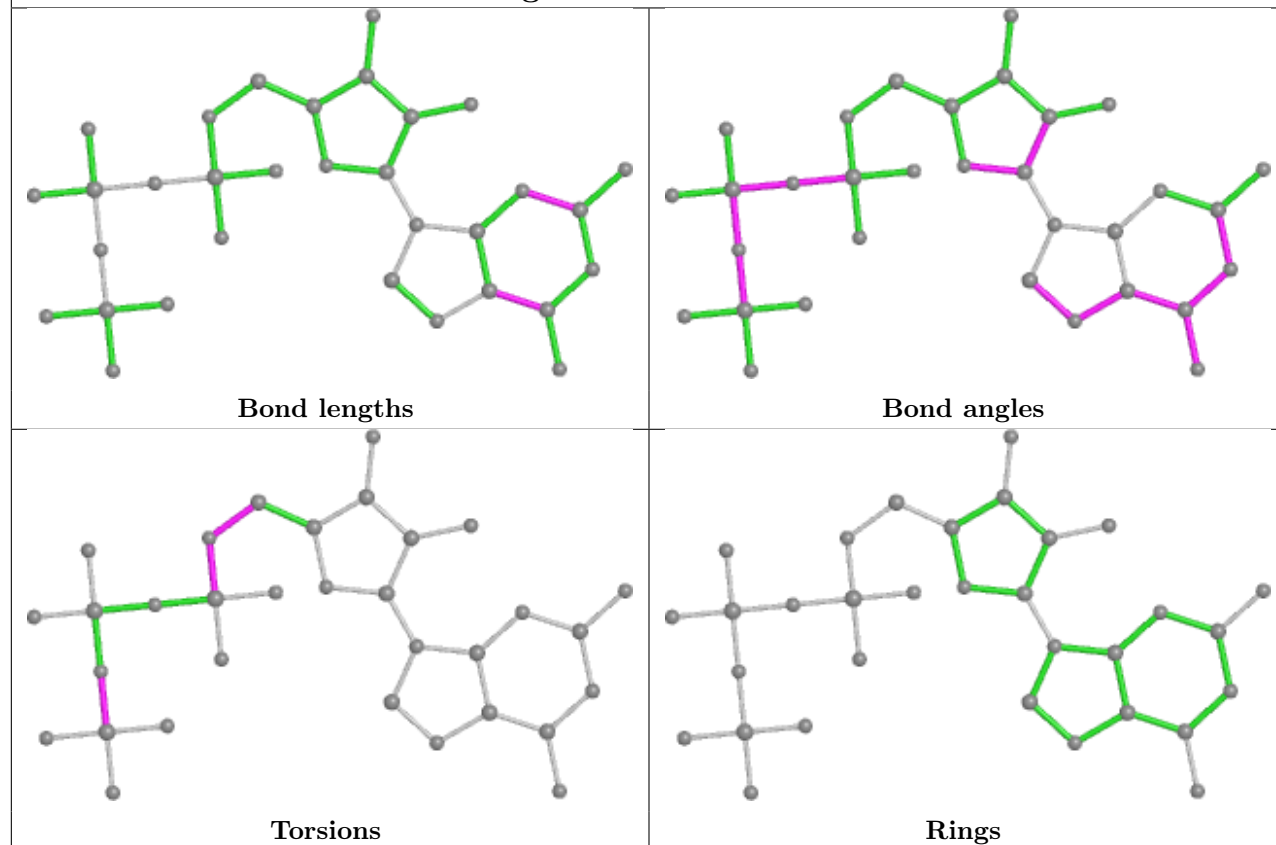




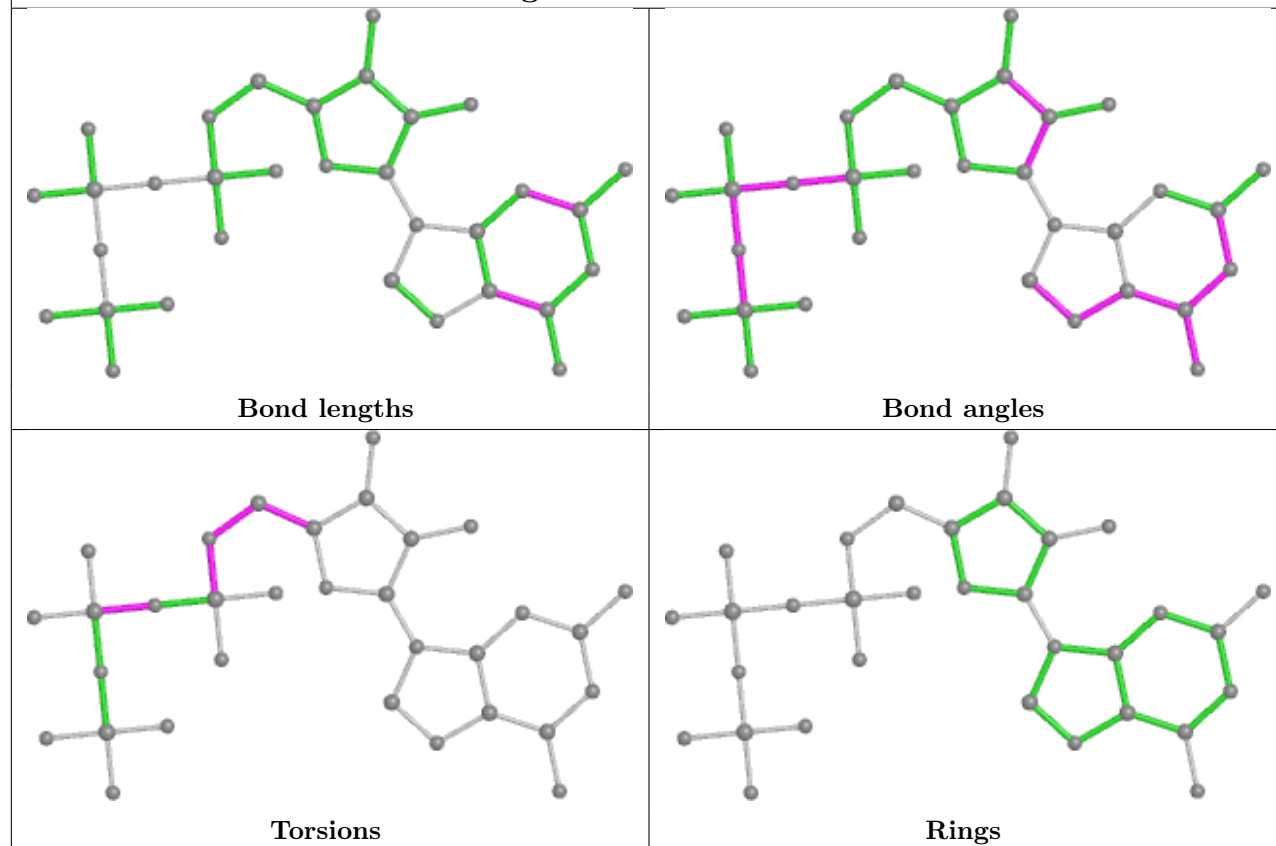


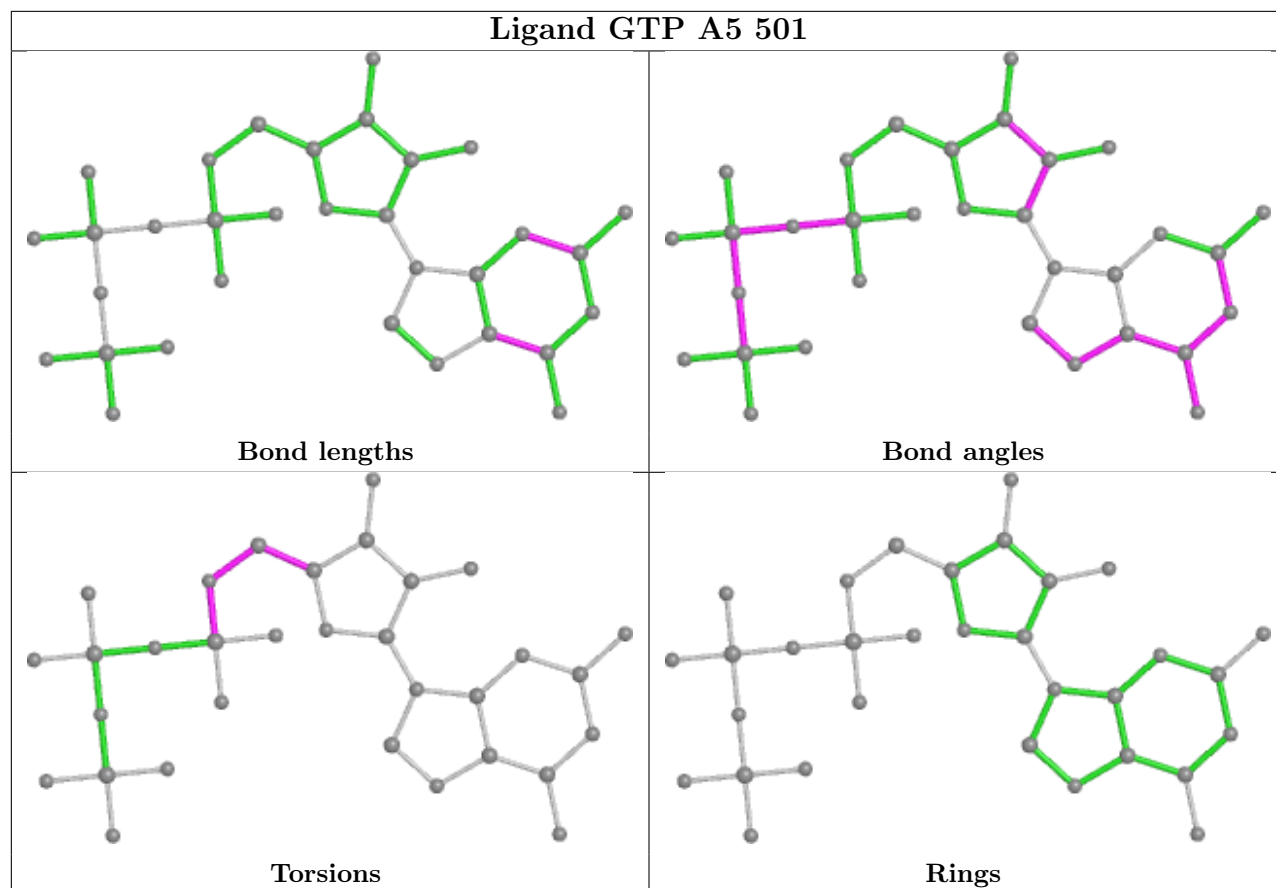


Ligand GTP B2 501



Ligand GTP A3 501





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.

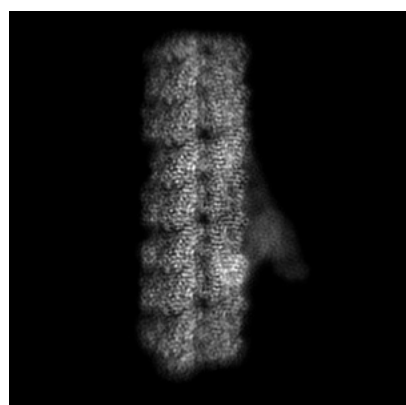
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23084. These allow visual inspection of the internal detail of the map and identification of artifacts.

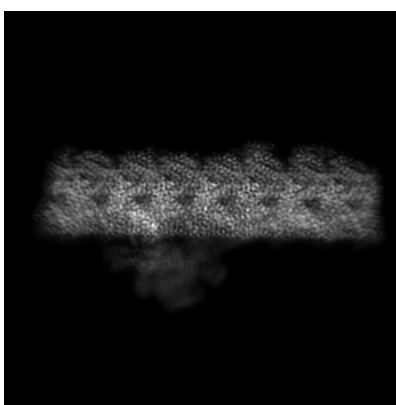
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

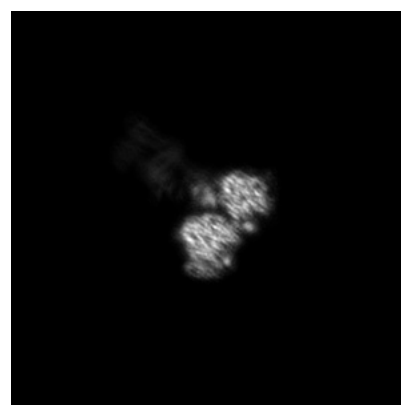
6.1.1 Primary map



X



Y

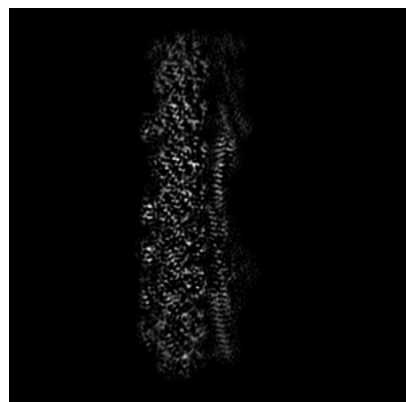


Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

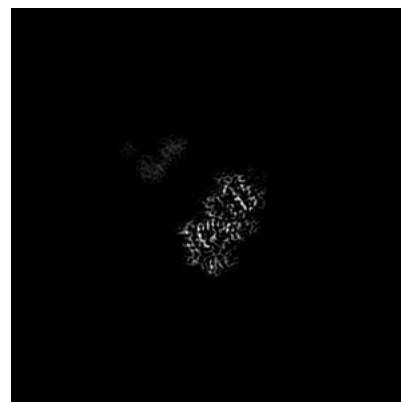
6.2.1 Primary map



X Index: 145



Y Index: 145



Z Index: 145

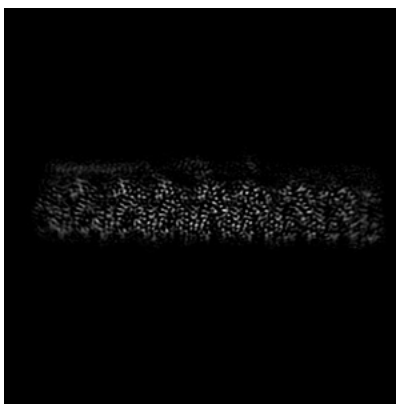
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

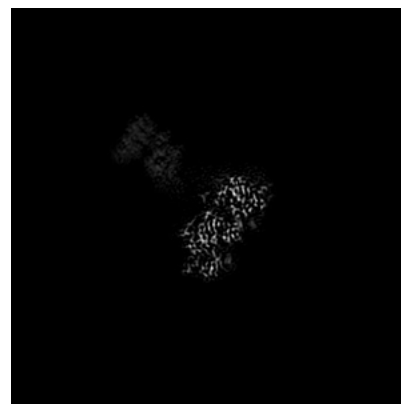
6.3.1 Primary map



X Index: 141



Y Index: 129



Z Index: 115

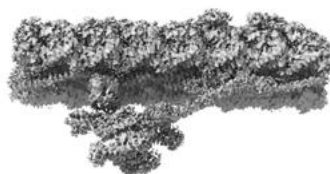
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

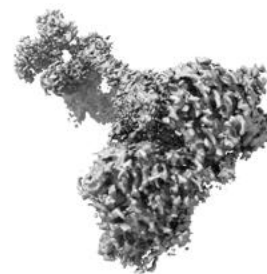
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

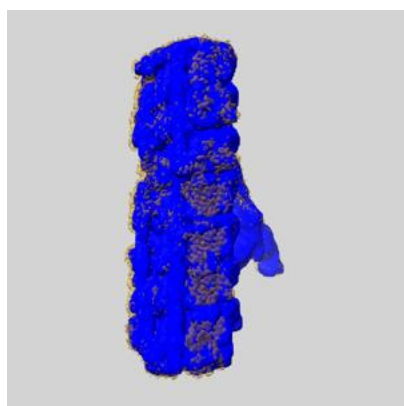
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

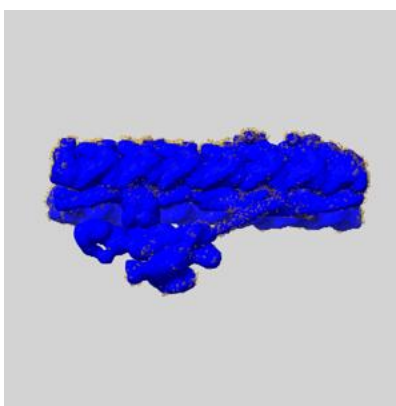
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

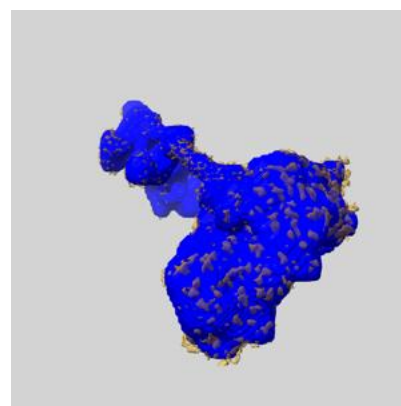
6.5.1 emd_23084_msk_1.map [i](#)



X



Y

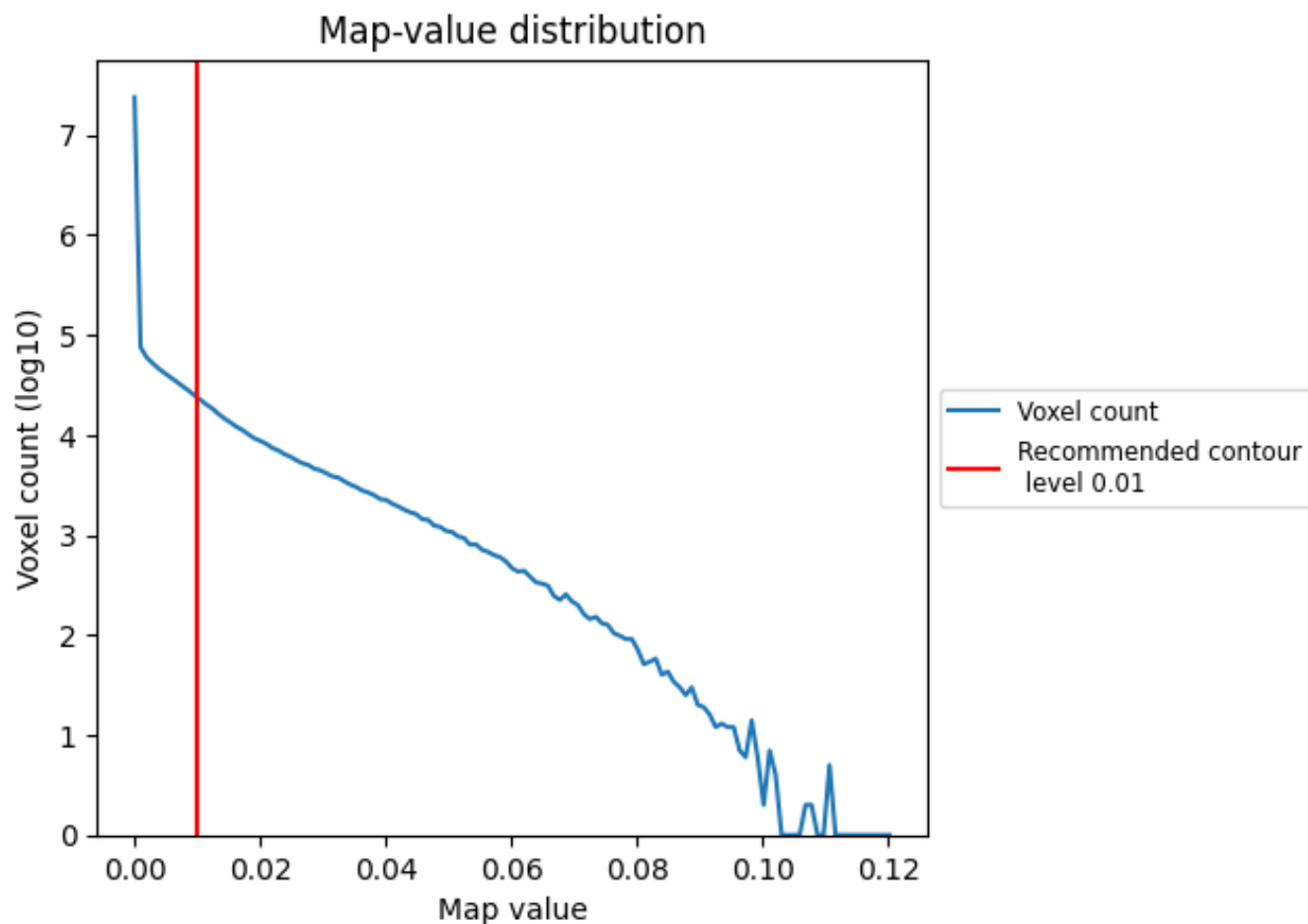


Z

7 Map analysis [i](#)

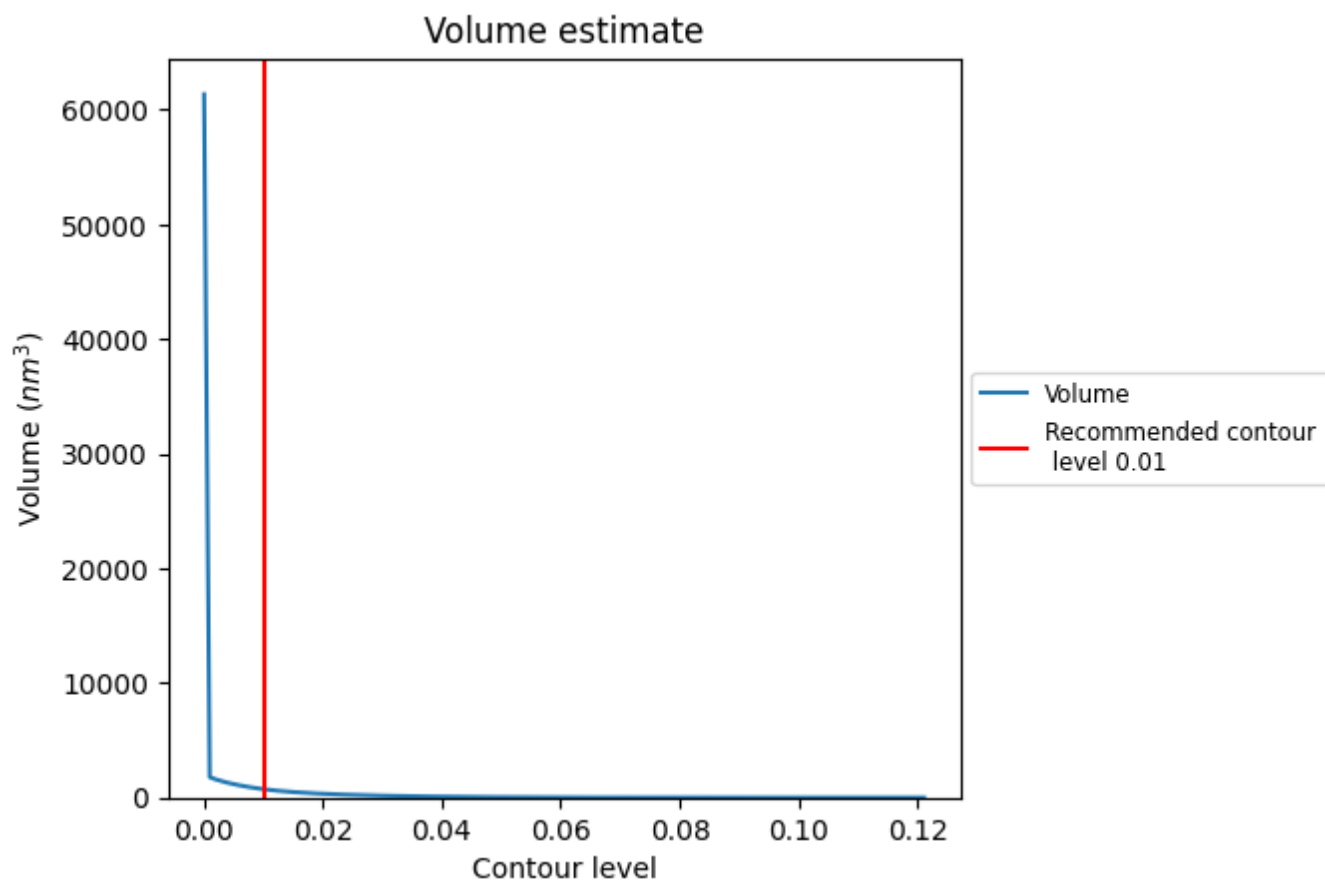
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

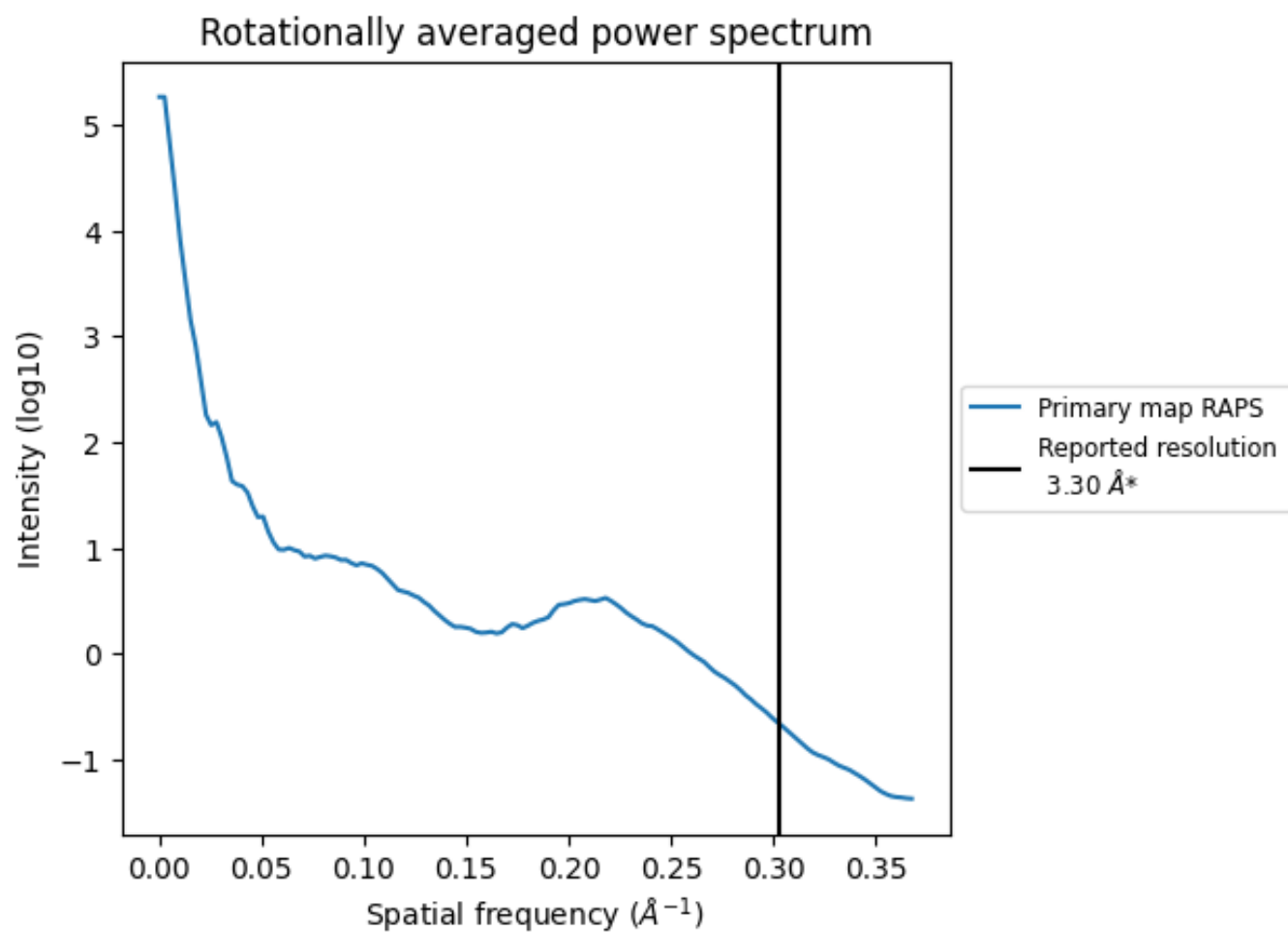
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 732 nm³; this corresponds to an approximate mass of 662 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

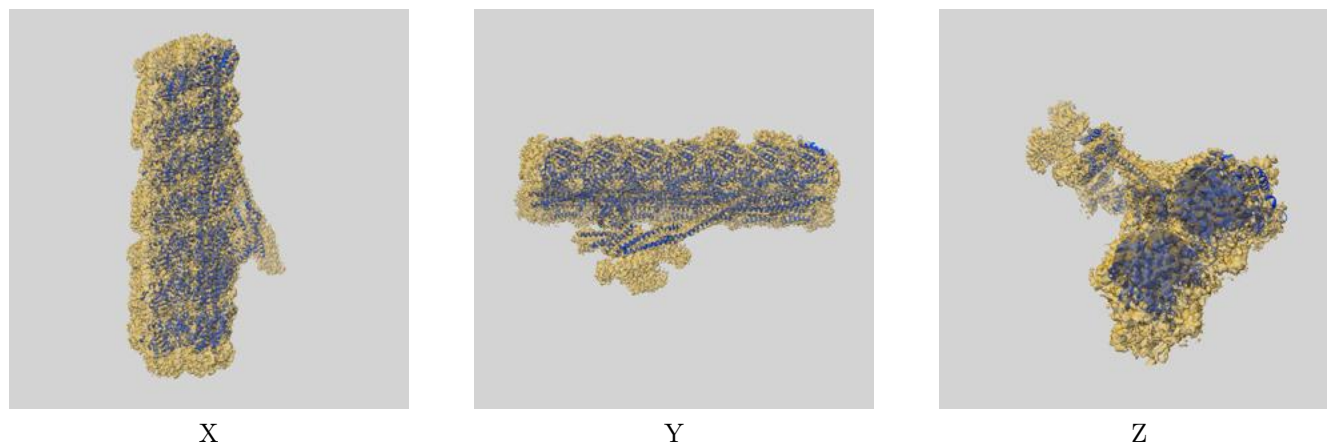
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23084 and PDB model 7KZO. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)

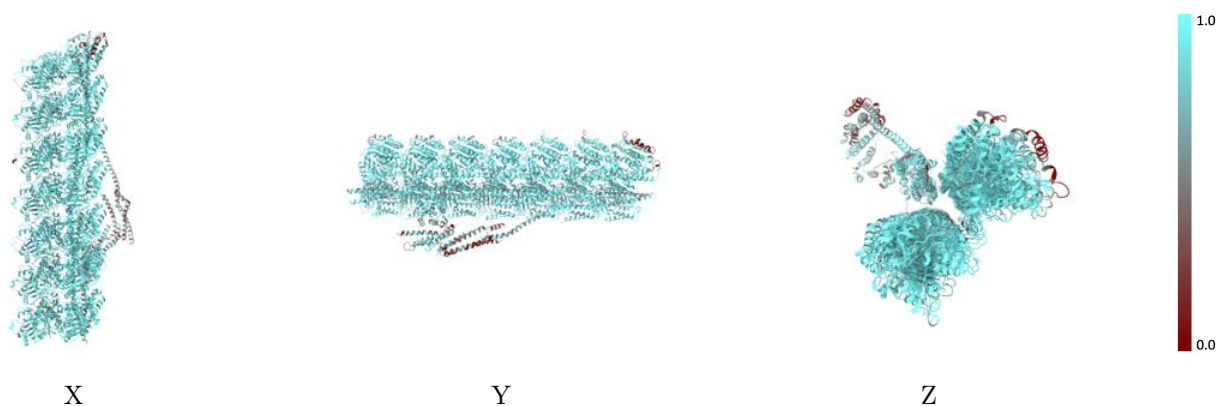


The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

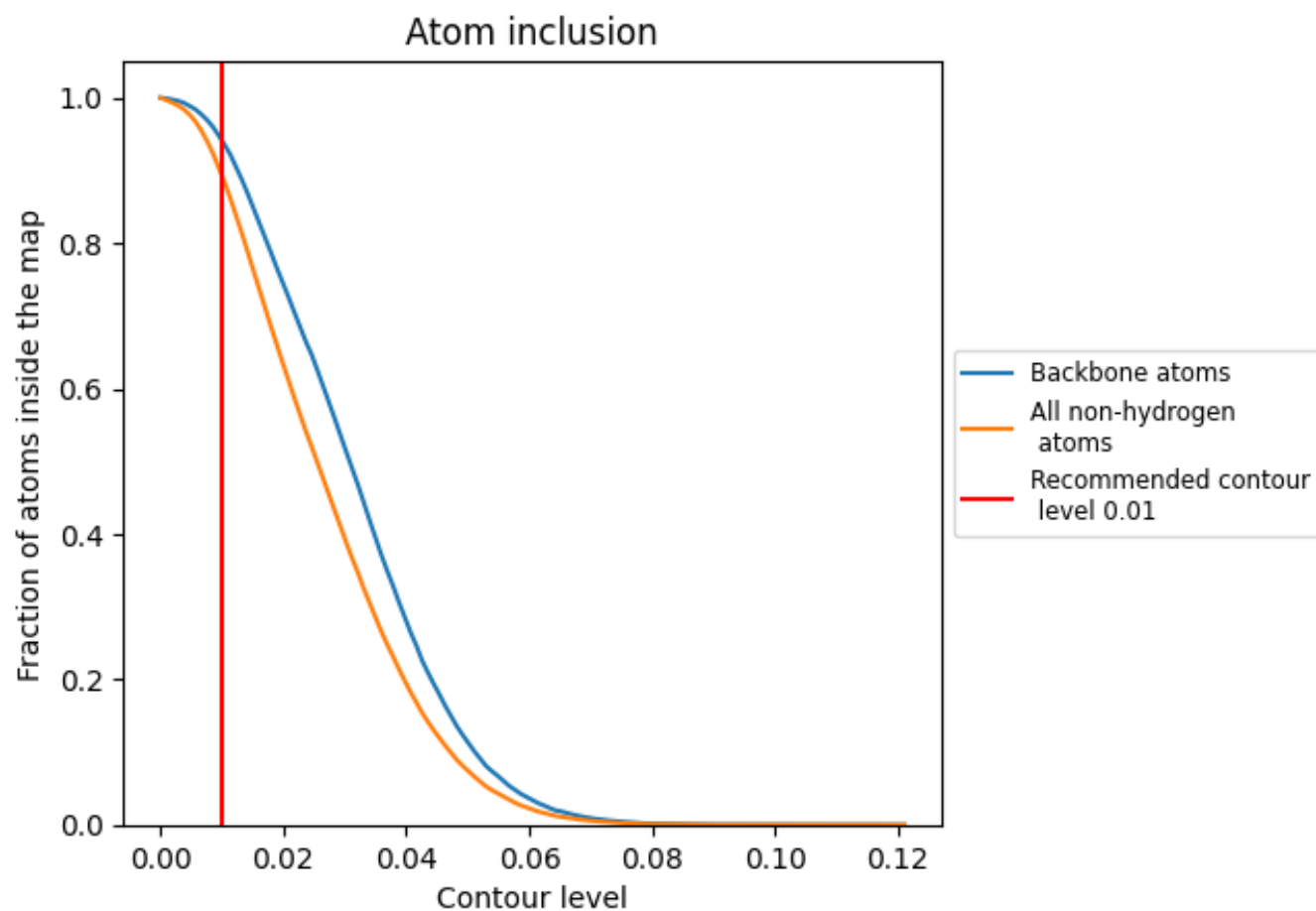
This section was not generated.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	<div></div> 0.8928
A1	<div></div> 0.9067
A2	<div></div> 0.9225
A3	<div></div> 0.9285
A4	<div></div> 0.9362
A5	<div></div> 0.9315
A6	<div></div> 0.9185
A7	<div></div> 0.9183
B1	<div></div> 0.9054
B2	<div></div> 0.9225
B3	<div></div> 0.9346
B4	<div></div> 0.9291
B5	<div></div> 0.9477
B6	<div></div> 0.9202
B7	<div></div> 0.8439
C	<div></div> 0.6236
X	<div></div> 0.6829
X1	<div></div> 0.8400
Y	<div></div> 0.6634
Y1	<div></div> 0.8591
Z	<div></div> 0.7194

