



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 02:12 PM UTC

PDB ID : 7JU4 / pdb_00007ju4
EMDB ID : EMD-22481
Title : Radial spoke 2 stalk, IDAc, and N-DRC attached with doublet microtubule
Authors : Gui, M.; Ma, M.; Sze-Tu, E.; Wang, X.; Koh, F.; Zhong, E.; Berger, B.; Davis, J.; Dutcher, S.; Zhang, R.; Brown, A.
Deposited on : 2020-08-19
Resolution : 3.40 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:

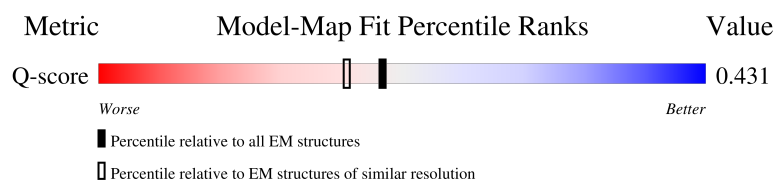
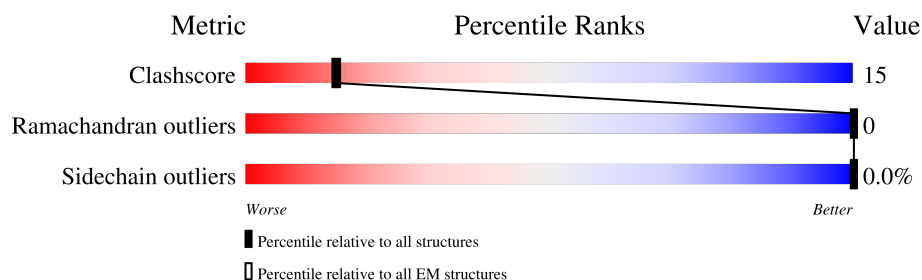
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



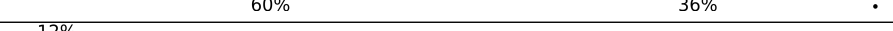
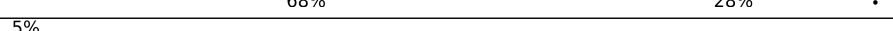
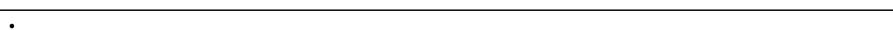
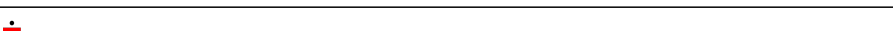
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	0	471	7% 24% 13% 63%
1	4	471	5% 22% 11% 67%
2	1	698	16% 8% 76%
3	2	573	23% 9% 68%

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Mol	Chain	Length	Quality of chain
4	3	72	 88% 12%
5	6	443	 65% 31% .
5	8	443	 64% 33% .
5	C	443	 5% 62% 34% .
5	G	443	 66% 30% .
5	I	443	 65% 31% .
5	K	443	 62% 34% .
5	O	443	 65% 31% .
5	Q	443	 63% 33% .
5	S	443	 60% 36% .
5	W	443	 12% 68% 28% .
5	Y	443	 5% 70% 27% .
5	i	443	 64% 32% .
5	k	443	 63% 33% .
5	y	443	 63% 33% .
6	7	451	 65% 30% 5%
6	9	451	 65% 30% 5%
6	D	451	 66% 30% .
6	H	451	 64% 33% .
6	J	451	 65% 32% .
6	L	451	 66% 31% .
6	P	451	 65% 32% .
6	R	451	 69% 27% .
6	T	451	 63% 34% .
6	X	451	 63% 31% 5%

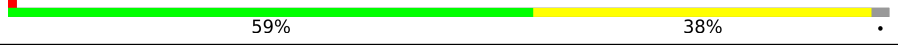
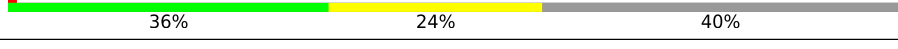
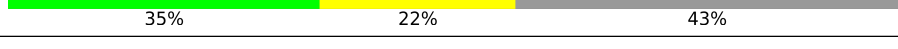
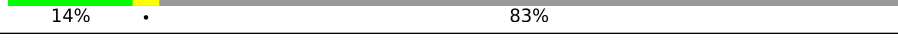
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Mol	Chain	Length	Quality of chain
6	Z	451	
6	j	451	
6	t	451	
6	z	451	
7	A	925	
8	B	904	
9	E	516	
9	F	516	
10	M	500	
10	N	500	
11	U	204	
11	V	204	
12	a	91	
12	b	91	
12	c	91	
12	d	91	
12	e	91	
12	f	91	
12	g	91	
12	h	91	
12	o	91	
12	p	91	
12	q	91	
12	r	91	
13	l	331	

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Mol	Chain	Length	Quality of chain
14	m	256	
15	n	378	
16	s	682	
17	u	377	
18	v	253	
18	w	253	
19	x	1298	

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 133504 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 Dynein regulatory complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	173	Total	C	N	O	S	0	0
			1364	858	235	270	1		
1	4	154	Total	C	N	O	S	0	0
			1246	788	214	243	1		

- Molecule 2 is a protein called Dynein regulatory complex protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	168	Total	C	N	O	S	0	0
			1431	896	265	267	3		

- Molecule 3 is a protein called Dynein regulatory complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	183	Total	C	N	O	S	0	0
			1497	933	281	279	4		

- Molecule 4 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	3	72	Total	C	N	O	0	0
			360	216	72	72		

- Molecule 5 is a protein called Tubulin beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
5	8	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		
5	C	426	Total	C	N	O	S	0	0
			3346	2103	574	639	30		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	I	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	K	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	O	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	Q	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	S	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	W	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	Y	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	i	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	k	426	Total 3346	C 2103	N 574	O 639	S 30	0	0
5	y	426	Total 3346	C 2103	N 574	O 639	S 30	0	0

- Molecule 6 is a protein called Tubulin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
6	9	427	Total 3318	C 2103	N 565	O 629	S 21	0	0
6	D	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
6	H	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
6	J	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
6	L	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
6	P	436	Total 3376	C 2136	N 575	O 644	S 21	0	0
6	R	436	Total 3376	C 2136	N 575	O 644	S 21	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	436	Total	C	N	O	S	0	0
			3376	2136	575	644	21		
6	X	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
6	Z	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
6	j	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
6	t	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		
6	z	427	Total	C	N	O	S	0	0
			3318	2103	565	629	21		

- Molecule 7 is a protein called Flagellar-associated protein 59.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	435	Total	C	N	O	S	0	0
			3535	2170	665	686	14		

- Molecule 8 is a protein called Flagellar-associated protein 172.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	435	Total	C	N	O	S	0	0
			3479	2134	655	674	16		

- Molecule 9 is a protein called Radial spoke protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	86	Total	C	N	O	S	0	0
			685	432	109	142	2		
9	F	117	Total	C	N	O	S	0	0
			931	583	150	195	3		

- Molecule 10 is a protein called Radial spoke protein 7.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	M	44	Total	C	N	O	0	0
			353	232	59	62		
10	N	40	Total	C	N	O	0	0
			316	208	53	55		

- Molecule 11 is a protein called Radial spoke protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	U	49	Total	C	N	O	S	0	0
			391	255	65	70	1		
11	V	160	Total	C	N	O		0	0
			891	544	172	175			

- Molecule 12 is a protein called Dynein 8 kDa light chain, flagellar outer arm.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	a	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	b	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	c	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	d	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	e	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	f	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	g	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	h	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	o	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	p	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	q	84	Total	C	N	O	S	0	0
			686	442	115	125	4		
12	r	84	Total	C	N	O	S	0	0
			686	442	115	125	4		

- Molecule 13 is a protein called Radial spoke protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	l	327	Total	C	N	O	S	0	0
			2438	1529	434	465	10		

- Molecule 14 is a protein called FAP207.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	m	204	Total	C	N	O	S	0	0
			1639	1029	294	310	6		

- Molecule 15 is a protein called Radial spike protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	n	307	Total	C	N	O	S	0	0
			1516	902	307	307			

- Molecule 16 is a protein called FAP253.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	s	176	Total	C	N	O	S	0	0
			1465	924	265	273	3		

- Molecule 17 is a protein called Actin.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	u	370	Total	C	N	O	S	0	0
			2880	1828	487	542	23		

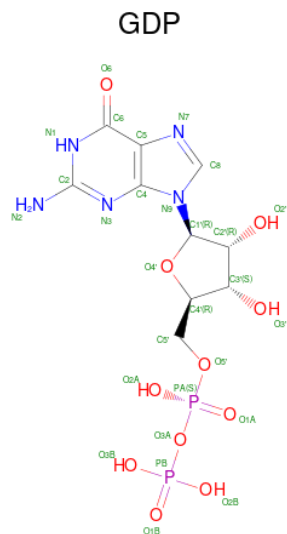
- Molecule 18 is a protein called 28 kDa inner dynein arm light chain, axonemal.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	v	152	Total	C	N	O	S	0	0
			1256	776	229	245	6		
18	w	143	Total	C	N	O	S	0	0
			1186	736	213	232	5		

- Molecule 19 is a protein called CFAP91 domain-containing protein.

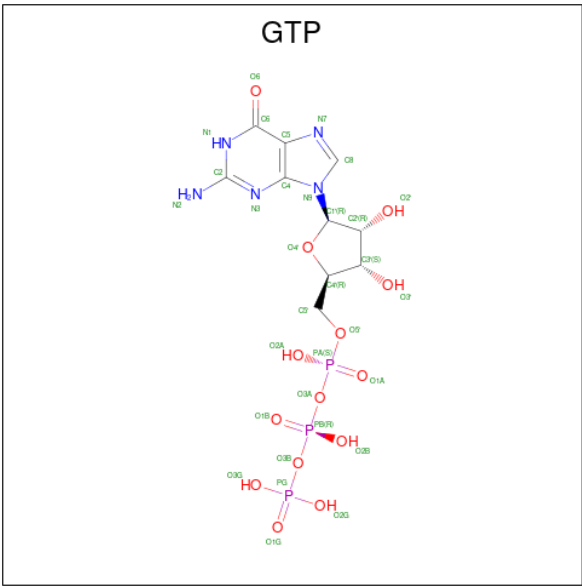
Mol	Chain	Residues	Atoms					AltConf	Trace
19	x	224	Total	C	N	O	S	0	0
			1826	1135	343	343	5		

- Molecule 20 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					AltConf
20	6	1	Total 28	C 10	N 5	O 11	P 2	0
20	8	1	Total 28	C 10	N 5	O 11	P 2	0
20	C	1	Total 28	C 10	N 5	O 11	P 2	0
20	G	1	Total 28	C 10	N 5	O 11	P 2	0
20	I	1	Total 28	C 10	N 5	O 11	P 2	0
20	K	1	Total 28	C 10	N 5	O 11	P 2	0
20	O	1	Total 28	C 10	N 5	O 11	P 2	0
20	Q	1	Total 28	C 10	N 5	O 11	P 2	0
20	S	1	Total 28	C 10	N 5	O 11	P 2	0
20	W	1	Total 28	C 10	N 5	O 11	P 2	0
20	Y	1	Total 28	C 10	N 5	O 11	P 2	0
20	i	1	Total 28	C 10	N 5	O 11	P 2	0
20	k	1	Total 28	C 10	N 5	O 11	P 2	0
20	y	1	Total 28	C 10	N 5	O 11	P 2	0

- Molecule 21 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
21	7	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	9	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	D	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	H	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	J	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	L	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	P	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	R	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	T	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	X	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	Z	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	j	1	Total	C	N	O	P	0
			32	10	5	14	3	
21	y	1	Total	C	N	O	P	0
			32	10	5	14	3	

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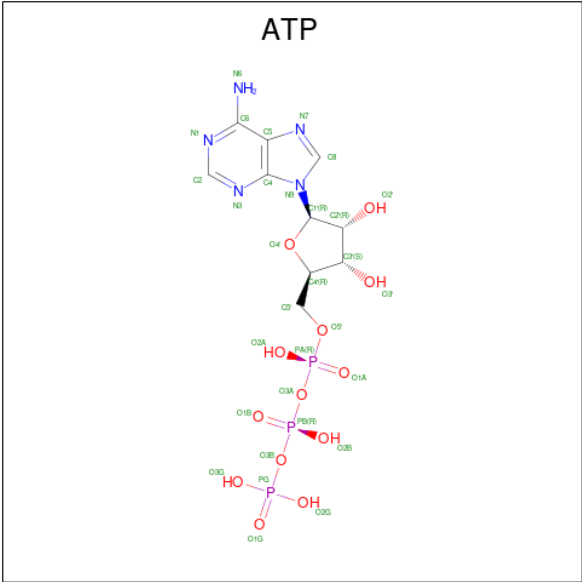
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Mol	Chain	Residues	Atoms					AltConf
21	z	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
22	7	1	Total	Mg	0
			1	1	
22	9	1	Total	Mg	0
			1	1	
22	D	1	Total	Mg	0
			1	1	
22	H	1	Total	Mg	0
			1	1	
22	J	1	Total	Mg	0
			1	1	
22	L	1	Total	Mg	0
			1	1	
22	P	1	Total	Mg	0
			1	1	
22	R	1	Total	Mg	0
			1	1	
22	T	1	Total	Mg	0
			1	1	
22	X	1	Total	Mg	0
			1	1	
22	Z	1	Total	Mg	0
			1	1	
22	j	1	Total	Mg	0
			1	1	
22	t	1	Total	Mg	0
			1	1	
22	z	1	Total	Mg	0
			1	1	

- Molecule 23 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

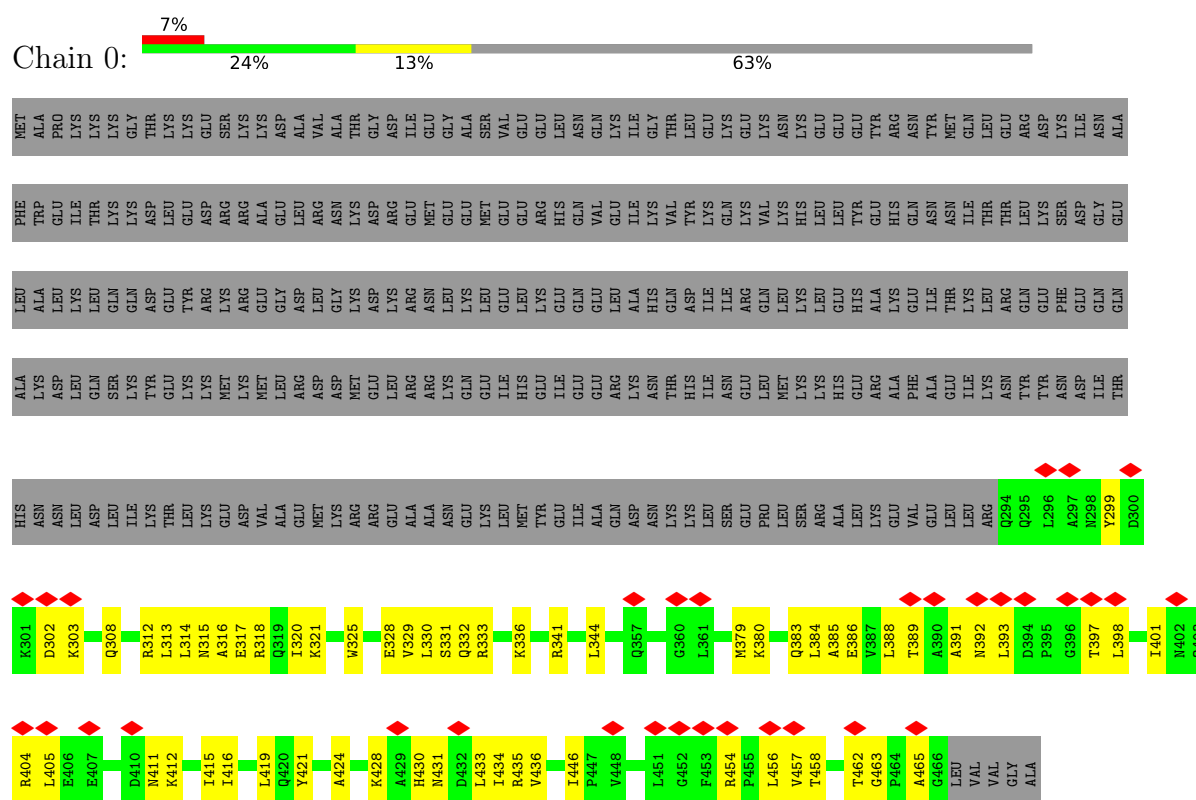


Mol	Chain	Residues	Atoms					AltConf
23	u	1	Total	C	N	O	P	0
			31	10	5	13	3	

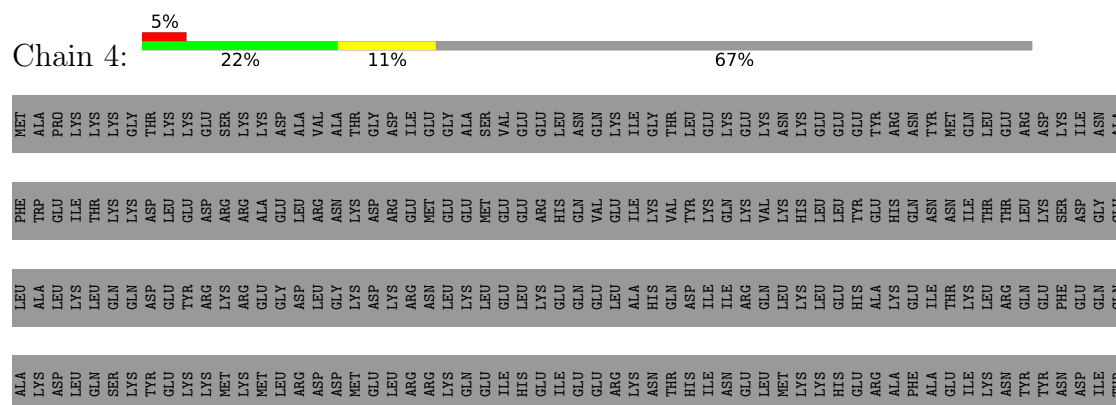
3 Residue-property plots

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: Dynein regulatory complex subunit 4

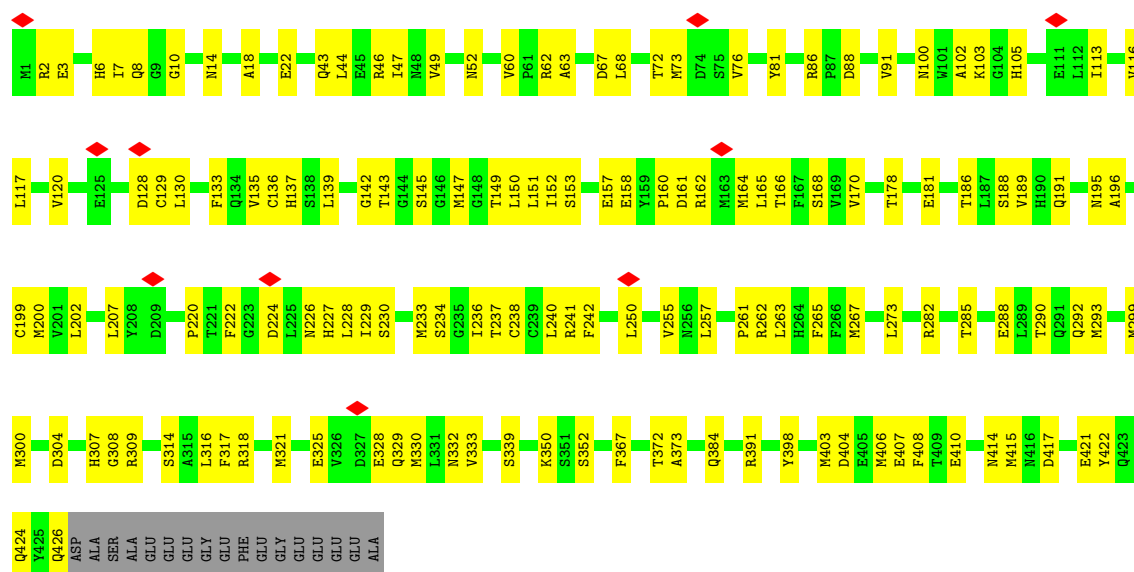


• Molecule 1: Dynein regulatory complex subunit 4

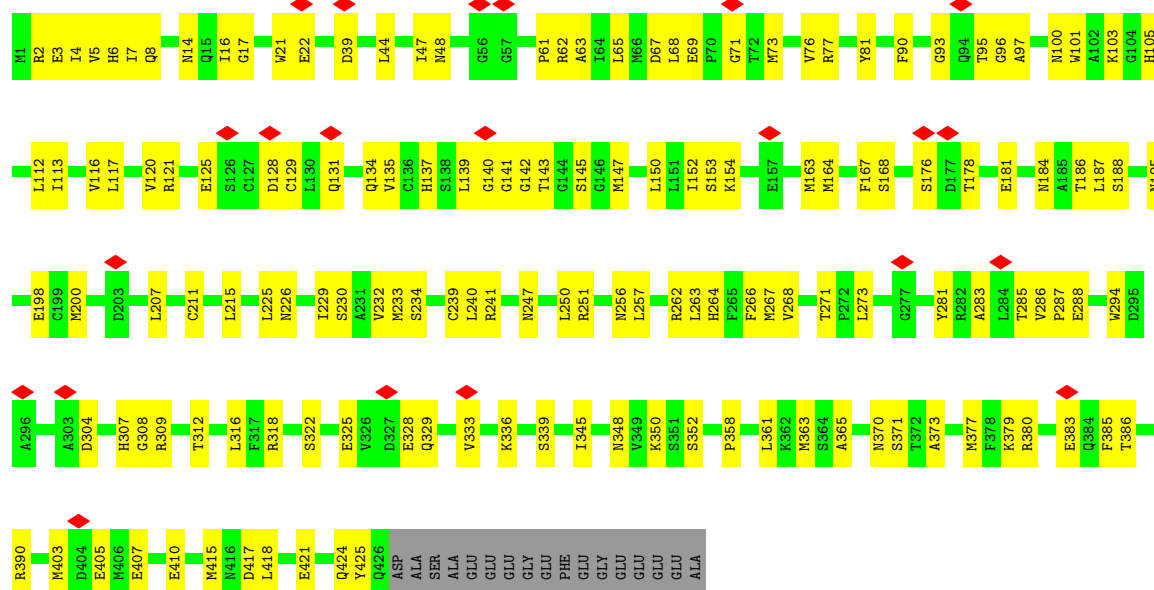




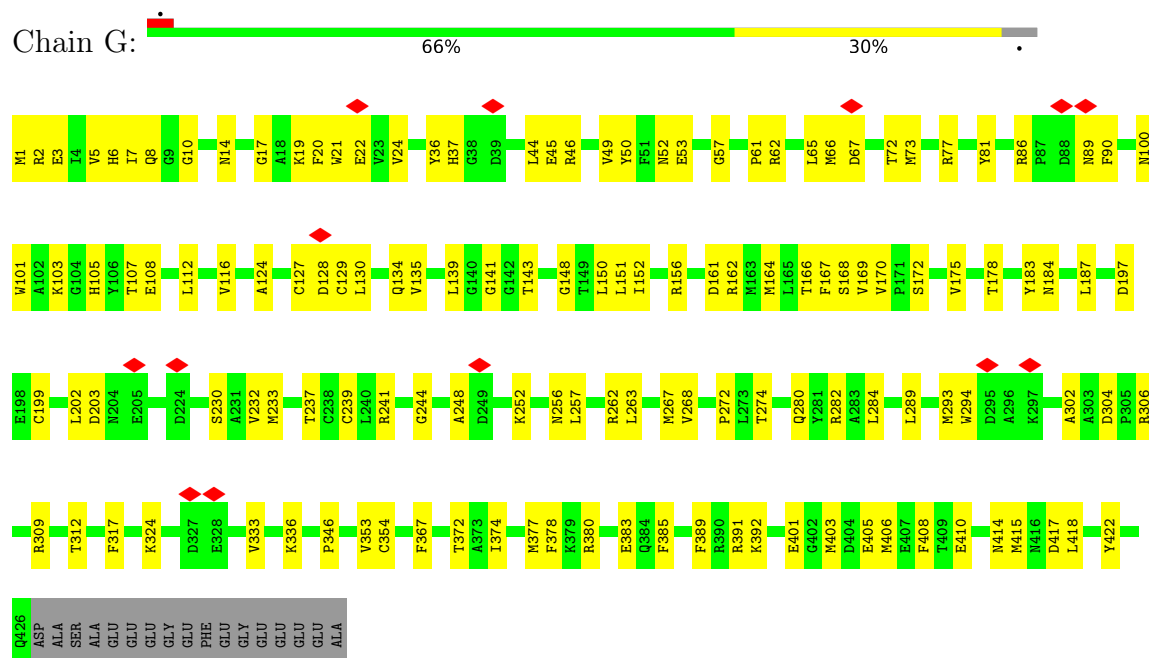
- Molecule 5: Tubulin beta



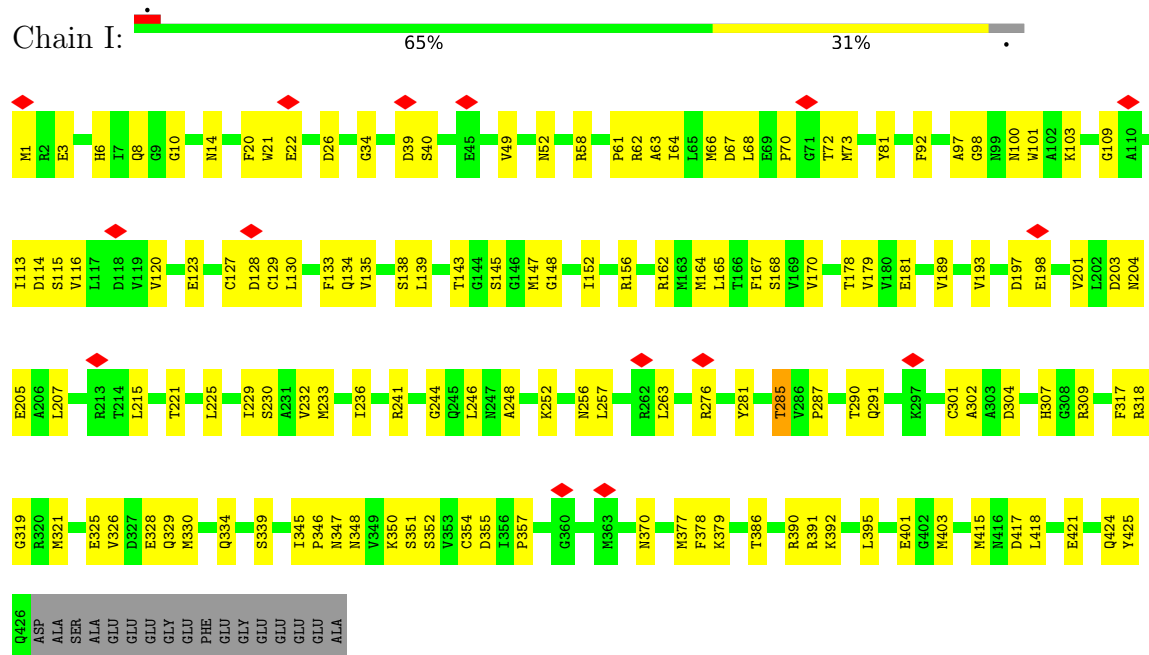
- Molecule 5: Tubulin beta



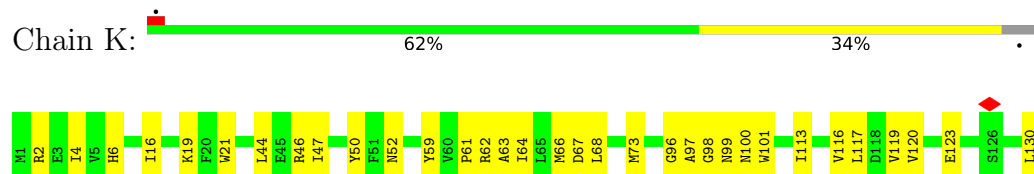
- Molecule 5: Tubulin beta

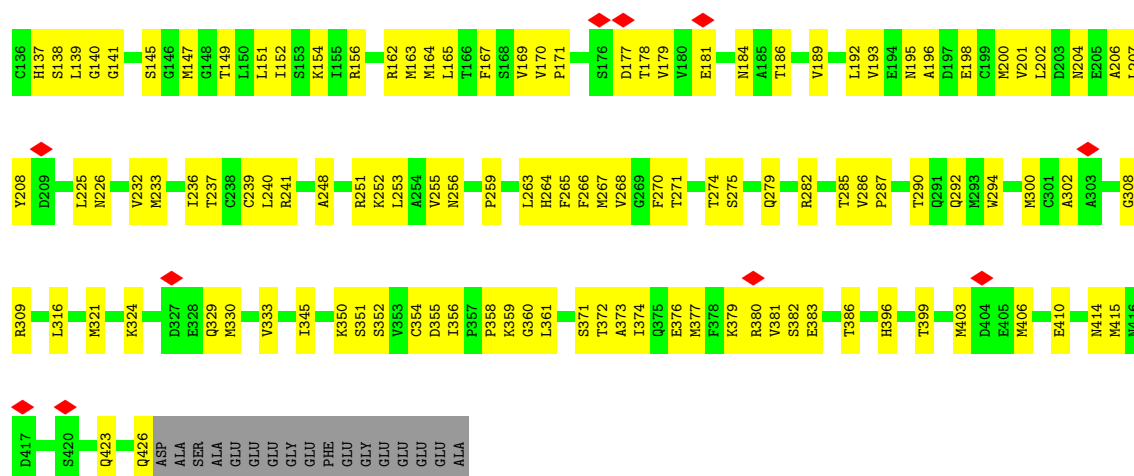


• Molecule 5: Tubulin beta

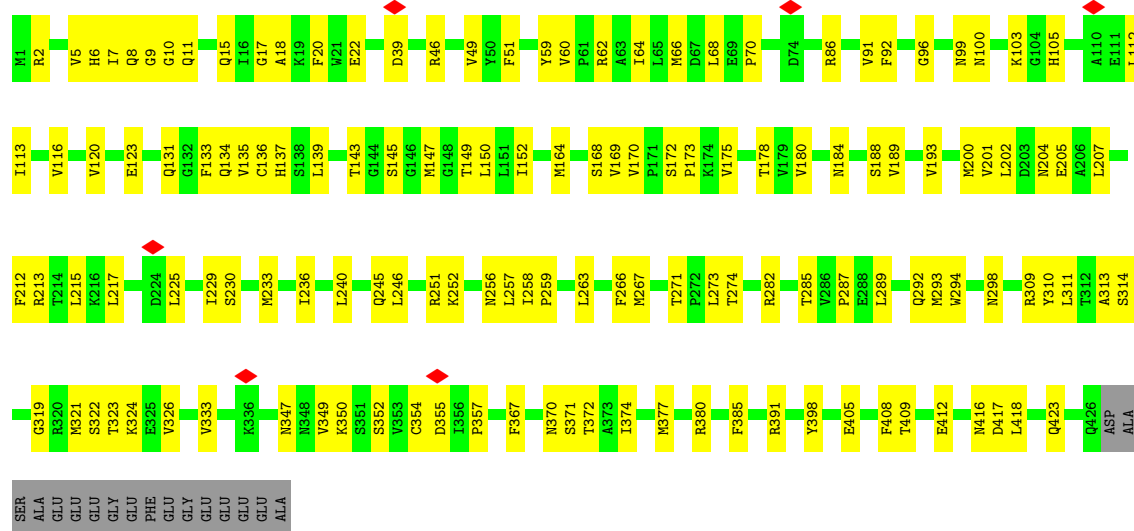


• Molecule 5: Tubulin beta

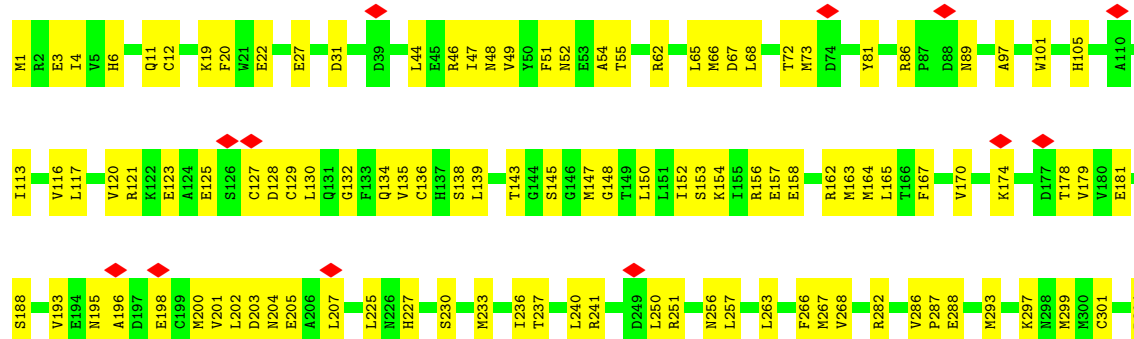




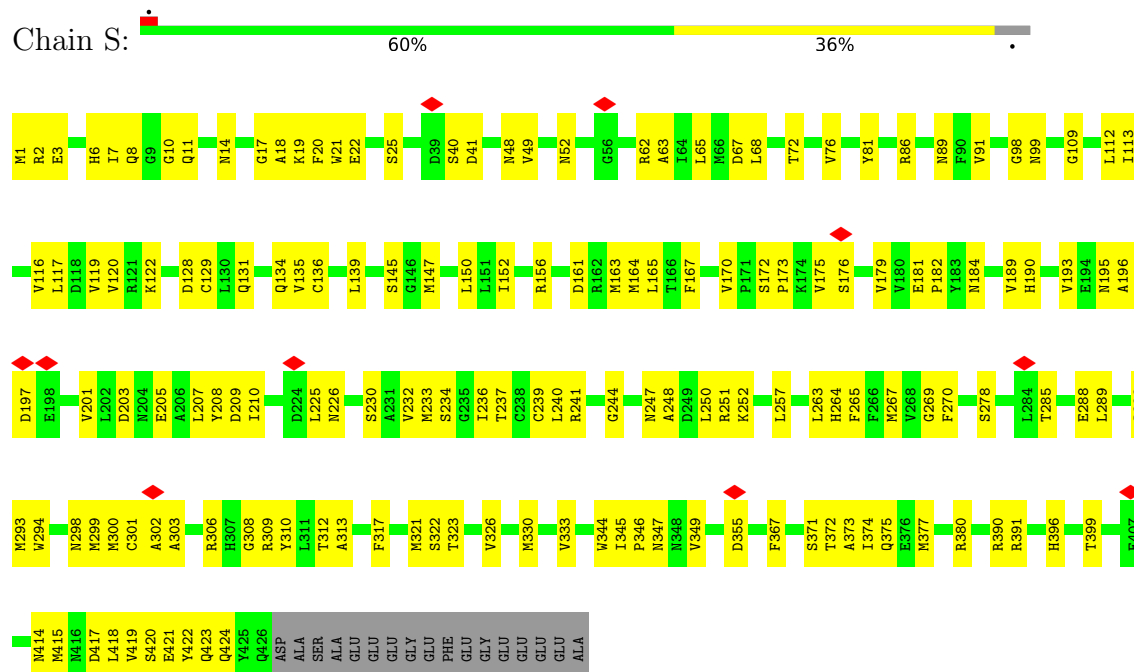
• Molecule 5: Tubulin beta



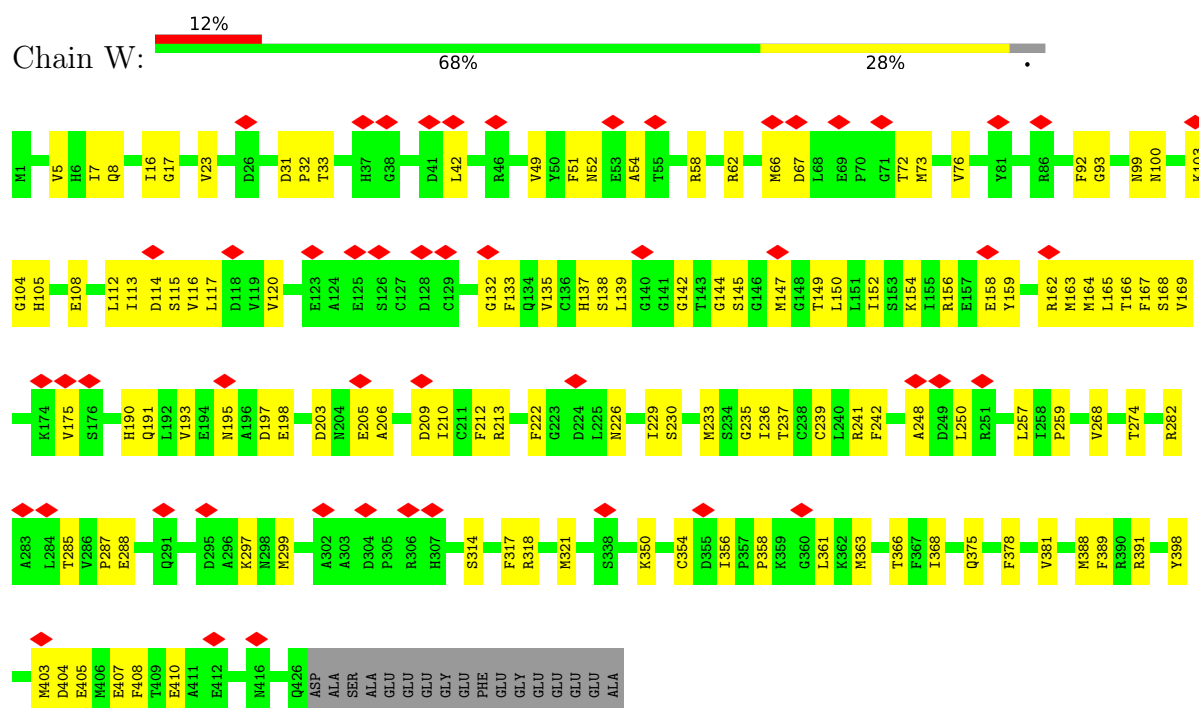
• Molecule 5: Tubulin beta



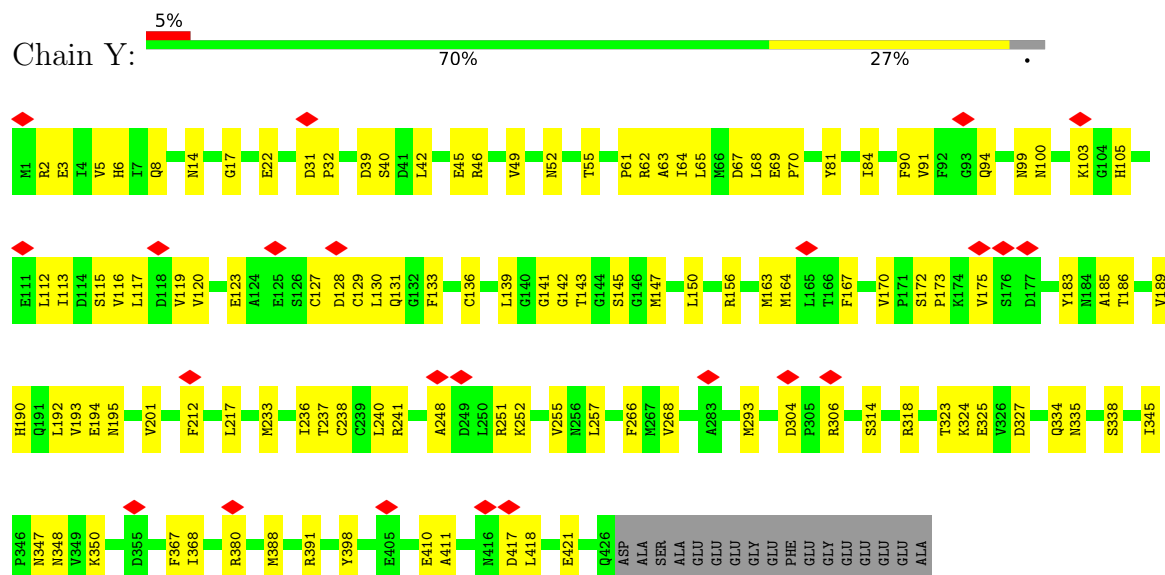
- Molecule 5: Tubulin beta



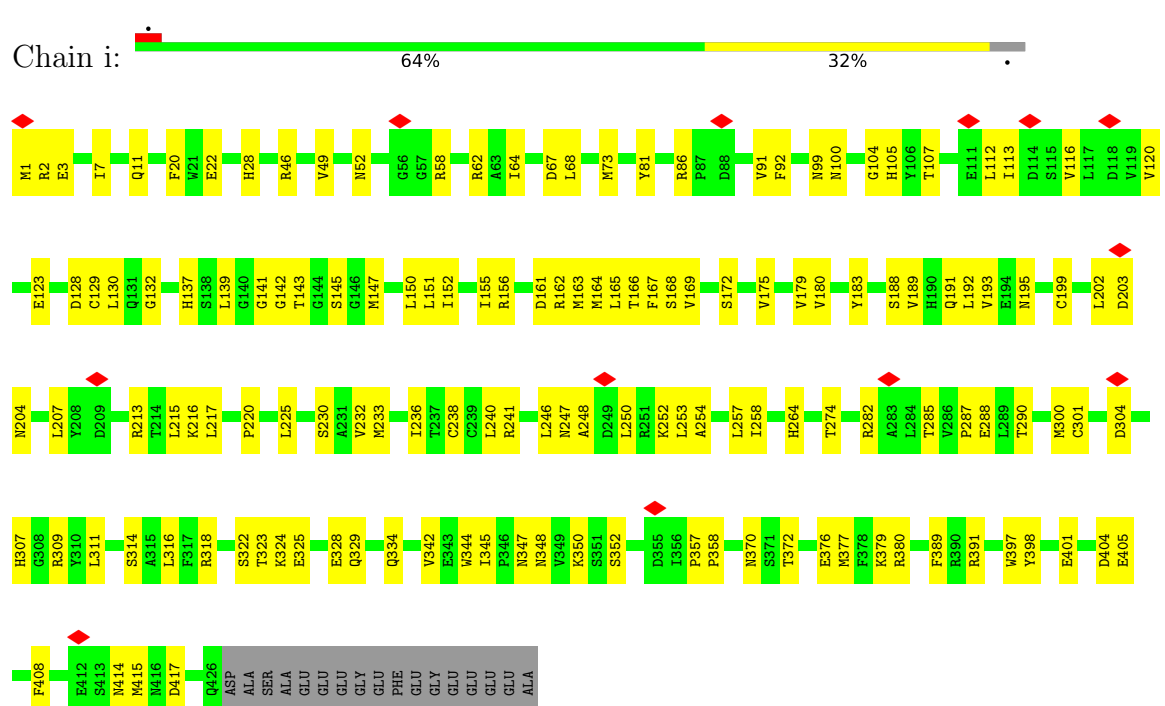
- Molecule 5: Tubulin beta



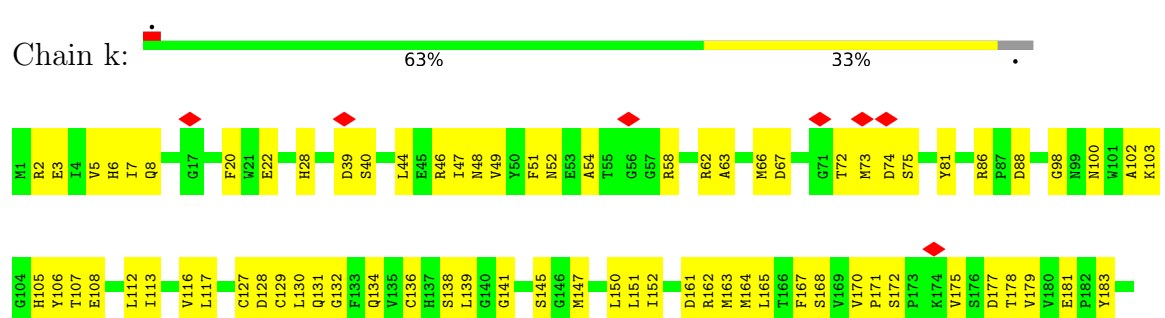
- Molecule 5: Tubulin beta

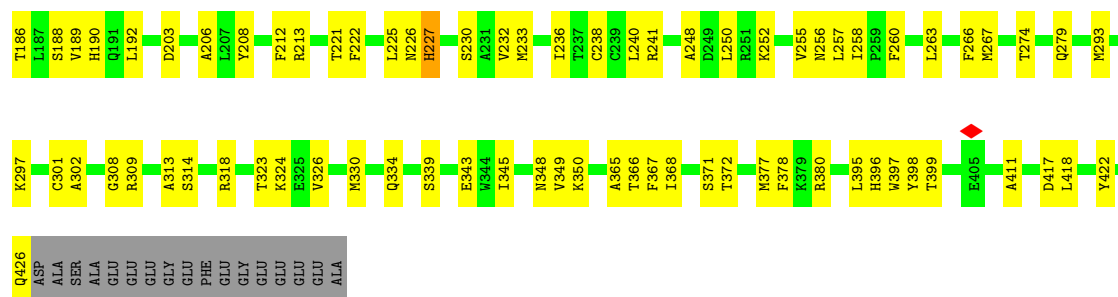


- Molecule 5: Tubulin beta

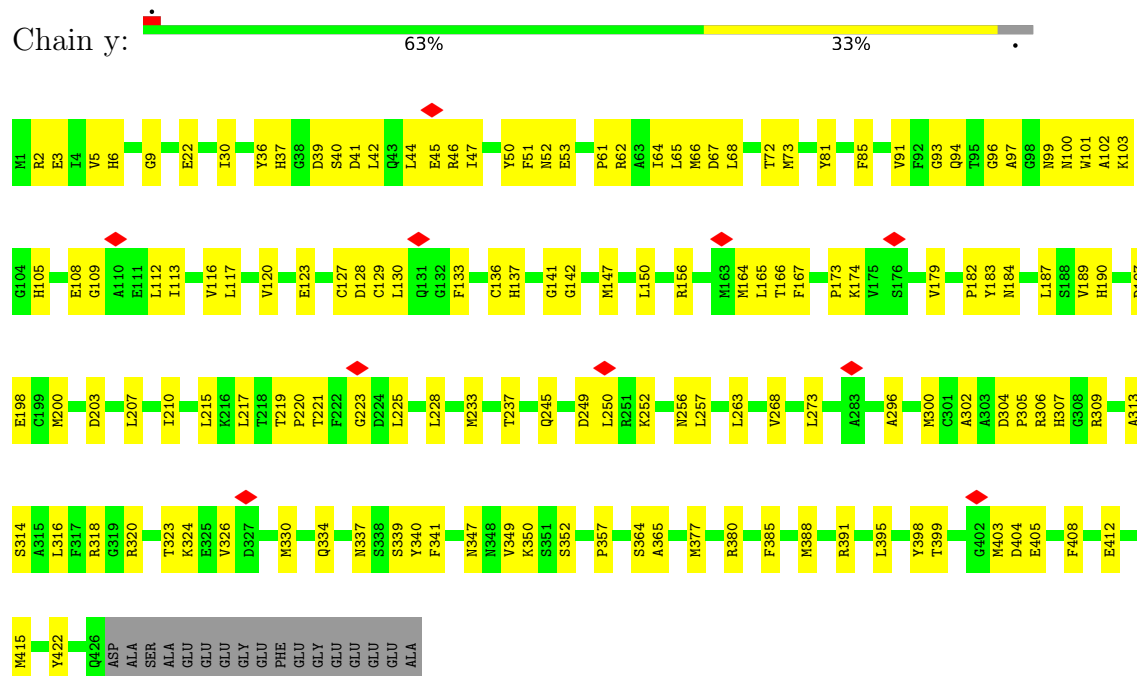


- Molecule 5: Tubulin beta

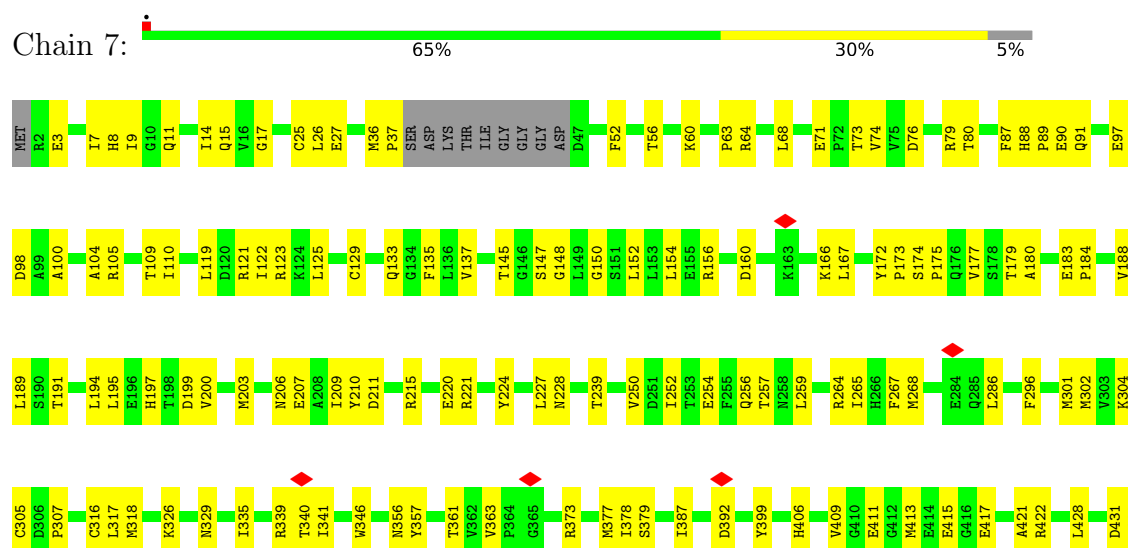


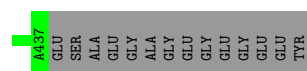


- Molecule 5: Tubulin beta



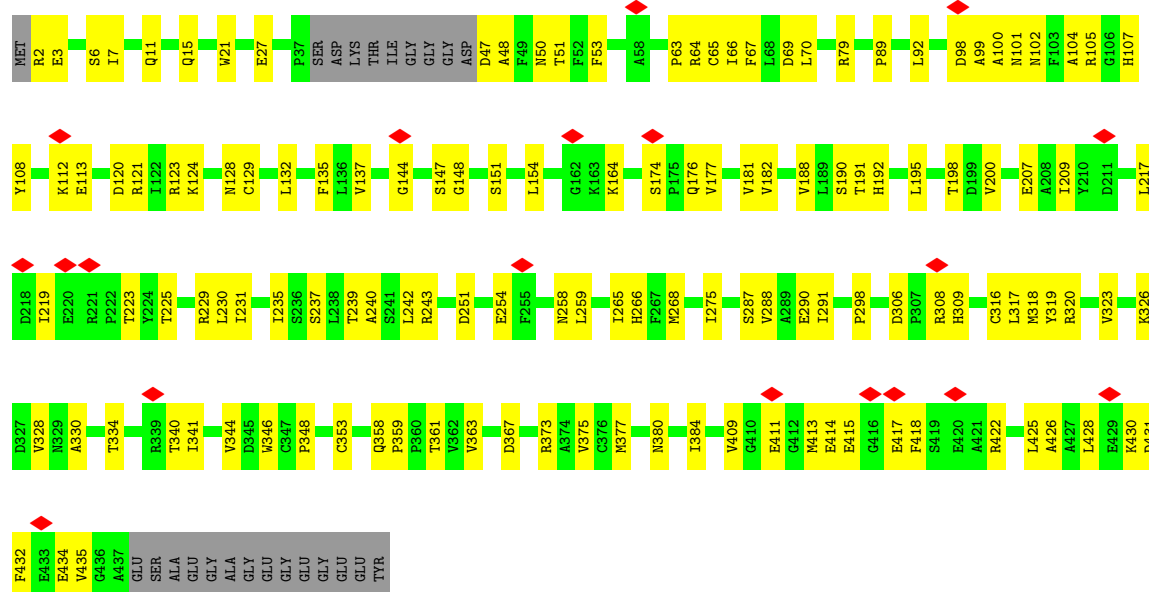
- Molecule 6: Tubulin alpha





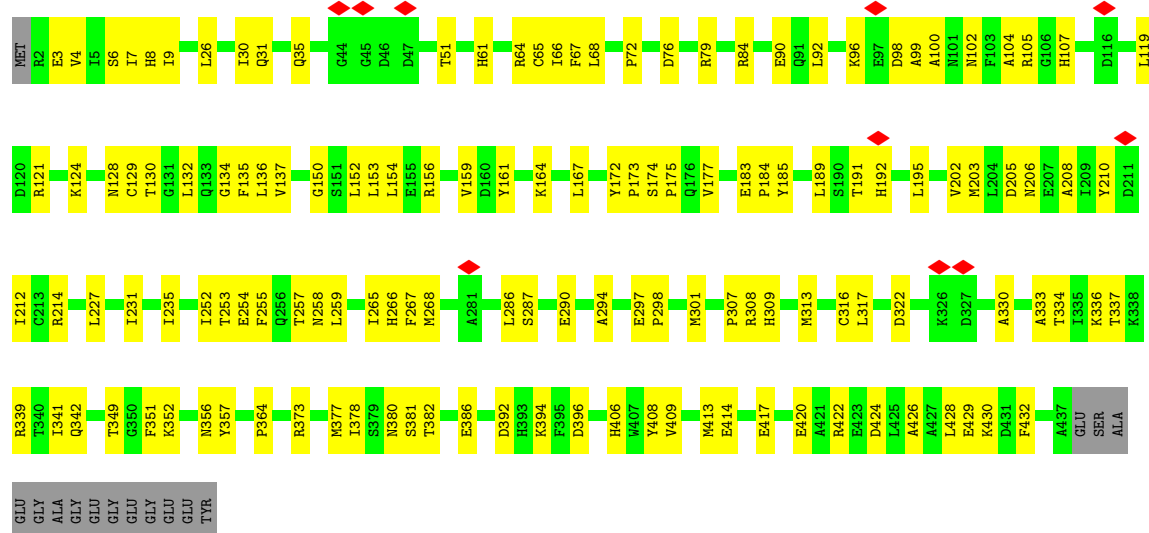
• Molecule 6: Tubulin alpha

Chain 9: 65% 30% 5%



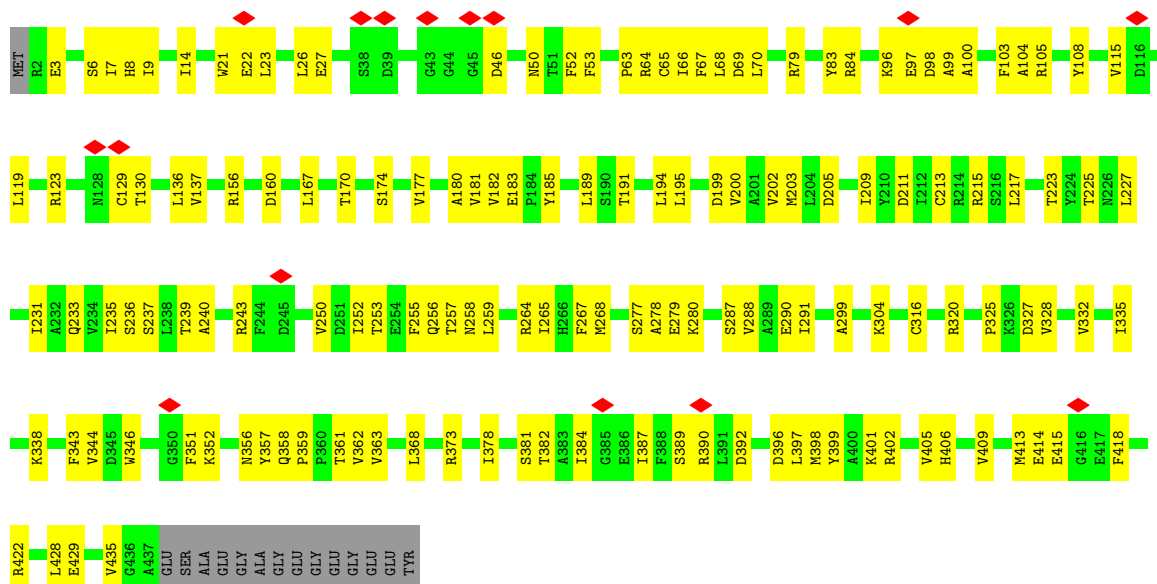
• Molecule 6: Tubulin alpha

Chain D: 66% 30% 4%



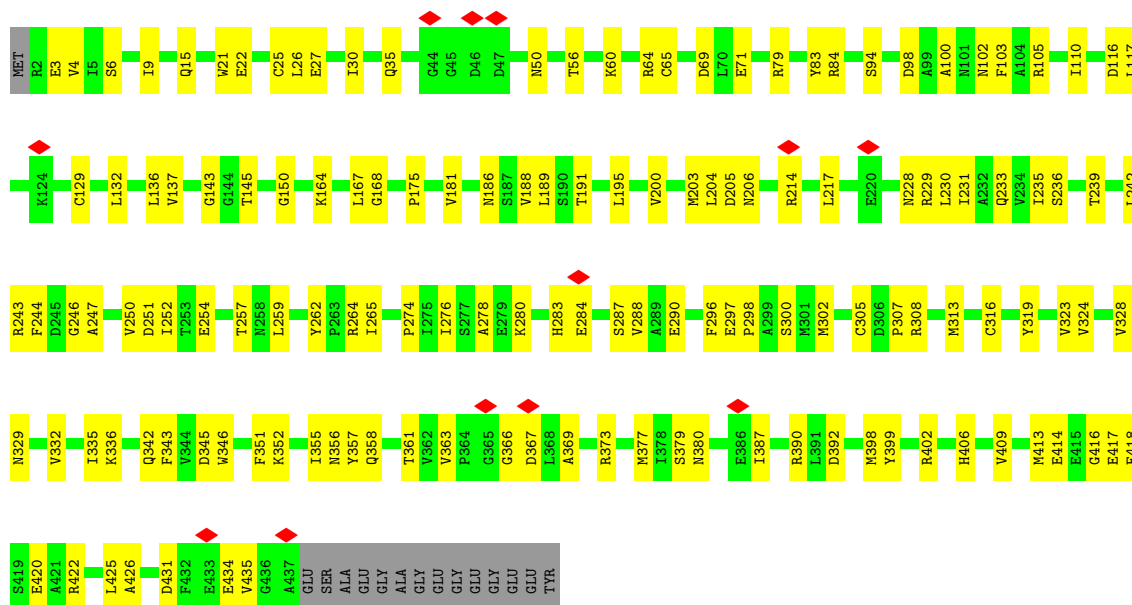
• Molecule 6: Tubulin alpha

Chain H: 64% 33% 3%



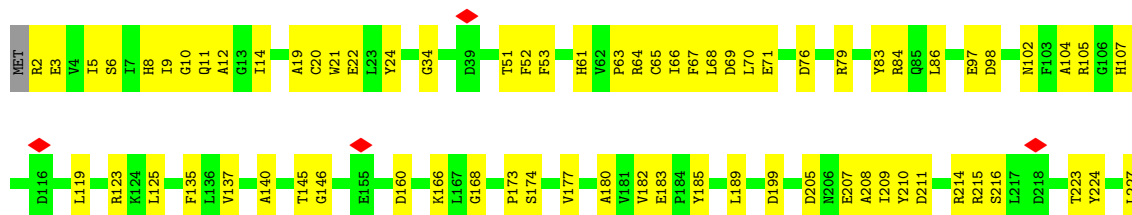
• Molecule 6: Tubulin alpha

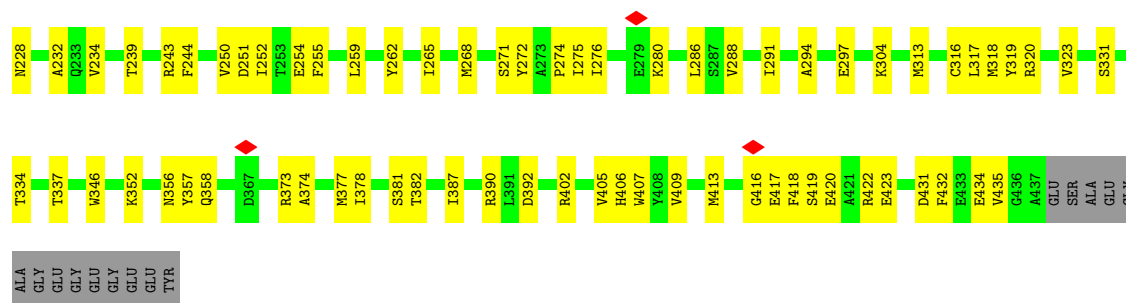
Chain J: 65% 32%



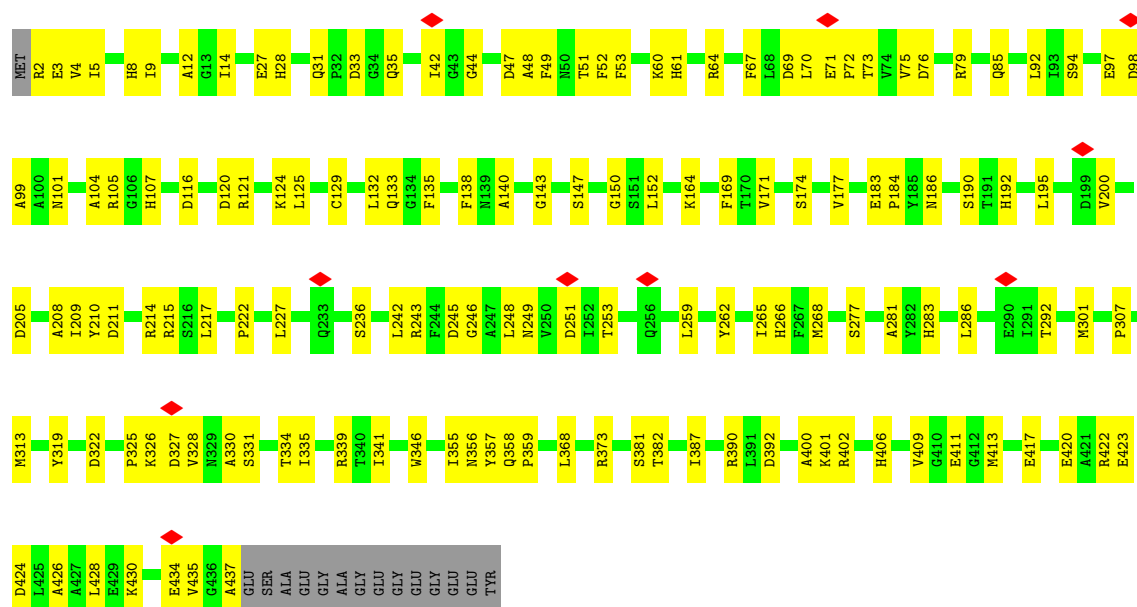
• Molecule 6: Tubulin alpha

Chain L: 66% 31%

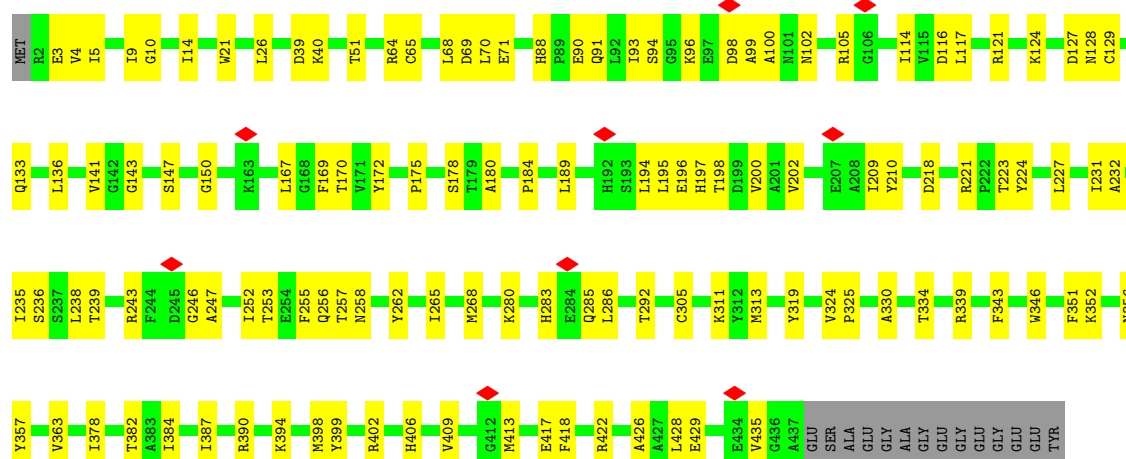




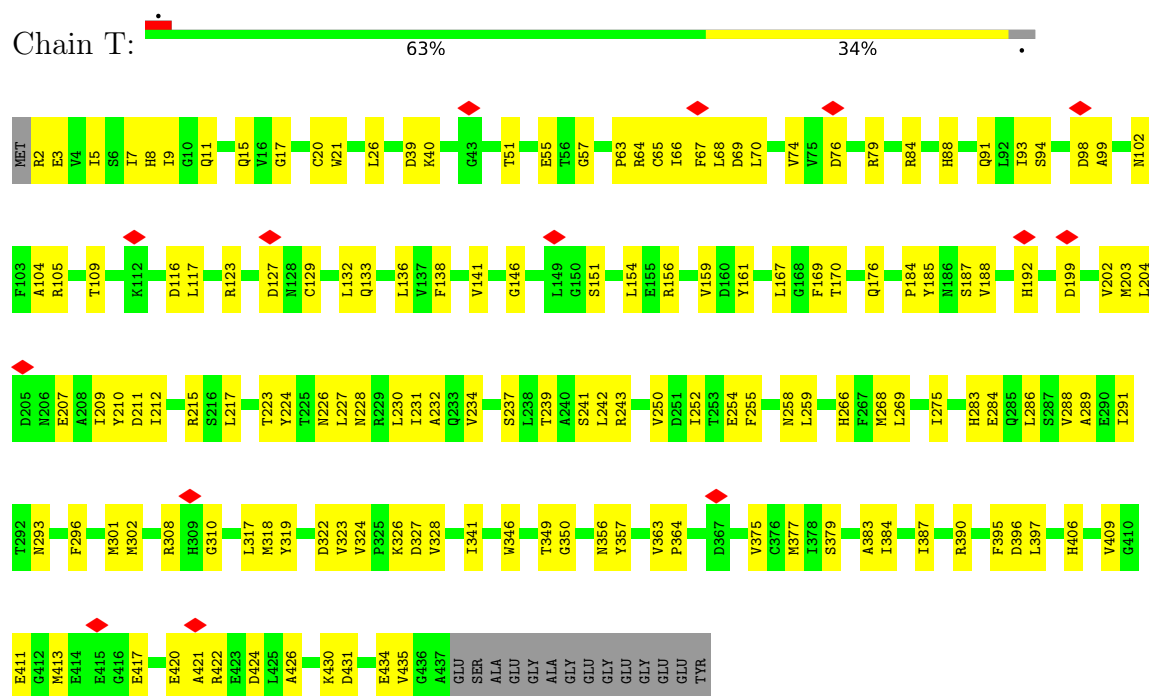
• Molecule 6: Tubulin alpha



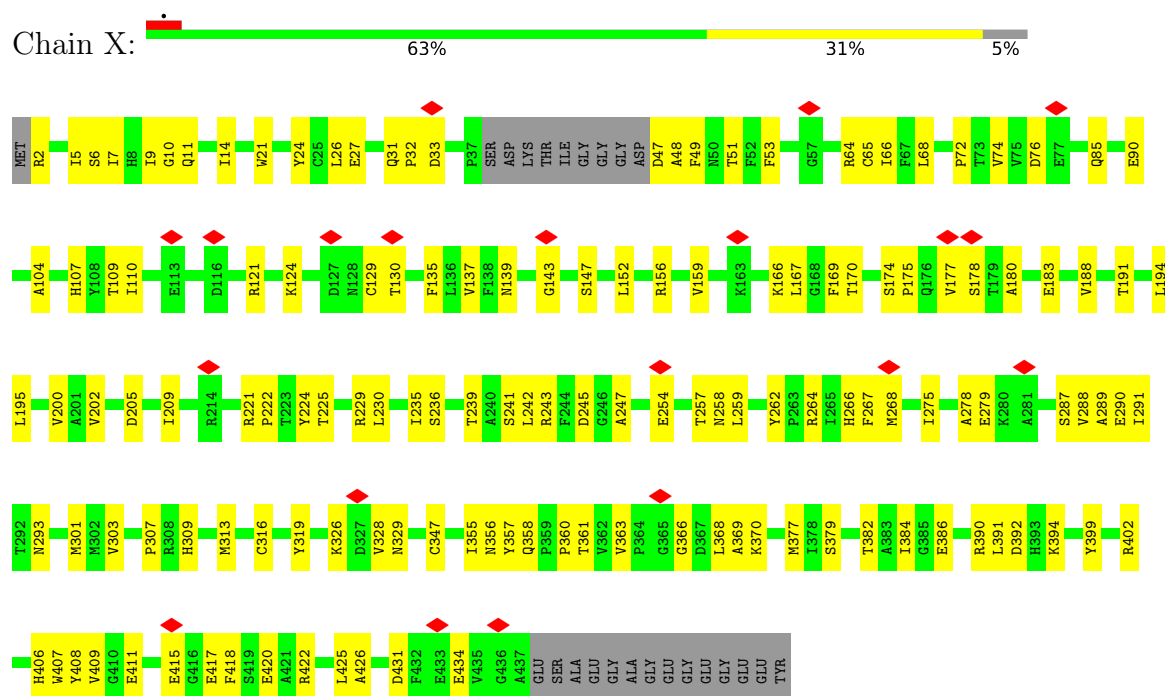
• Molecule 6: Tubulin alpha



- Molecule 6: Tubulin alpha

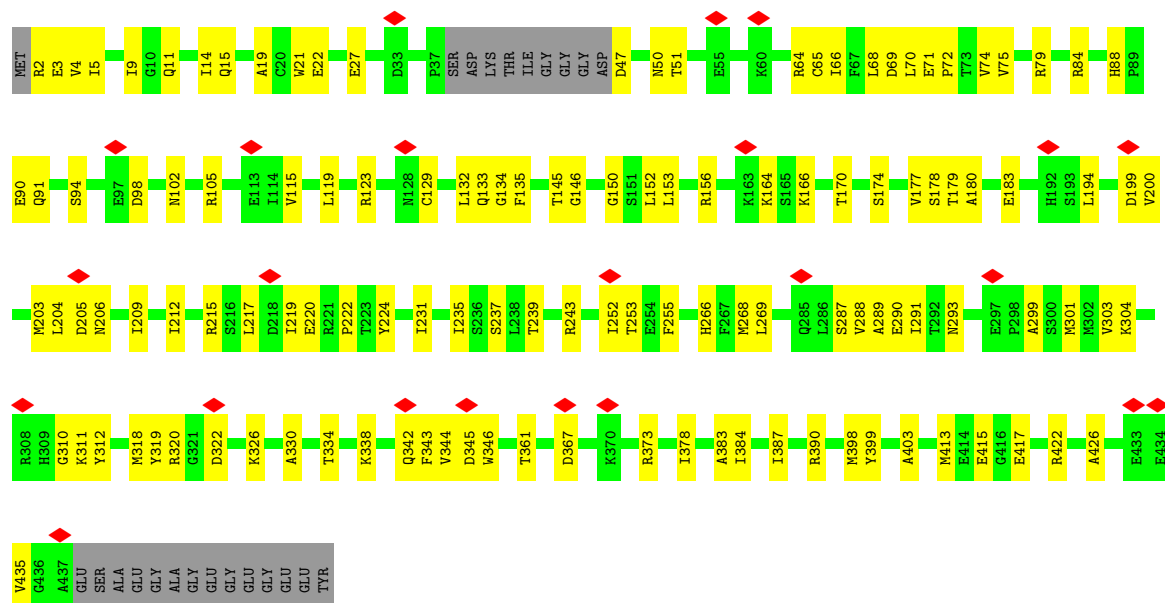


- Molecule 6: Tubulin alpha

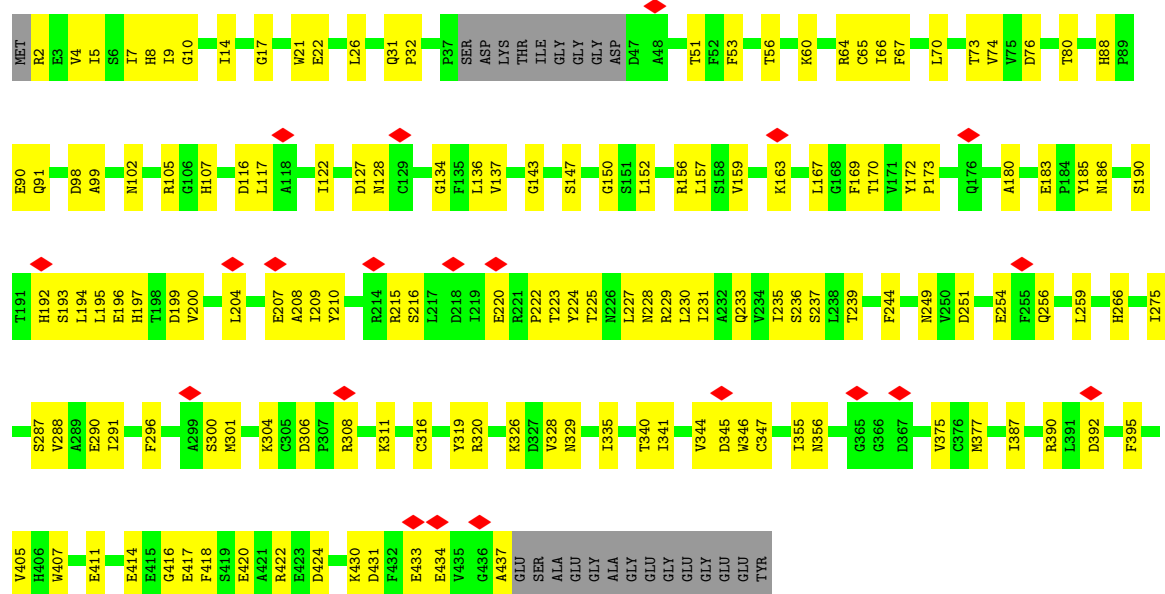


- Molecule 6: Tubulin alpha

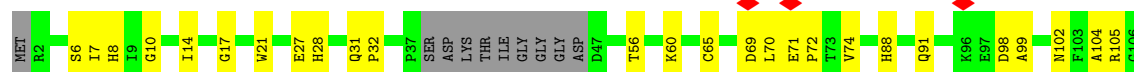


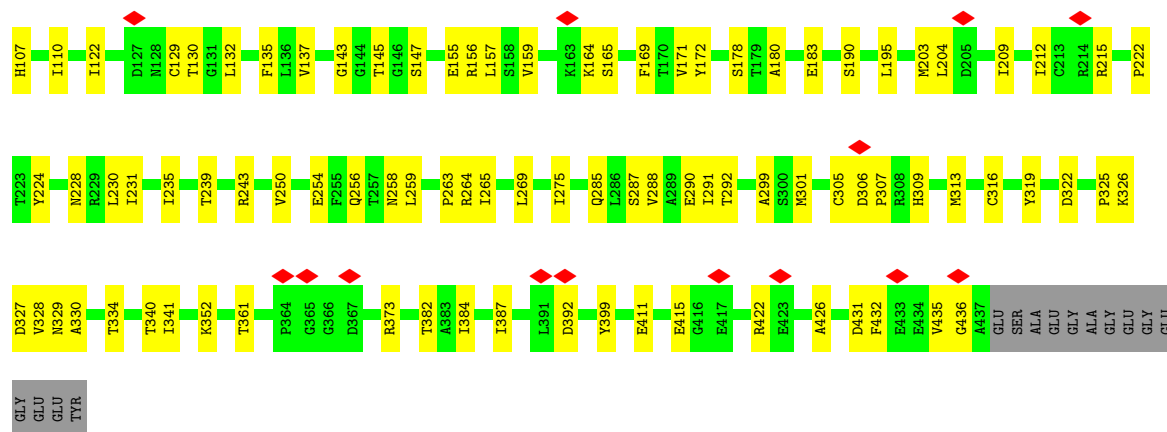


• Molecule 6: Tubulin alpha

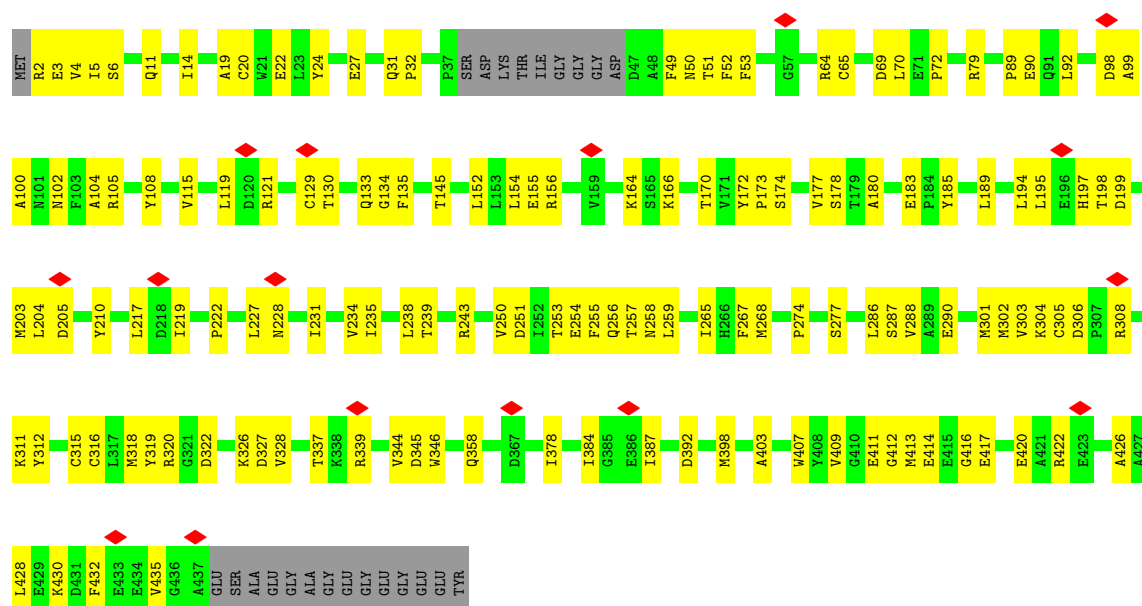


• Molecule 6: Tubulin alpha

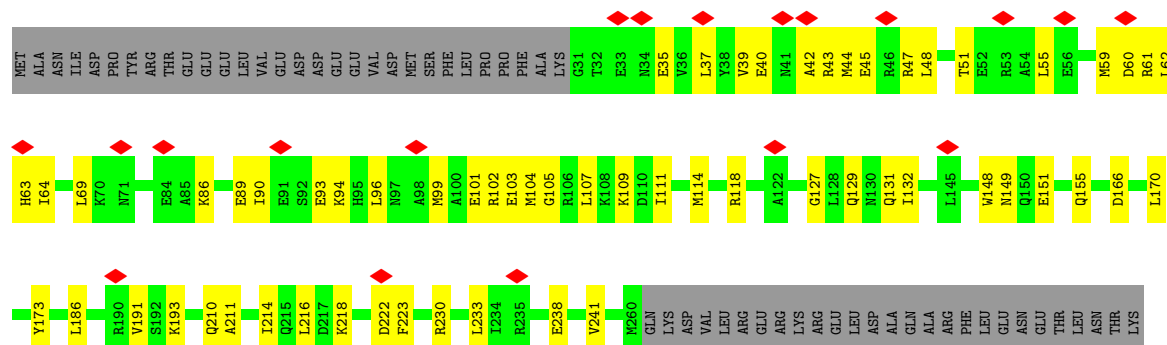
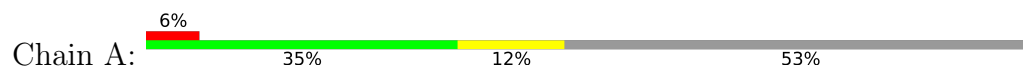


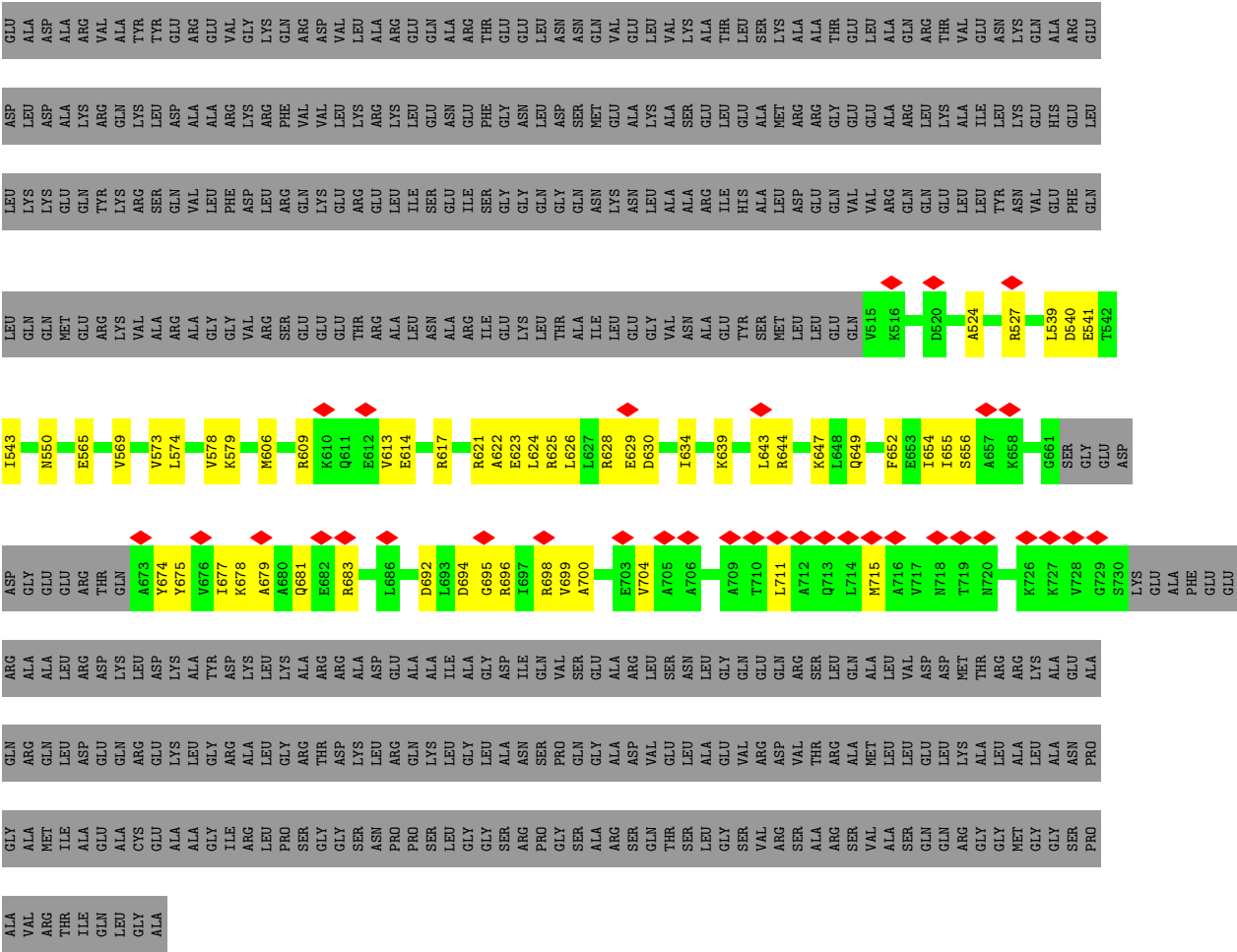


• Molecule 6: Tubulin alpha

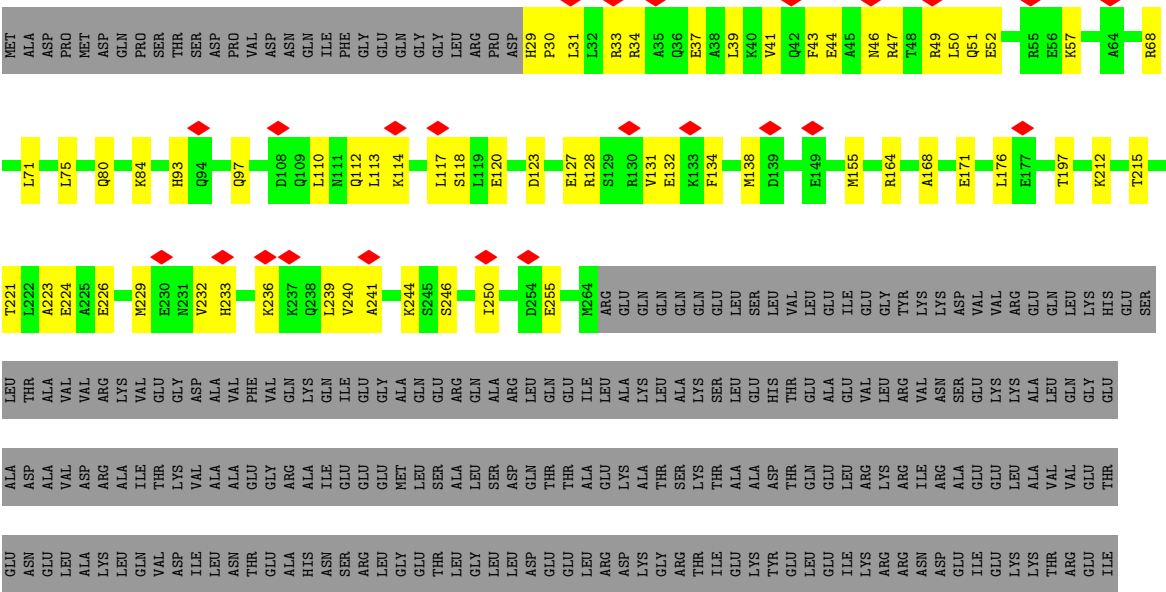
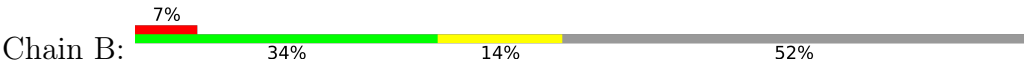


• Molecule 7: Flagellar-associated protein 59

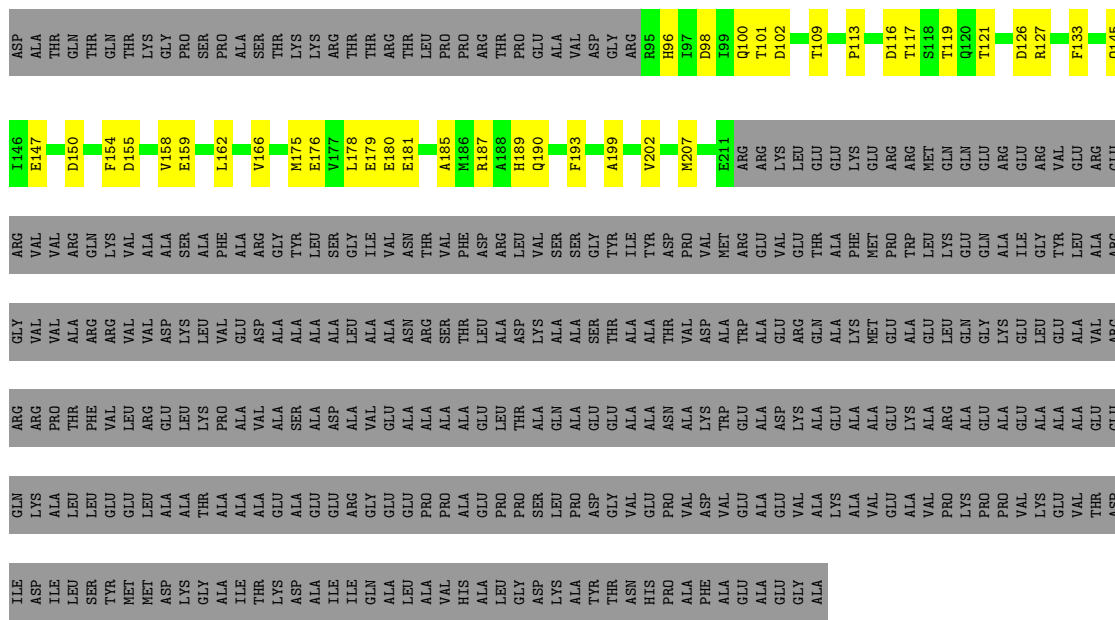




• Molecule 8: Flagellar-associated protein 172





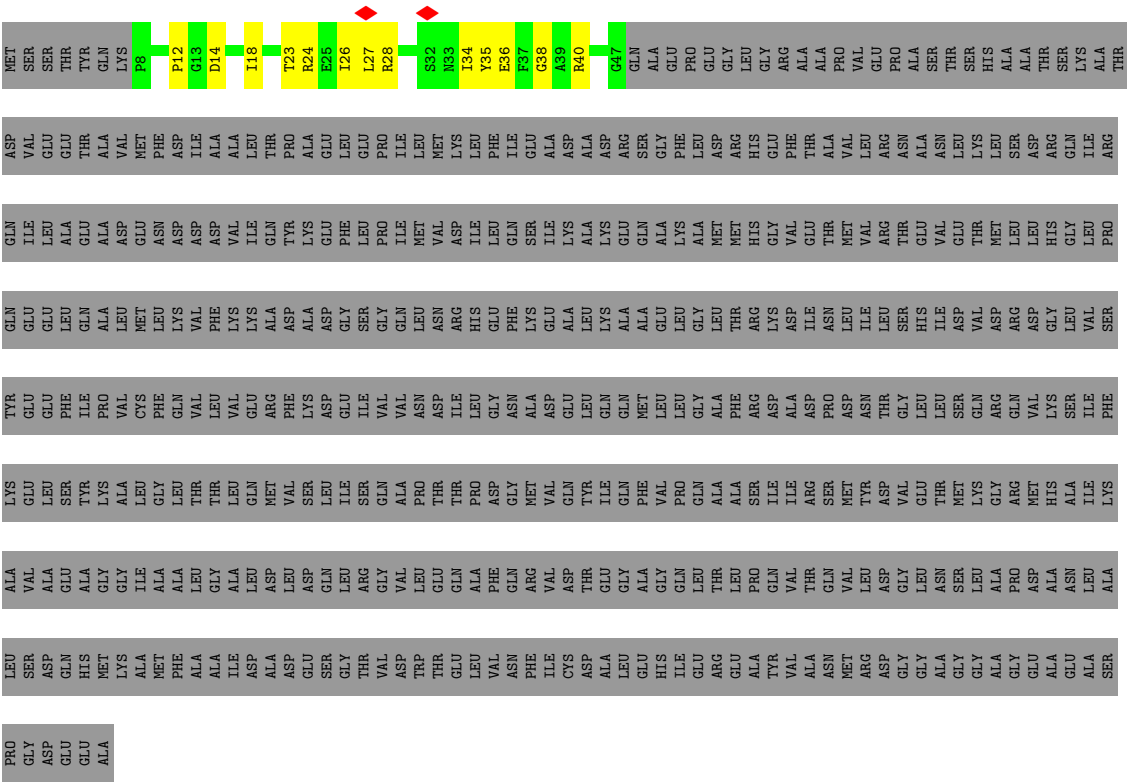


- Molecule 10: Radial spoke protein 7

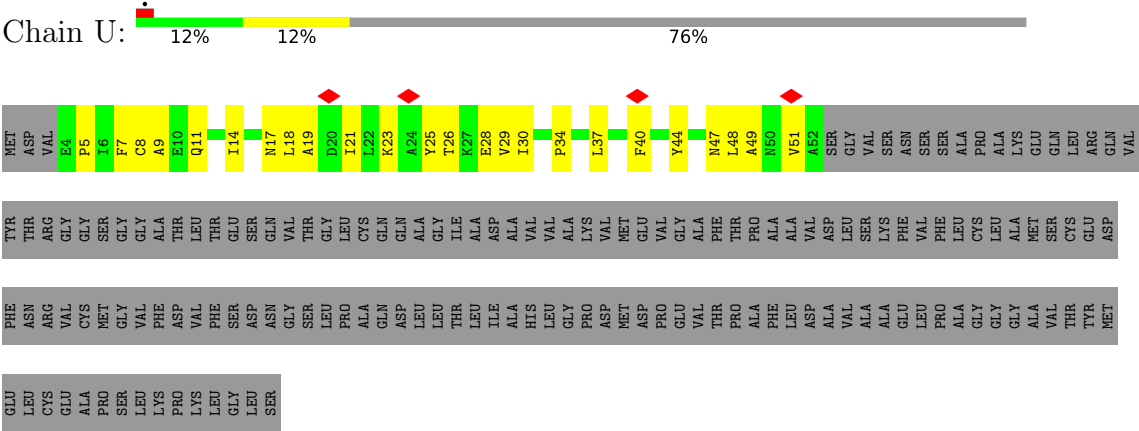


- Molecule 10: Radial spoke protein 7

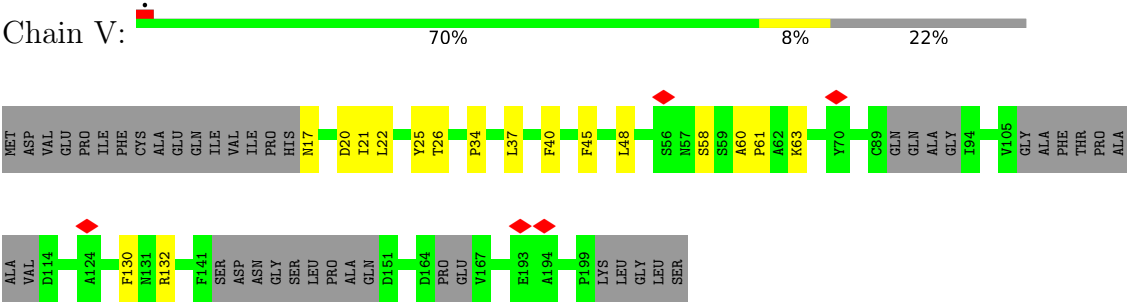




• Molecule 11: Radial spoke protein 11

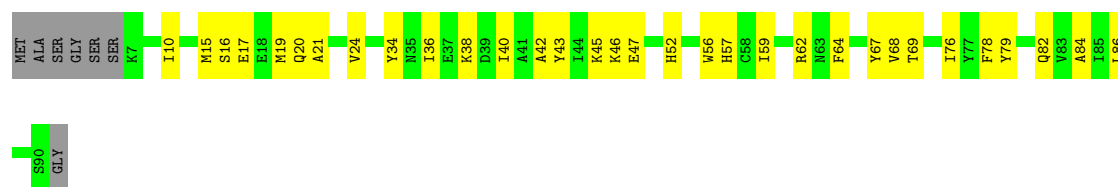


• Molecule 11: Radial spoke protein 11

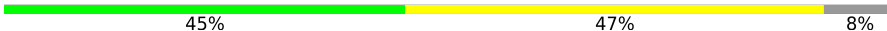


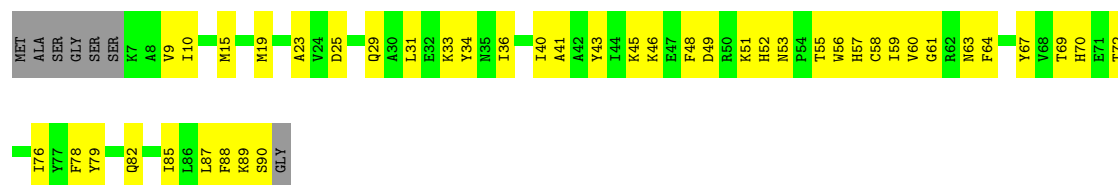
• Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

Chain a: 



- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

Chain b: 



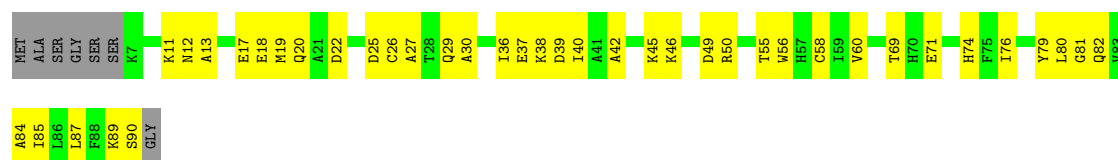
- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

Chain c: 



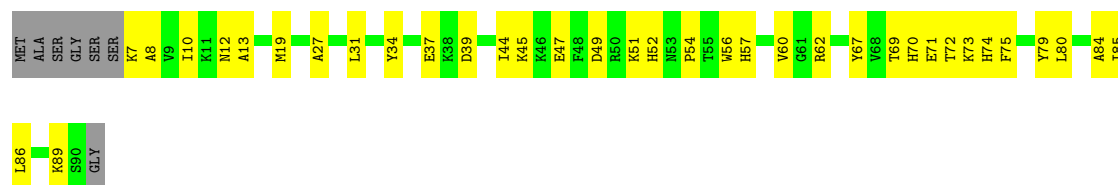
- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

Chain d: 



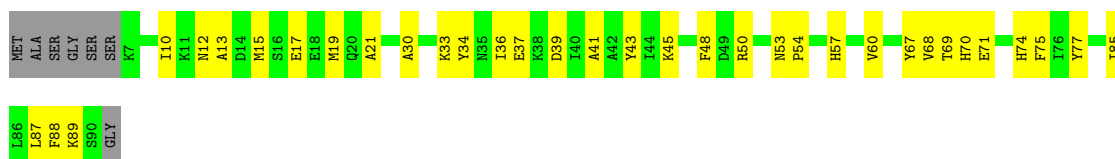
- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

Chain e: 

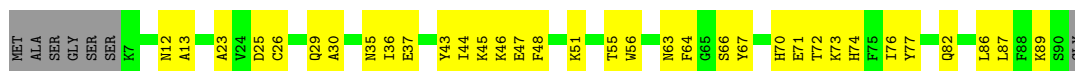


- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

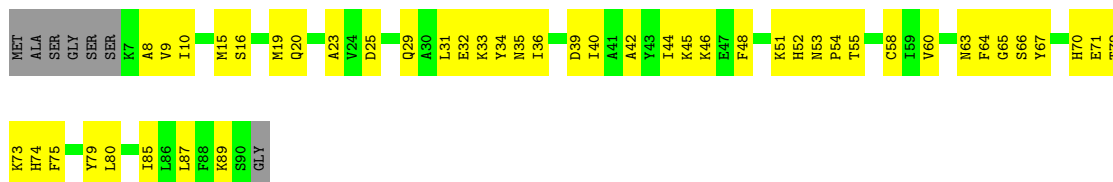
Chain f: 



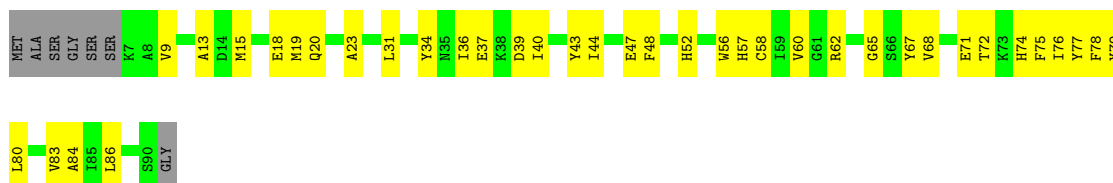
- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm



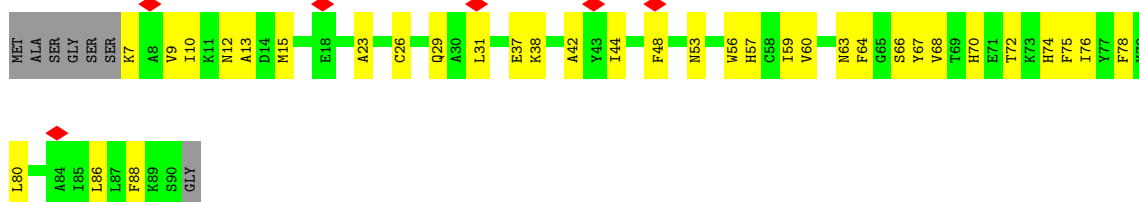
- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm



- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

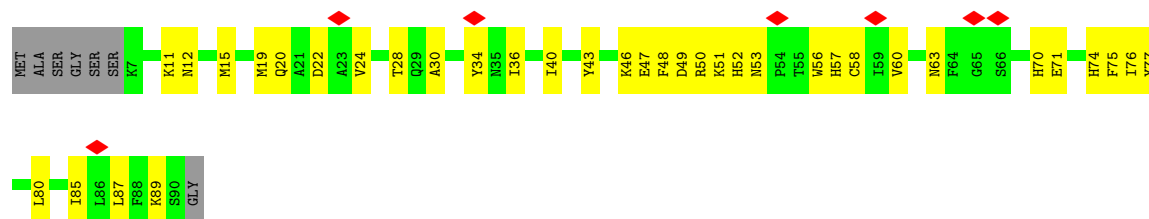


- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

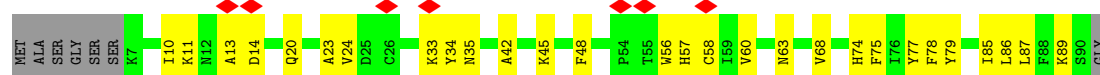


- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm

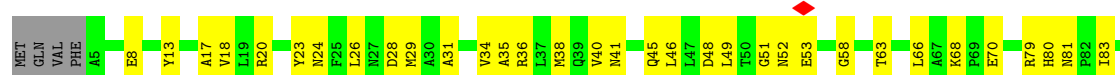




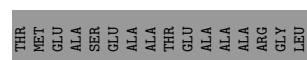
- Molecule 12: Dynein 8 kDa light chain, flagellar outer arm



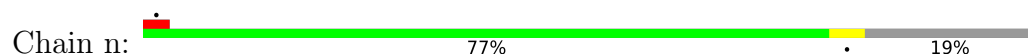
- Molecule 13: Radial spoke protein 15

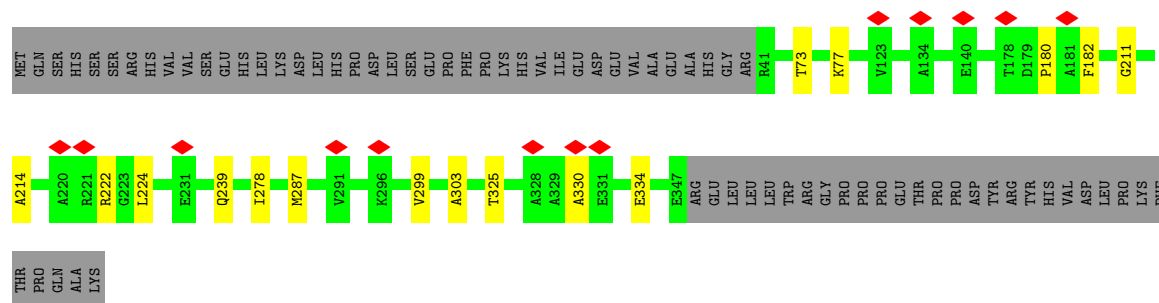


- Molecule 14: FAP207

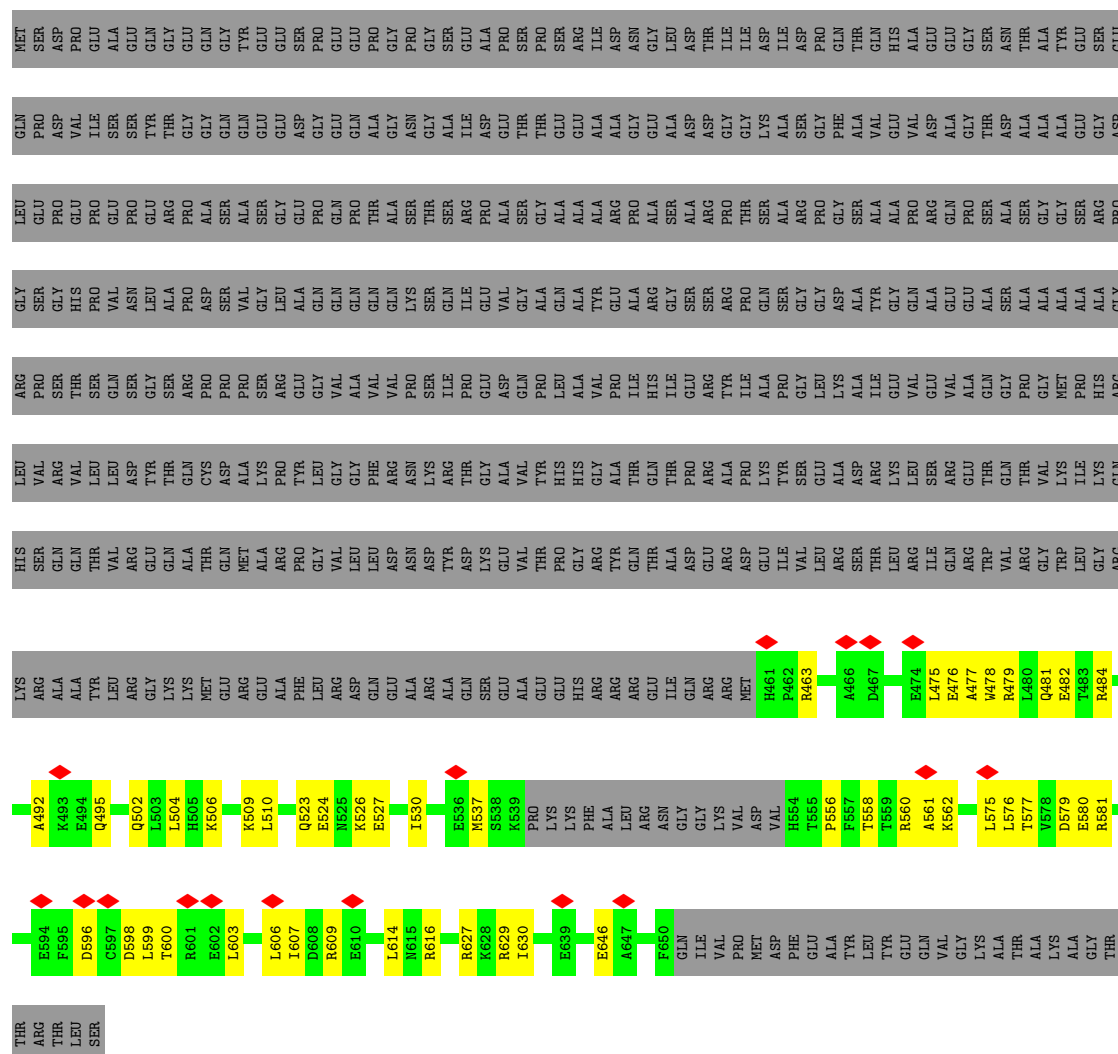


- Molecule 15: Radial spike protein 8



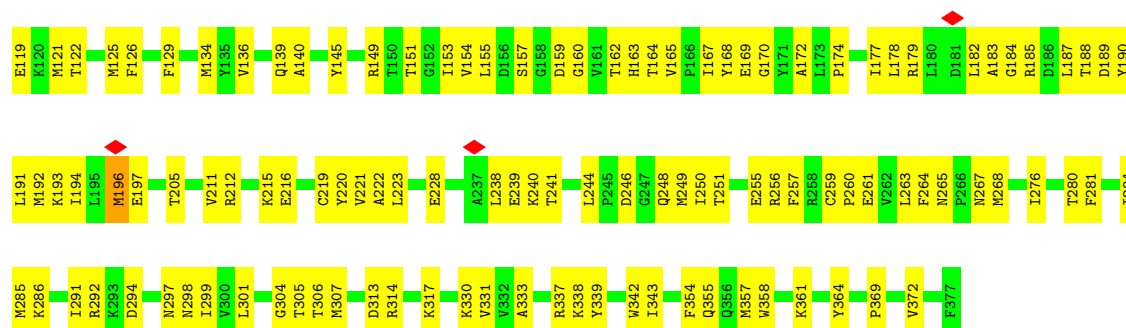


- Molecule 16: FAP253

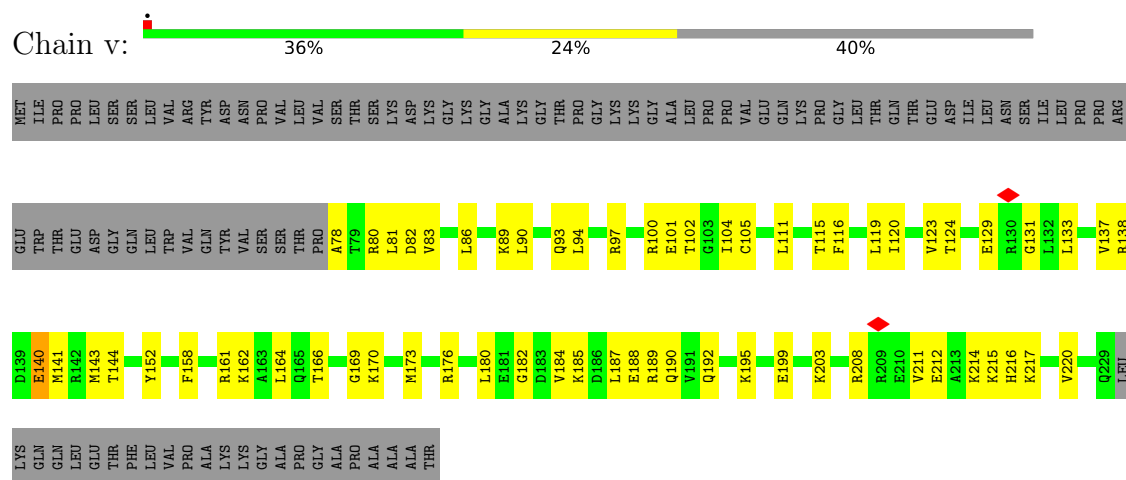


- Molecule 17: Actin

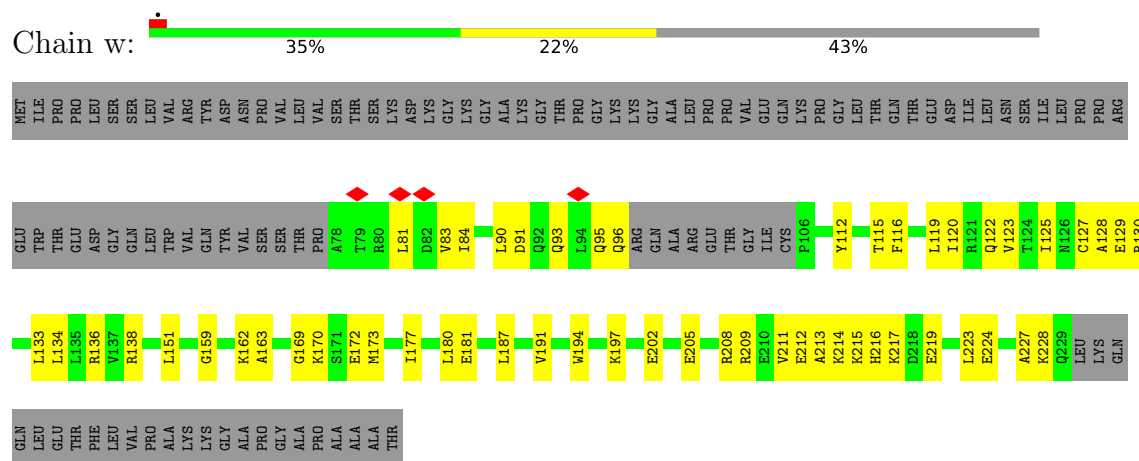




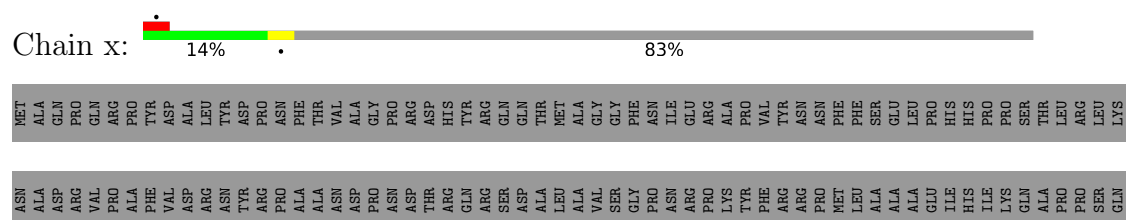
- Molecule 18: 28 kDa inner dynein arm light chain, axonemal



- Molecule 18: 28 kDa inner dynein arm light chain, axonemal



- Molecule 19: CFAP91 domain-containing protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	202168	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38.9	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	1167.296, 1167.296, 1167.296	wwPDB
Map dimensions	832, 832, 832	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.403, 1.403, 1.403	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: GDP, MG, GTP, ATP

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	0	0.17	0/1379	0.49	0/1860
1	4	0.19	0/1258	0.45	0/1690
2	1	0.18	0/1458	0.42	0/1962
3	2	0.33	0/1517	0.59	0/2038
5	6	0.17	0/3420	0.39	0/4628
5	8	0.18	0/3420	0.38	0/4628
5	C	0.16	0/3420	0.37	0/4628
5	G	0.17	0/3420	0.37	0/4628
5	I	0.18	0/3420	0.40	2/4628 (0.0%)
5	K	0.20	0/3420	0.41	0/4628
5	O	0.20	0/3420	0.40	0/4628
5	Q	0.18	0/3420	0.39	0/4628
5	S	0.18	0/3420	0.38	0/4628
5	W	0.16	0/3420	0.39	0/4628
5	Y	0.17	0/3420	0.38	0/4628
5	i	0.17	0/3420	0.37	0/4628
5	k	0.19	0/3420	0.39	0/4628
5	y	0.19	0/3420	0.39	0/4628
6	7	0.18	0/3389	0.39	0/4595
6	9	0.17	0/3389	0.38	0/4595
6	D	0.18	0/3448	0.39	0/4675
6	H	0.19	0/3448	0.41	0/4675
6	J	0.18	0/3448	0.39	0/4675
6	L	0.19	0/3448	0.41	0/4675
6	P	0.18	0/3448	0.38	0/4675
6	R	0.18	0/3448	0.38	0/4675
6	T	0.17	0/3448	0.38	0/4675
6	X	0.17	0/3389	0.37	0/4595
6	Z	0.16	0/3389	0.37	0/4595
6	j	0.17	0/3389	0.40	0/4595
6	t	0.17	0/3389	0.41	0/4595
6	z	0.22	0/3389	0.43	0/4595

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	A	0.18	0/3562	0.38	0/4763
8	B	0.21	0/3499	0.42	0/4674
9	E	0.22	0/698	0.47	0/948
9	F	0.21	0/946	0.52	0/1287
10	M	0.20	0/363	0.41	0/491
10	N	0.20	0/325	0.50	0/439
11	U	0.22	0/399	0.49	0/543
11	V	0.17	0/891	0.39	0/1221
12	a	0.26	0/702	0.49	0/945
12	b	0.25	0/702	0.49	0/945
12	c	0.27	0/702	0.49	0/945
12	d	0.26	0/702	0.48	0/945
12	e	0.23	0/702	0.43	0/945
12	f	0.26	0/702	0.50	0/945
12	g	0.21	0/702	0.48	0/945
12	h	0.22	0/702	0.42	0/945
12	o	0.15	0/702	0.41	0/945
12	p	0.17	0/702	0.45	0/945
12	q	0.12	0/702	0.38	0/945
12	r	0.15	0/702	0.40	0/945
13	l	0.23	0/2469	0.48	0/3363
14	m	0.19	0/1688	0.51	0/2273
15	n	0.14	0/1515	0.34	0/2108
16	s	0.14	0/1487	0.34	0/2004
17	u	0.15	0/2942	0.39	2/3985 (0.1%)
18	v	0.17	0/1267	0.48	2/1696 (0.1%)
18	w	0.17	0/1196	0.40	0/1599
19	x	0.23	0/1847	0.41	0/2473
All	All	0.19	0/134869	0.40	6/182439 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	v	140	GLU	CA-C-N	-5.44	111.62	121.14
18	v	140	GLU	C-N-CA	-5.44	111.62	121.14
17	u	196	MET	CA-C-N	-5.22	112.01	120.72
17	u	196	MET	C-N-CA	-5.22	112.01	120.72
5	I	285	THR	CA-C-N	5.20	123.52	120.24

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	0	1364	0	1390	60	0
1	4	1246	0	1277	54	0
2	1	1431	0	1408	56	0
3	2	1497	0	1515	51	0
4	3	360	0	87	8	0
5	6	3346	0	3240	107	0
5	8	3346	0	3240	111	0
5	C	3346	0	3239	109	0
5	G	3346	0	3240	96	0
5	I	3346	0	3240	107	0
5	K	3346	0	3238	114	0
5	O	3346	0	3240	97	0
5	Q	3346	0	3240	114	0
5	S	3346	0	3240	130	0
5	W	3346	0	3237	80	0
5	Y	3346	0	3240	83	0
5	i	3346	0	3240	104	0
5	k	3346	0	3240	122	0
5	y	3346	0	3239	111	0
6	7	3318	0	3259	96	0
6	9	3318	0	3259	99	0
6	D	3376	0	3313	97	0
6	H	3376	0	3313	111	0
6	J	3376	0	3313	108	0
6	L	3376	0	3309	104	0
6	P	3376	0	3312	106	0
6	R	3376	0	3313	93	0
6	T	3376	0	3313	115	0
6	X	3318	0	3259	99	0
6	Z	3318	0	3259	90	0
6	j	3318	0	3259	110	0
6	t	3318	0	3257	88	0
6	z	3318	0	3259	107	0
7	A	3535	0	3570	115	0
8	B	3479	0	3554	119	0
9	E	685	0	652	30	0
9	F	931	0	885	41	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	M	353	0	352	14	0
10	N	316	0	316	18	0
11	U	391	0	400	21	0
11	V	891	0	581	14	0
12	a	686	0	672	34	0
12	b	686	0	672	41	0
12	c	686	0	672	25	0
12	d	686	0	672	35	0
12	e	686	0	672	29	0
12	f	686	0	672	27	0
12	g	686	0	672	33	0
12	h	686	0	672	37	0
12	o	686	0	672	35	0
12	p	686	0	672	30	0
12	q	686	0	672	30	0
12	r	686	0	672	24	0
13	l	2438	0	2518	82	0
14	m	1639	0	1507	81	0
15	n	1516	0	795	8	0
16	s	1465	0	1489	31	0
17	u	2880	0	2867	111	0
18	v	1256	0	1265	62	0
18	w	1186	0	1194	48	0
19	x	1826	0	1863	45	0
20	6	28	0	12	2	0
20	8	28	0	12	3	0
20	C	28	0	12	1	0
20	G	28	0	12	0	0
20	I	28	0	12	2	0
20	K	28	0	12	4	0
20	O	28	0	12	4	0
20	Q	28	0	12	1	0
20	S	28	0	12	2	0
20	W	28	0	12	1	0
20	Y	28	0	12	1	0
20	i	28	0	12	1	0
20	k	28	0	11	1	0
20	y	28	0	12	0	0
21	7	32	0	12	3	0
21	9	32	0	12	1	0
21	D	32	0	12	0	0
21	H	32	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	J	32	0	12	1	0
21	L	32	0	11	3	0
21	P	32	0	12	1	0
21	R	32	0	11	0	0
21	T	32	0	12	1	0
21	X	32	0	12	0	0
21	Z	32	0	12	1	0
21	j	32	0	12	2	0
21	y	32	0	11	2	0
21	z	32	0	12	2	0
22	7	1	0	0	0	0
22	9	1	0	0	0	0
22	D	1	0	0	0	0
22	H	1	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
22	P	1	0	0	0	0
22	R	1	0	0	0	0
22	T	1	0	0	0	0
22	X	1	0	0	0	0
22	Z	1	0	0	0	0
22	j	1	0	0	0	0
22	t	1	0	0	0	0
22	z	1	0	0	0	0
23	u	31	0	12	2	0
All	All	133504	0	129242	3938	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 15.

The worst 5 of 3938 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)
5:y:113:ILE:HD13	5:y:150:LEU:HD22	1.40	1.03
7:A:606:MET:HG3	8:B:613:ILE:HD12	1.45	0.98
10:N:14:ASP:HB2	11:V:37:LEU:HD12	1.52	0.92
5:k:113:ILE:HA	5:k:116:VAL:HG12	1.55	0.89
5:i:113:ILE:HD13	5:i:150:LEU:HD22	1.53	0.88

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	0	171/471 (36%)	166 (97%)	5 (3%)	0	100	100
1	4	150/471 (32%)	148 (99%)	2 (1%)	0	100	100
2	1	164/698 (24%)	157 (96%)	7 (4%)	0	100	100
3	2	179/573 (31%)	176 (98%)	3 (2%)	0	100	100
5	6	424/443 (96%)	398 (94%)	26 (6%)	0	100	100
5	8	424/443 (96%)	399 (94%)	25 (6%)	0	100	100
5	C	424/443 (96%)	410 (97%)	14 (3%)	0	100	100
5	G	424/443 (96%)	393 (93%)	31 (7%)	0	100	100
5	I	424/443 (96%)	398 (94%)	26 (6%)	0	100	100
5	K	424/443 (96%)	396 (93%)	28 (7%)	0	100	100
5	O	424/443 (96%)	401 (95%)	23 (5%)	0	100	100
5	Q	424/443 (96%)	396 (93%)	28 (7%)	0	100	100
5	S	424/443 (96%)	398 (94%)	26 (6%)	0	100	100
5	W	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
5	Y	424/443 (96%)	405 (96%)	19 (4%)	0	100	100
5	i	424/443 (96%)	404 (95%)	20 (5%)	0	100	100
5	k	424/443 (96%)	398 (94%)	26 (6%)	0	100	100
5	y	424/443 (96%)	400 (94%)	24 (6%)	0	100	100
6	7	423/451 (94%)	396 (94%)	27 (6%)	0	100	100
6	9	423/451 (94%)	393 (93%)	30 (7%)	0	100	100
6	D	434/451 (96%)	413 (95%)	21 (5%)	0	100	100
6	H	434/451 (96%)	410 (94%)	24 (6%)	0	100	100
6	J	434/451 (96%)	402 (93%)	32 (7%)	0	100	100
6	L	434/451 (96%)	404 (93%)	30 (7%)	0	100	100
6	P	434/451 (96%)	405 (93%)	29 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	R	434/451 (96%)	410 (94%)	24 (6%)	0	100	100
6	T	434/451 (96%)	410 (94%)	24 (6%)	0	100	100
6	X	423/451 (94%)	407 (96%)	16 (4%)	0	100	100
6	Z	423/451 (94%)	401 (95%)	22 (5%)	0	100	100
6	j	423/451 (94%)	402 (95%)	21 (5%)	0	100	100
6	t	423/451 (94%)	399 (94%)	24 (6%)	0	100	100
6	z	423/451 (94%)	398 (94%)	25 (6%)	0	100	100
7	A	429/925 (46%)	428 (100%)	1 (0%)	0	100	100
8	B	429/904 (48%)	428 (100%)	1 (0%)	0	100	100
9	E	84/516 (16%)	81 (96%)	3 (4%)	0	100	100
9	F	115/516 (22%)	105 (91%)	10 (9%)	0	100	100
10	M	42/500 (8%)	38 (90%)	4 (10%)	0	100	100
10	N	38/500 (8%)	33 (87%)	5 (13%)	0	100	100
11	U	47/204 (23%)	42 (89%)	5 (11%)	0	100	100
11	V	150/204 (74%)	133 (89%)	17 (11%)	0	100	100
12	a	82/91 (90%)	72 (88%)	10 (12%)	0	100	100
12	b	82/91 (90%)	76 (93%)	6 (7%)	0	100	100
12	c	82/91 (90%)	79 (96%)	3 (4%)	0	100	100
12	d	82/91 (90%)	76 (93%)	6 (7%)	0	100	100
12	e	82/91 (90%)	76 (93%)	6 (7%)	0	100	100
12	f	82/91 (90%)	75 (92%)	7 (8%)	0	100	100
12	g	82/91 (90%)	77 (94%)	5 (6%)	0	100	100
12	h	82/91 (90%)	79 (96%)	3 (4%)	0	100	100
12	o	82/91 (90%)	73 (89%)	9 (11%)	0	100	100
12	p	82/91 (90%)	73 (89%)	9 (11%)	0	100	100
12	q	82/91 (90%)	73 (89%)	9 (11%)	0	100	100
12	r	82/91 (90%)	78 (95%)	4 (5%)	0	100	100
13	l	325/331 (98%)	285 (88%)	40 (12%)	0	100	100
14	m	202/256 (79%)	174 (86%)	28 (14%)	0	100	100
15	n	305/378 (81%)	270 (88%)	35 (12%)	0	100	100
16	s	172/682 (25%)	160 (93%)	12 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	u	368/377 (98%)	350 (95%)	18 (5%)	0	100	100
18	v	150/253 (59%)	144 (96%)	6 (4%)	0	100	100
18	w	139/253 (55%)	138 (99%)	1 (1%)	0	100	100
19	x	216/1298 (17%)	206 (95%)	10 (5%)	0	100	100
All	All	16794/23918 (70%)	15820 (94%)	974 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	0	146/418 (35%)	146 (100%)	0	100	100
1	4	135/418 (32%)	135 (100%)	0	100	100
2	1	153/573 (27%)	153 (100%)	0	100	100
3	2	158/470 (34%)	157 (99%)	1 (1%)	78	80
5	6	367/379 (97%)	367 (100%)	0	100	100
5	8	367/379 (97%)	367 (100%)	0	100	100
5	C	367/379 (97%)	367 (100%)	0	100	100
5	G	367/379 (97%)	367 (100%)	0	100	100
5	I	367/379 (97%)	367 (100%)	0	100	100
5	K	367/379 (97%)	367 (100%)	0	100	100
5	O	367/379 (97%)	367 (100%)	0	100	100
5	Q	367/379 (97%)	367 (100%)	0	100	100
5	S	367/379 (97%)	367 (100%)	0	100	100
5	W	367/379 (97%)	367 (100%)	0	100	100
5	Y	367/379 (97%)	367 (100%)	0	100	100
5	i	367/379 (97%)	367 (100%)	0	100	100
5	k	367/379 (97%)	366 (100%)	1 (0%)	86	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	y	367/379 (97%)	367 (100%)	0	100	100
6	7	359/374 (96%)	358 (100%)	1 (0%)	86	84
6	9	359/374 (96%)	359 (100%)	0	100	100
6	D	365/374 (98%)	364 (100%)	1 (0%)	86	84
6	H	365/374 (98%)	365 (100%)	0	100	100
6	J	365/374 (98%)	365 (100%)	0	100	100
6	L	365/374 (98%)	365 (100%)	0	100	100
6	P	365/374 (98%)	365 (100%)	0	100	100
6	R	365/374 (98%)	365 (100%)	0	100	100
6	T	365/374 (98%)	365 (100%)	0	100	100
6	X	359/374 (96%)	359 (100%)	0	100	100
6	Z	359/374 (96%)	359 (100%)	0	100	100
6	j	359/374 (96%)	358 (100%)	1 (0%)	86	84
6	t	359/374 (96%)	359 (100%)	0	100	100
6	z	359/374 (96%)	358 (100%)	1 (0%)	86	84
7	A	368/766 (48%)	368 (100%)	0	100	100
8	B	362/742 (49%)	362 (100%)	0	100	100
9	E	76/406 (19%)	76 (100%)	0	100	100
9	F	102/406 (25%)	102 (100%)	0	100	100
10	M	36/406 (9%)	36 (100%)	0	100	100
10	N	32/406 (8%)	32 (100%)	0	100	100
11	U	42/162 (26%)	42 (100%)	0	100	100
11	V	28/162 (17%)	28 (100%)	0	100	100
12	a	72/76 (95%)	72 (100%)	0	100	100
12	b	72/76 (95%)	72 (100%)	0	100	100
12	c	72/76 (95%)	72 (100%)	0	100	100
12	d	72/76 (95%)	72 (100%)	0	100	100
12	e	72/76 (95%)	72 (100%)	0	100	100
12	f	72/76 (95%)	72 (100%)	0	100	100
12	g	72/76 (95%)	72 (100%)	0	100	100
12	h	72/76 (95%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	o	72/76 (95%)	72 (100%)	0	100	100
12	p	72/76 (95%)	72 (100%)	0	100	100
12	q	72/76 (95%)	72 (100%)	0	100	100
12	r	72/76 (95%)	72 (100%)	0	100	100
13	l	259/263 (98%)	259 (100%)	0	100	100
14	m	159/197 (81%)	159 (100%)	0	100	100
16	s	162/553 (29%)	162 (100%)	0	100	100
17	u	313/318 (98%)	313 (100%)	0	100	100
18	v	134/218 (62%)	134 (100%)	0	100	100
18	w	127/218 (58%)	127 (100%)	0	100	100
19	x	191/884 (22%)	191 (100%)	0	100	100
All	All	14053/19440 (72%)	14047 (100%)	6 (0%)	100	100

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	j	233	GLN
5	k	227	HIS
6	z	228	ASN
6	7	133	GLN
3	2	291	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
5	i	334	GLN
5	y	347	ASN
6	j	8	HIS
12	q	29	GLN
6	H	11	GLN

5.3.3 RNA ⓘ

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 43 ligands modelled in this entry, 14 are monoatomic - leaving 29 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$
20	GDP	I	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.78	8 (17%)
20	GDP	y	502	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
21	GTP	y	501	22	33,34,34	0.92	1 (3%)	50,54,54	1.57	8 (16%)
21	GTP	L	501	22	33,34,34	0.91	0	50,54,54	1.55	10 (20%)
20	GDP	K	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.72	6 (13%)
20	GDP	Q	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.79	6 (13%)
20	GDP	8	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.76	7 (15%)
20	GDP	O	501	-	29,30,30	1.18	3 (10%)	45,47,47	1.79	7 (15%)
21	GTP	Z	501	22	33,34,34	0.87	1 (3%)	50,54,54	1.57	9 (18%)
21	GTP	9	501	22	33,34,34	0.88	1 (3%)	50,54,54	1.64	9 (18%)
21	GTP	T	501	22	33,34,34	0.90	2 (6%)	50,54,54	1.58	8 (16%)
21	GTP	P	501	22	33,34,34	1.00	2 (6%)	50,54,54	1.62	9 (18%)
20	GDP	Y	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
20	GDP	G	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.74	6 (13%)
21	GTP	j	501	22	33,34,34	0.88	1 (3%)	50,54,54	1.58	9 (18%)
21	GTP	X	501	22	33,34,34	0.90	2 (6%)	50,54,54	1.58	9 (18%)
20	GDP	k	501	-	29,30,30	1.11	3 (10%)	45,47,47	1.92	9 (20%)
21	GTP	7	501	22	33,34,34	0.90	1 (3%)	50,54,54	1.62	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	GTP	R	501	22	33,34,34	0.90	1 (3%)	50,54,54	1.60	9 (18%)
21	GTP	z	501	22	33,34,34	0.94	1 (3%)	50,54,54	1.62	10 (20%)
21	GTP	J	501	22	33,34,34	0.88	1 (3%)	50,54,54	1.66	9 (18%)
20	GDP	i	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.81	7 (15%)
21	GTP	D	501	22	33,34,34	0.90	1 (3%)	50,54,54	1.57	9 (18%)
23	ATP	u	401	-	32,33,33	1.36	4 (12%)	48,52,52	1.76	9 (18%)
20	GDP	C	501	-	29,30,30	1.15	3 (10%)	45,47,47	1.76	8 (17%)
21	GTP	H	501	22	33,34,34	0.90	0	50,54,54	1.60	12 (24%)
20	GDP	W	501	-	29,30,30	1.14	3 (10%)	45,47,47	1.80	8 (17%)
20	GDP	S	501	-	29,30,30	1.16	3 (10%)	45,47,47	1.75	7 (15%)
20	GDP	6	501	-	29,30,30	1.13	3 (10%)	45,47,47	1.78	7 (15%)

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
20	GDP	I	501	-	-	6/16/32/32	0/3/3/3
20	GDP	y	502	-	-	4/16/32/32	0/3/3/3
21	GTP	y	501	22	-	4/22/38/38	0/3/3/3
21	GTP	L	501	22	-	5/22/38/38	0/3/3/3
20	GDP	K	501	-	-	4/16/32/32	0/3/3/3
20	GDP	Q	501	-	-	6/16/32/32	0/3/3/3
20	GDP	8	501	-	-	4/16/32/32	0/3/3/3
20	GDP	O	501	-	-	3/16/32/32	0/3/3/3
21	GTP	Z	501	22	-	4/22/38/38	0/3/3/3
21	GTP	9	501	22	-	6/22/38/38	0/3/3/3
21	GTP	T	501	22	-	3/22/38/38	0/3/3/3
21	GTP	P	501	22	-	5/22/38/38	0/3/3/3
20	GDP	Y	501	-	-	1/16/32/32	0/3/3/3
20	GDP	G	501	-	-	5/16/32/32	0/3/3/3
21	GTP	j	501	22	-	4/22/38/38	0/3/3/3
21	GTP	X	501	22	-	5/22/38/38	0/3/3/3
20	GDP	k	501	-	-	1/16/32/32	0/3/3/3
21	GTP	7	501	22	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	GTP	R	501	22	-	7/22/38/38	0/3/3/3
21	GTP	z	501	22	-	7/22/38/38	0/3/3/3
21	GTP	J	501	22	-	9/22/38/38	0/3/3/3
20	GDP	i	501	-	-	2/16/32/32	0/3/3/3
21	GTP	D	501	22	-	6/22/38/38	0/3/3/3
23	ATP	u	401	-	-	4/22/38/38	0/3/3/3
20	GDP	C	501	-	-	2/16/32/32	0/3/3/3
21	GTP	H	501	22	-	5/22/38/38	0/3/3/3
20	GDP	W	501	-	-	7/16/32/32	0/3/3/3
20	GDP	S	501	-	-	0/16/32/32	0/3/3/3
20	GDP	6	501	-	-	3/16/32/32	0/3/3/3

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	u	401	ATP	C5-C4	4.60	1.47	1.39
20	K	501	GDP	C5-C4	3.12	1.47	1.38
20	Y	501	GDP	C5-C4	3.09	1.47	1.38
20	8	501	GDP	C5-C4	3.07	1.47	1.38
20	C	501	GDP	C5-C4	3.06	1.47	1.38

The worst 5 of 236 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	k	501	GDP	C5-C4-N3	-6.72	117.70	128.39
20	O	501	GDP	C5-C4-N3	-6.23	118.48	128.39
20	I	501	GDP	C5-C4-N3	-6.21	118.51	128.39
20	i	501	GDP	C5-C4-N3	-6.17	118.58	128.39
20	W	501	GDP	C5-C4-N3	-6.13	118.64	128.39

There are no chirality outliers.

5 of 126 torsion outliers are listed below:

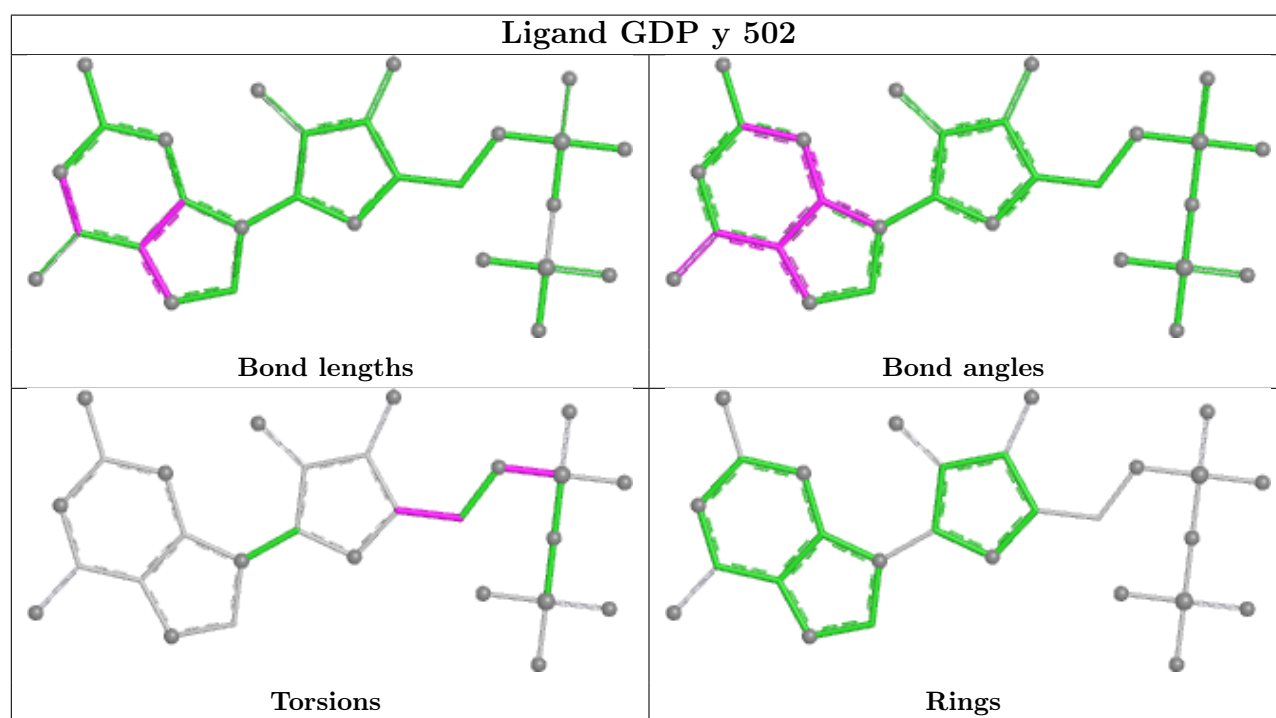
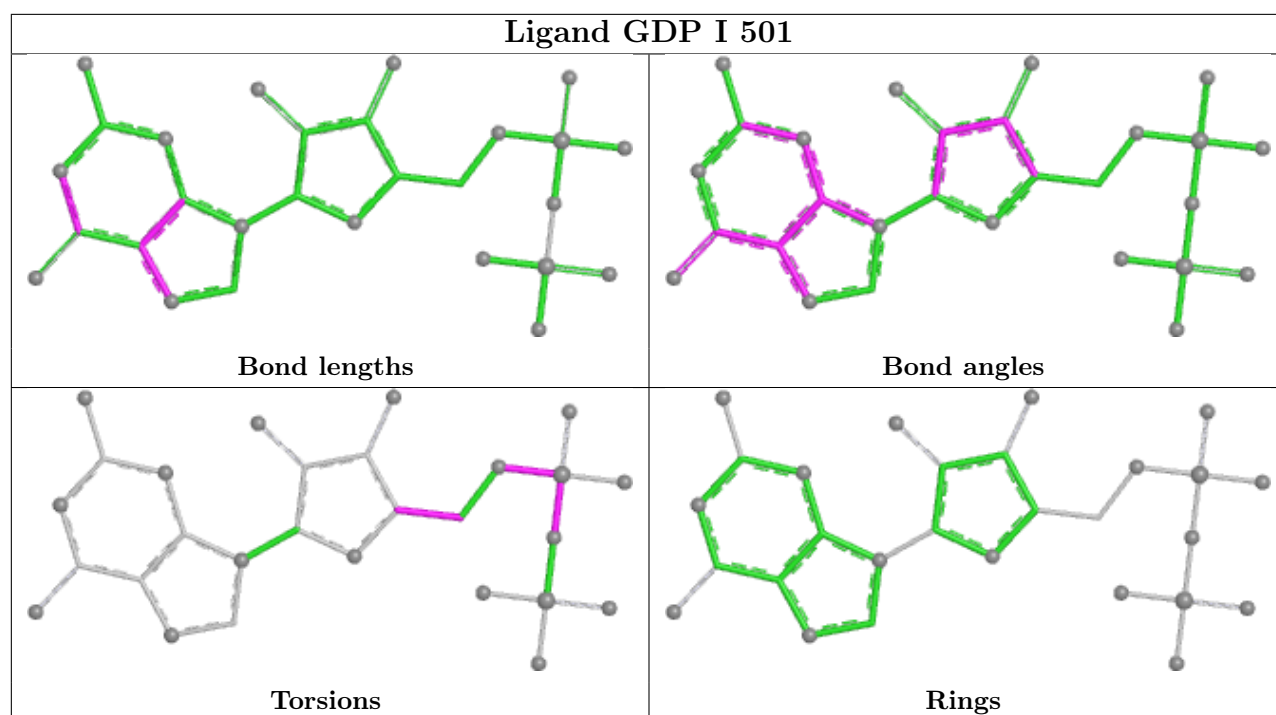
Mol	Chain	Res	Type	Atoms
20	6	501	GDP	C5'-O5'-PA-O3A
20	6	501	GDP	C5'-O5'-PA-O2A
20	8	501	GDP	C5'-O5'-PA-O3A
20	8	501	GDP	C5'-O5'-PA-O1A
20	C	501	GDP	C5'-O5'-PA-O3A

There are no ring outliers.

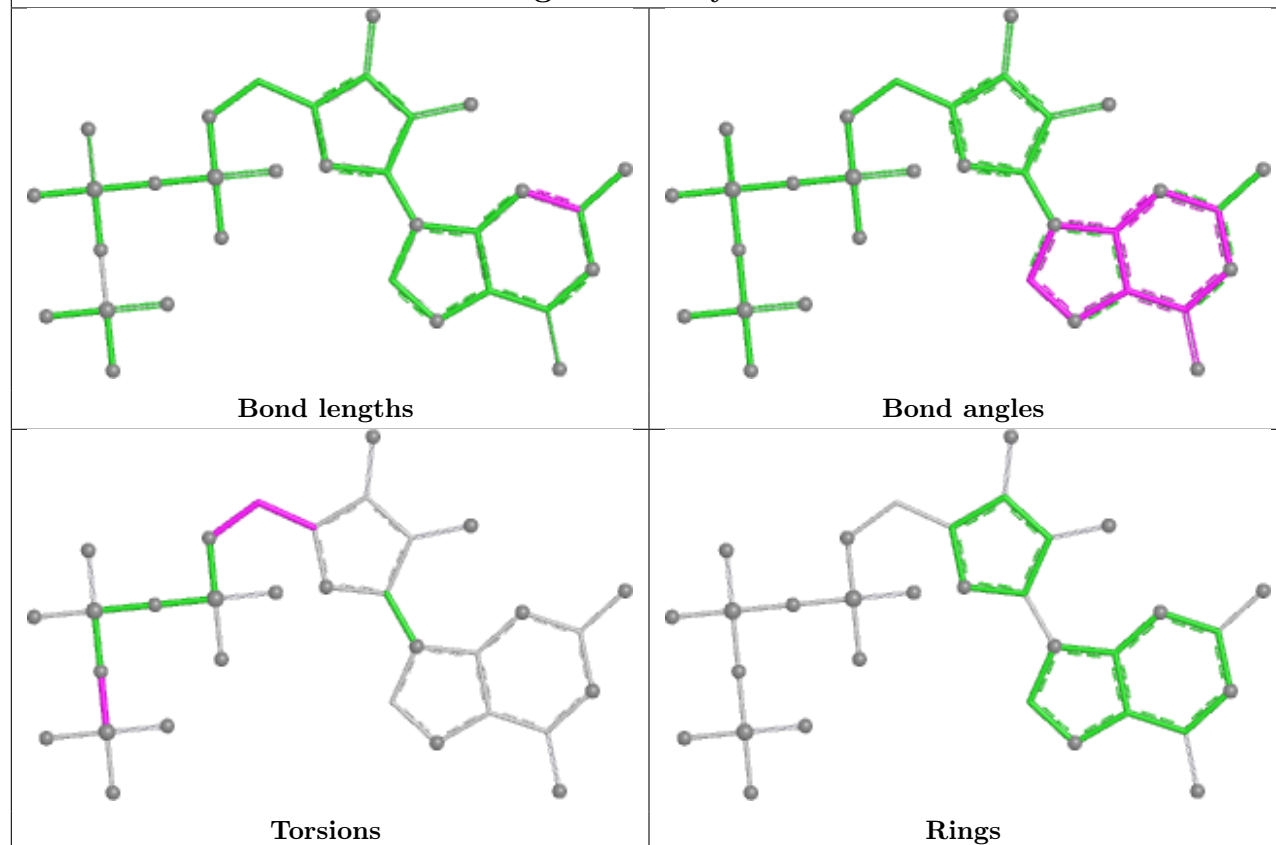
23 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	I	501	GDP	2	0
21	y	501	GTP	2	0
21	L	501	GTP	3	0
20	K	501	GDP	4	0
20	Q	501	GDP	1	0
20	8	501	GDP	3	0
20	O	501	GDP	4	0
21	Z	501	GTP	1	0
21	9	501	GTP	1	0
21	T	501	GTP	1	0
21	P	501	GTP	1	0
20	Y	501	GDP	1	0
21	j	501	GTP	2	0
20	k	501	GDP	1	0
21	7	501	GTP	3	0
21	z	501	GTP	2	0
21	J	501	GTP	1	0
20	i	501	GDP	1	0
23	u	401	ATP	2	0
20	C	501	GDP	1	0
20	W	501	GDP	1	0
20	S	501	GDP	2	0
20	6	501	GDP	2	0

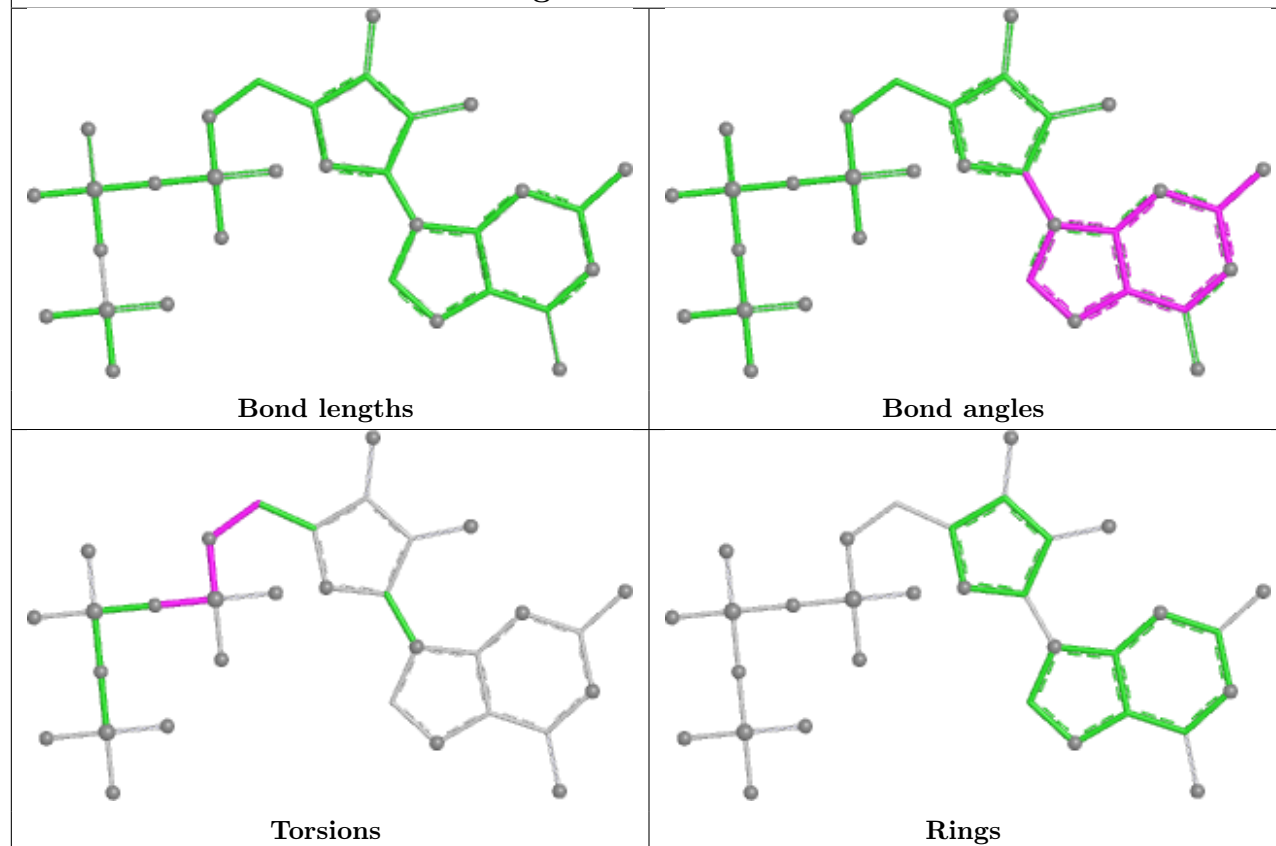
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

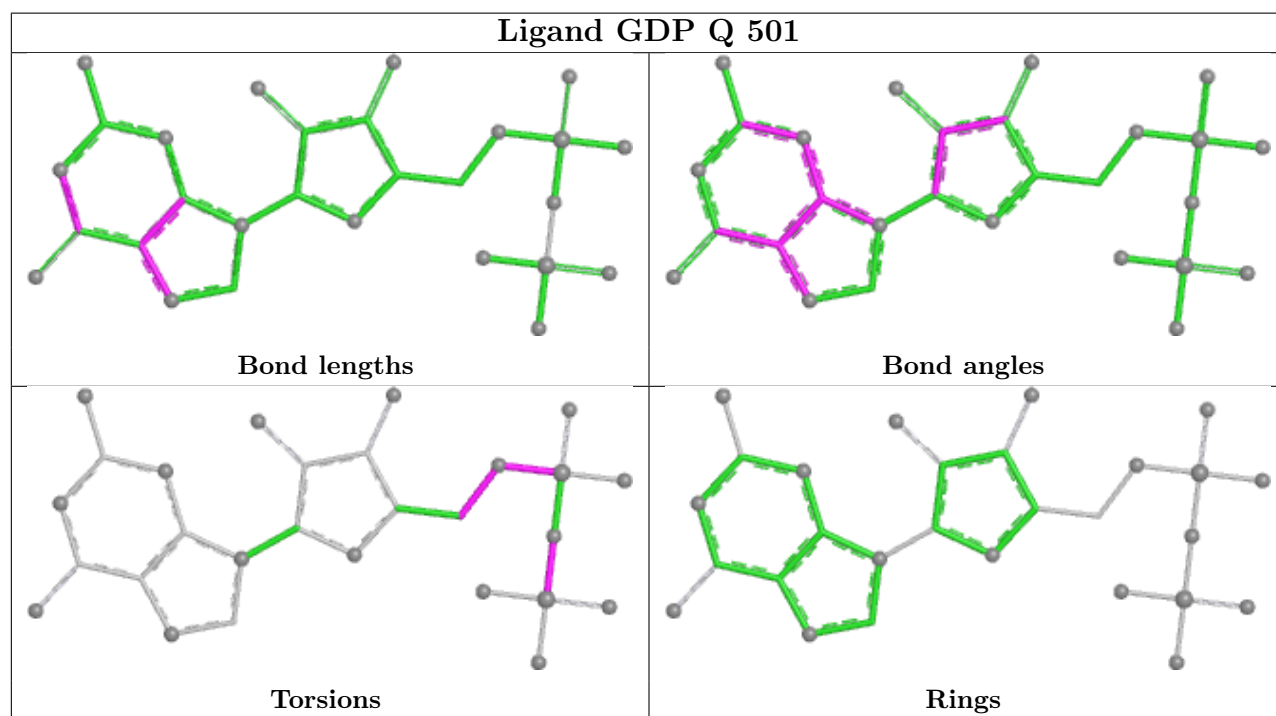
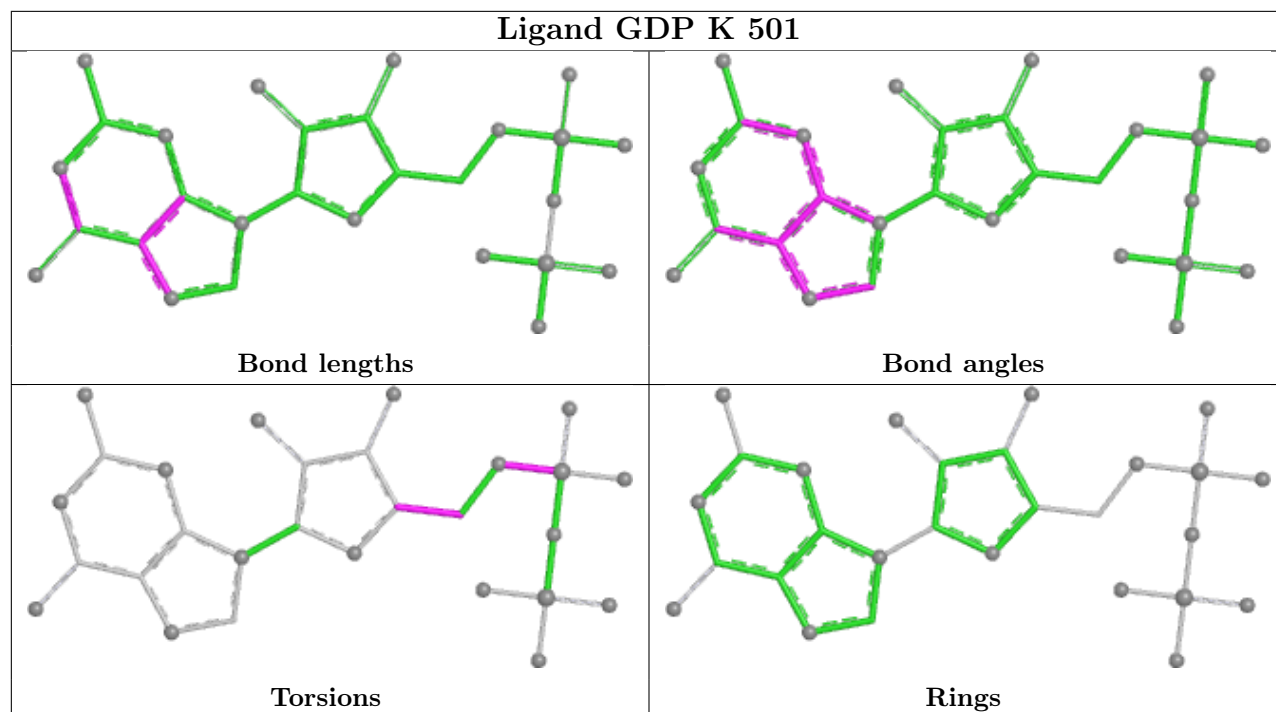


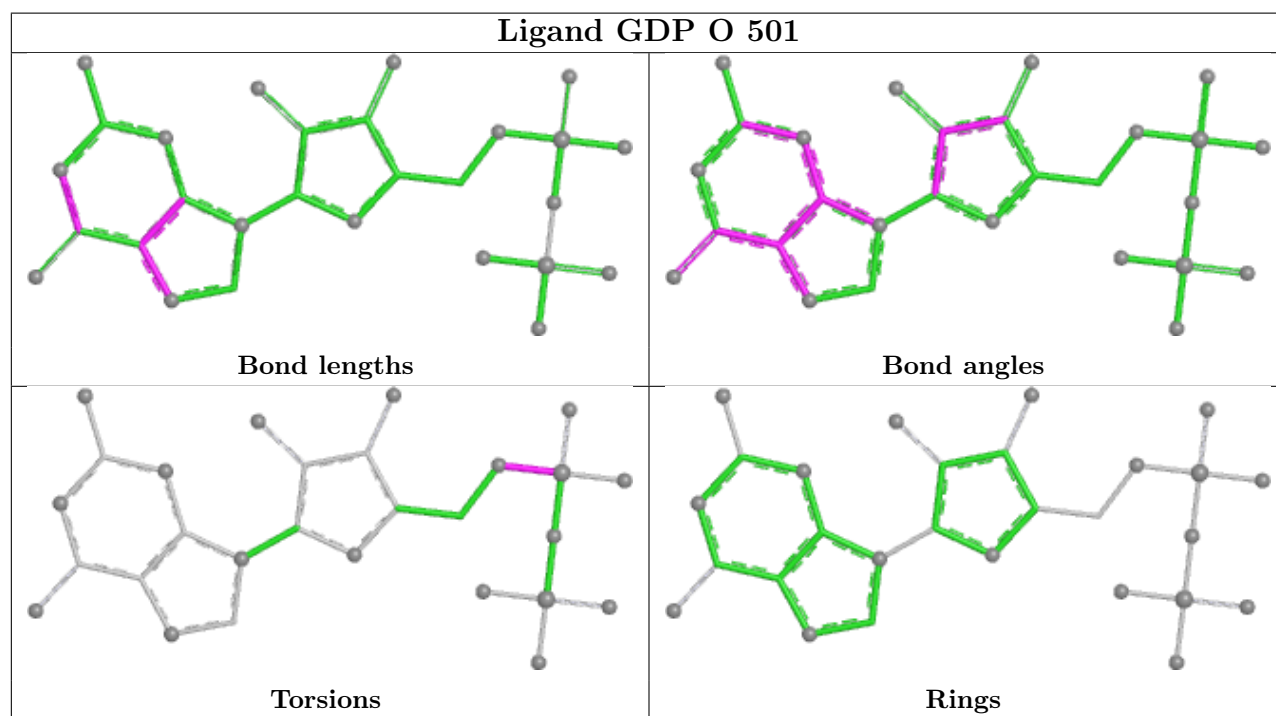
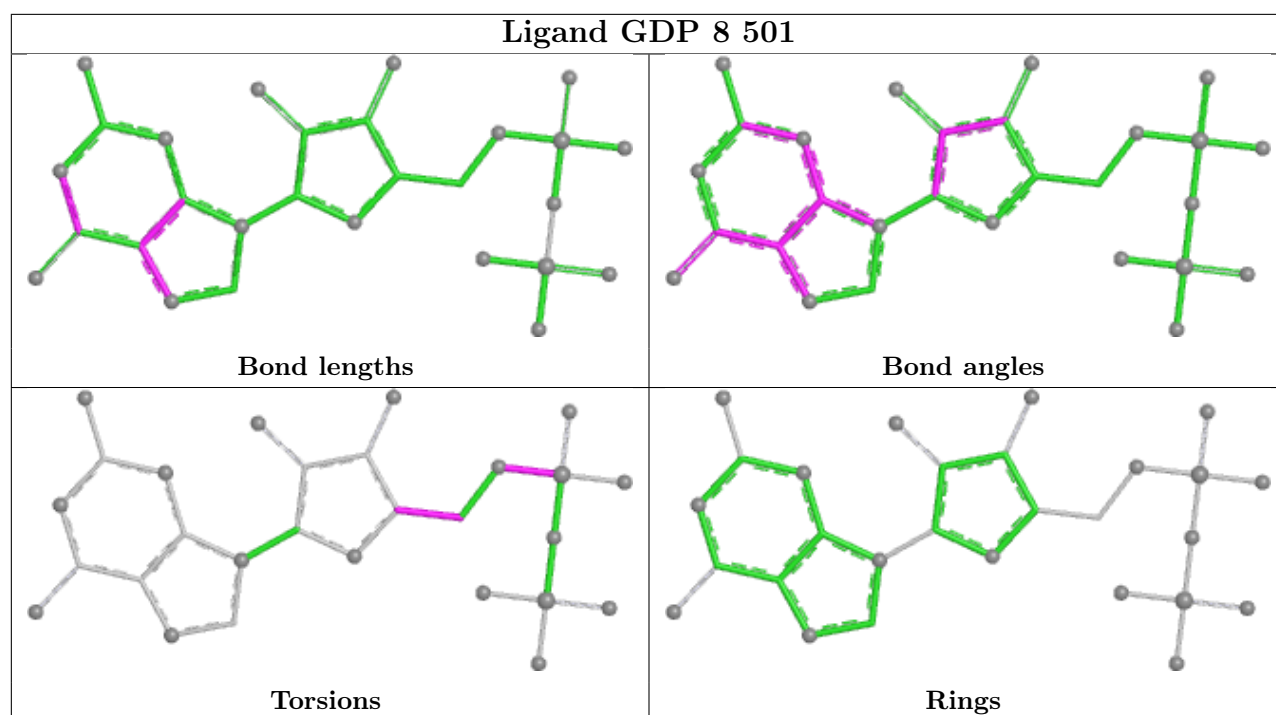
Ligand GTP y 501



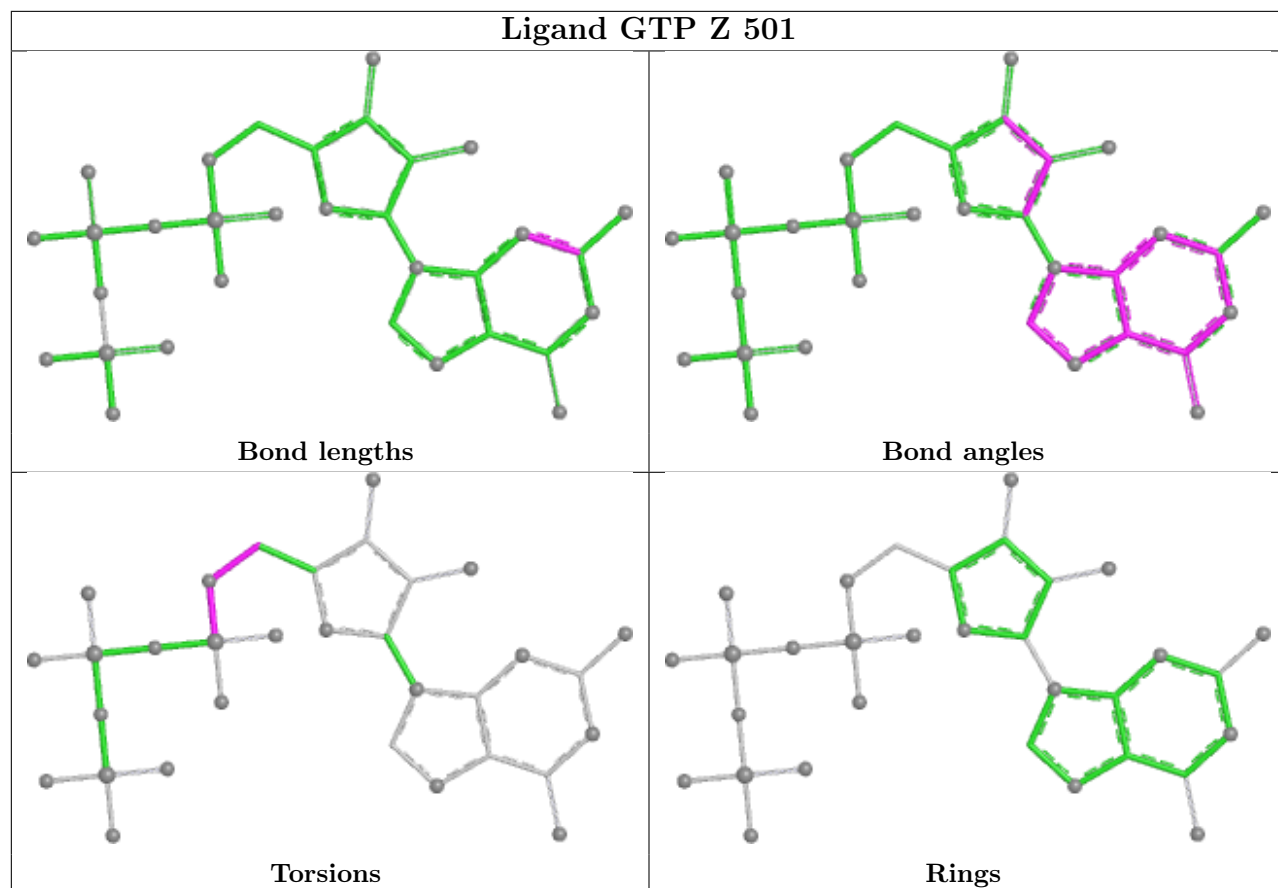
Ligand GTP L 501



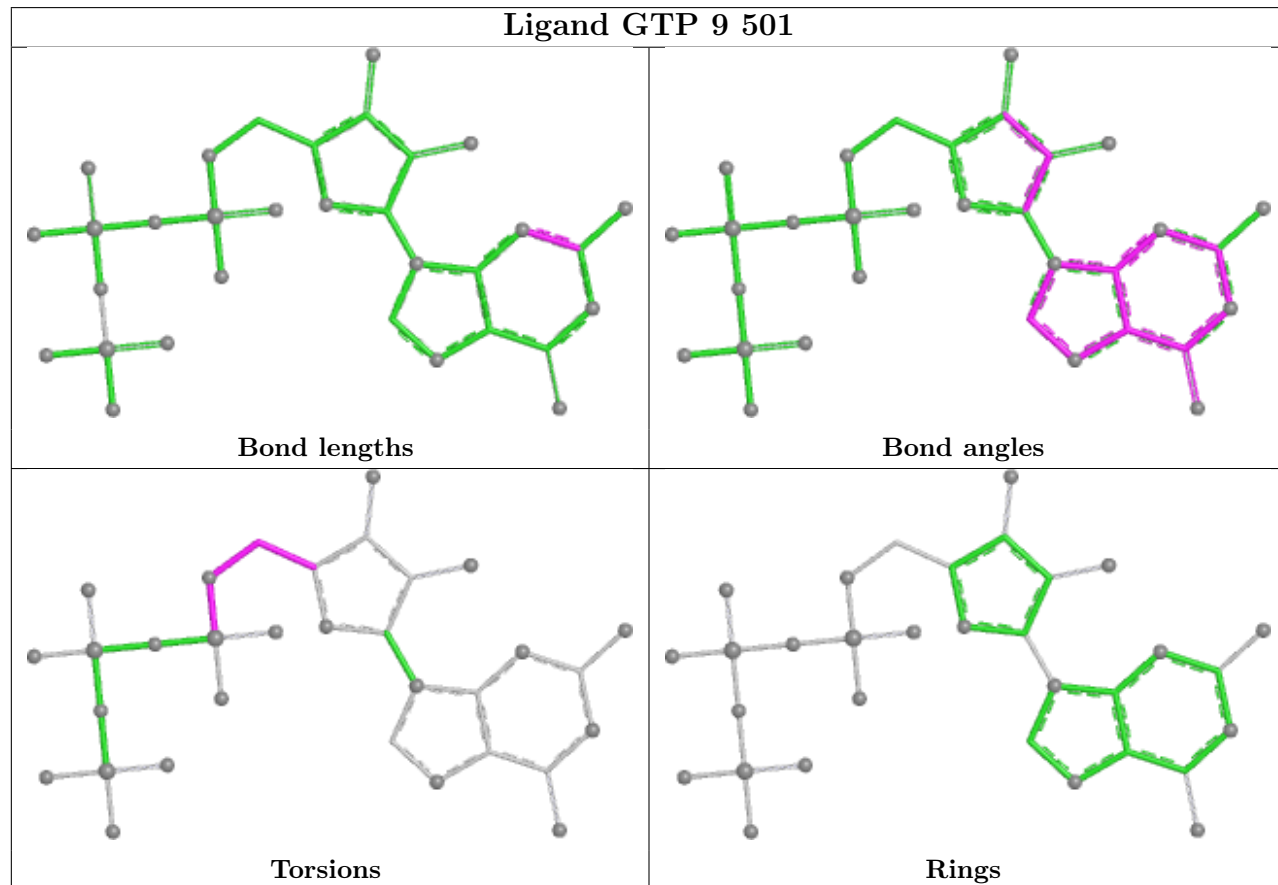


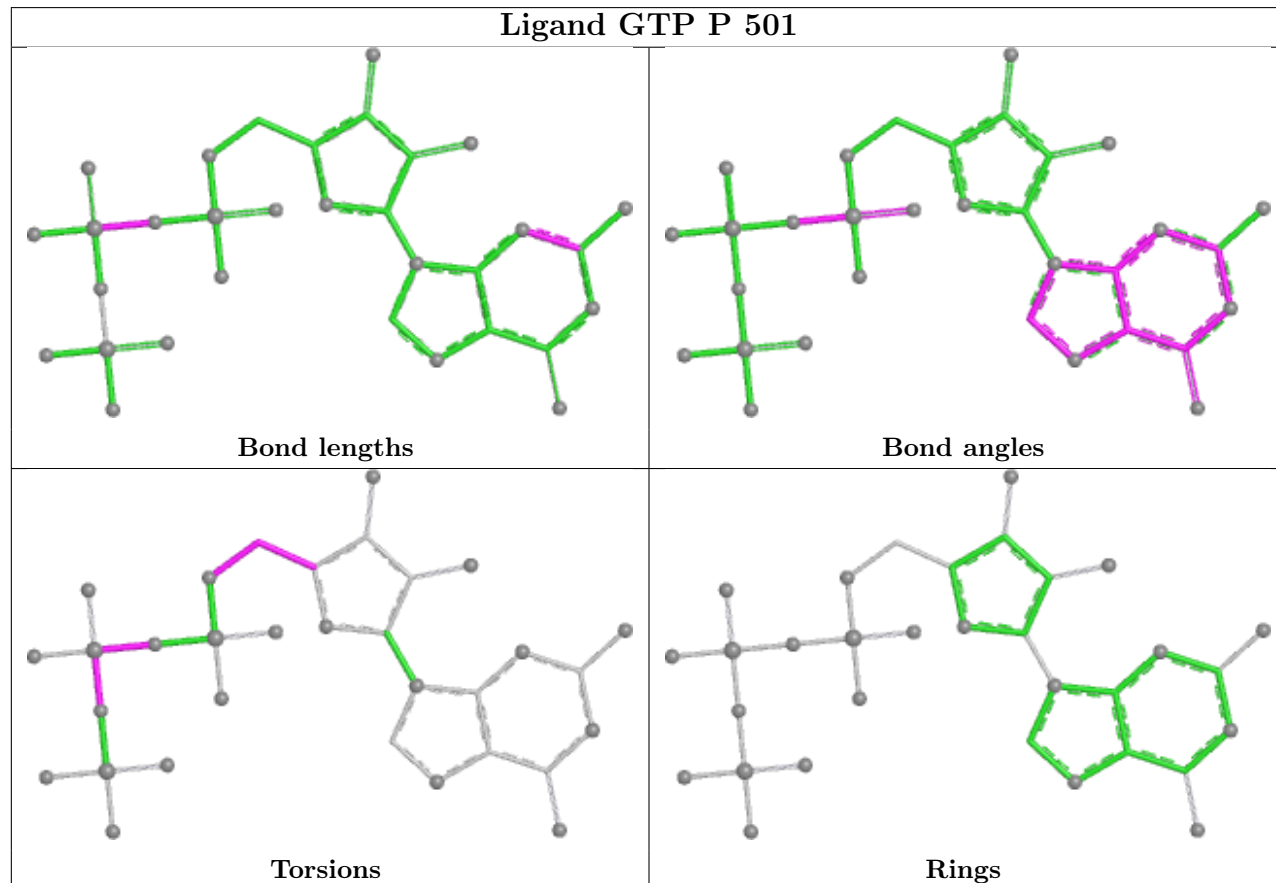
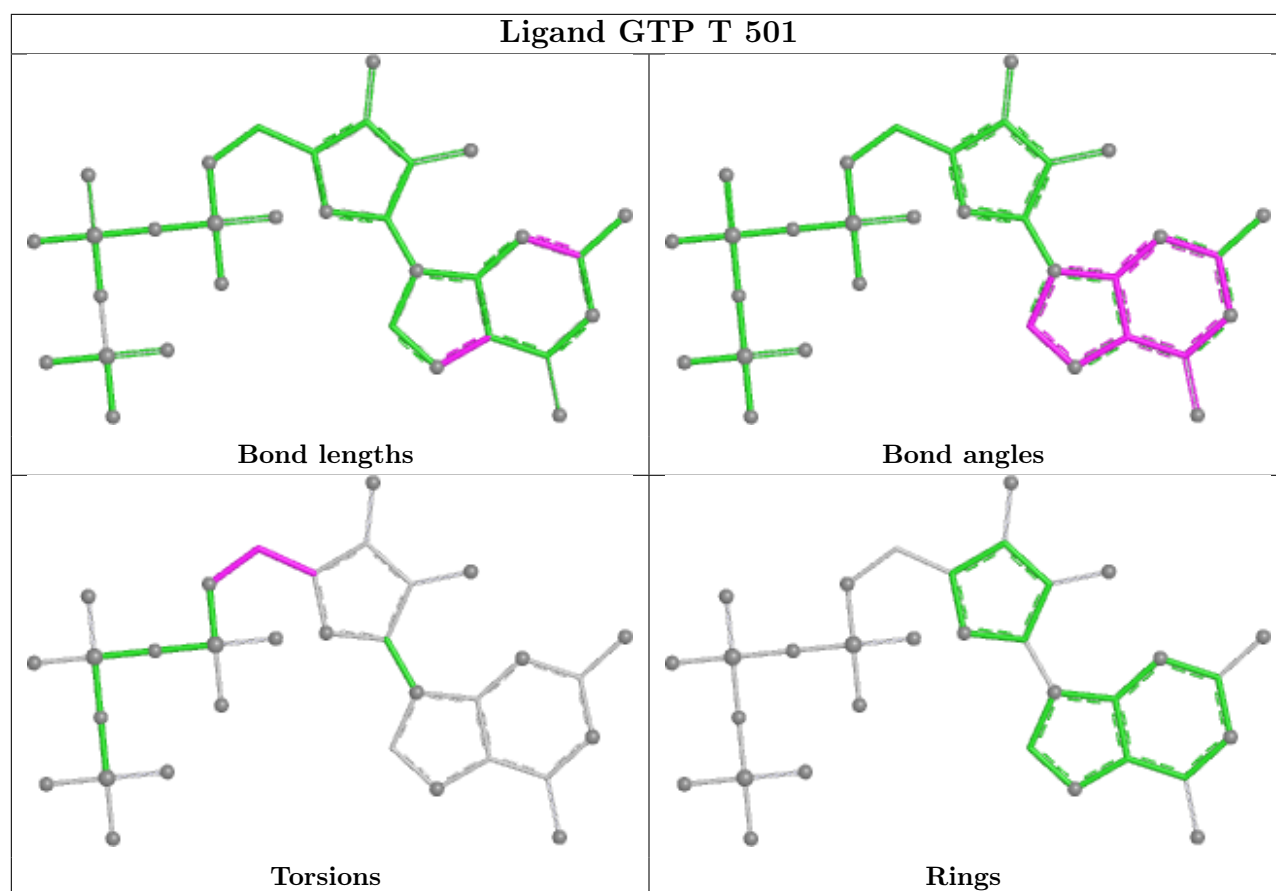


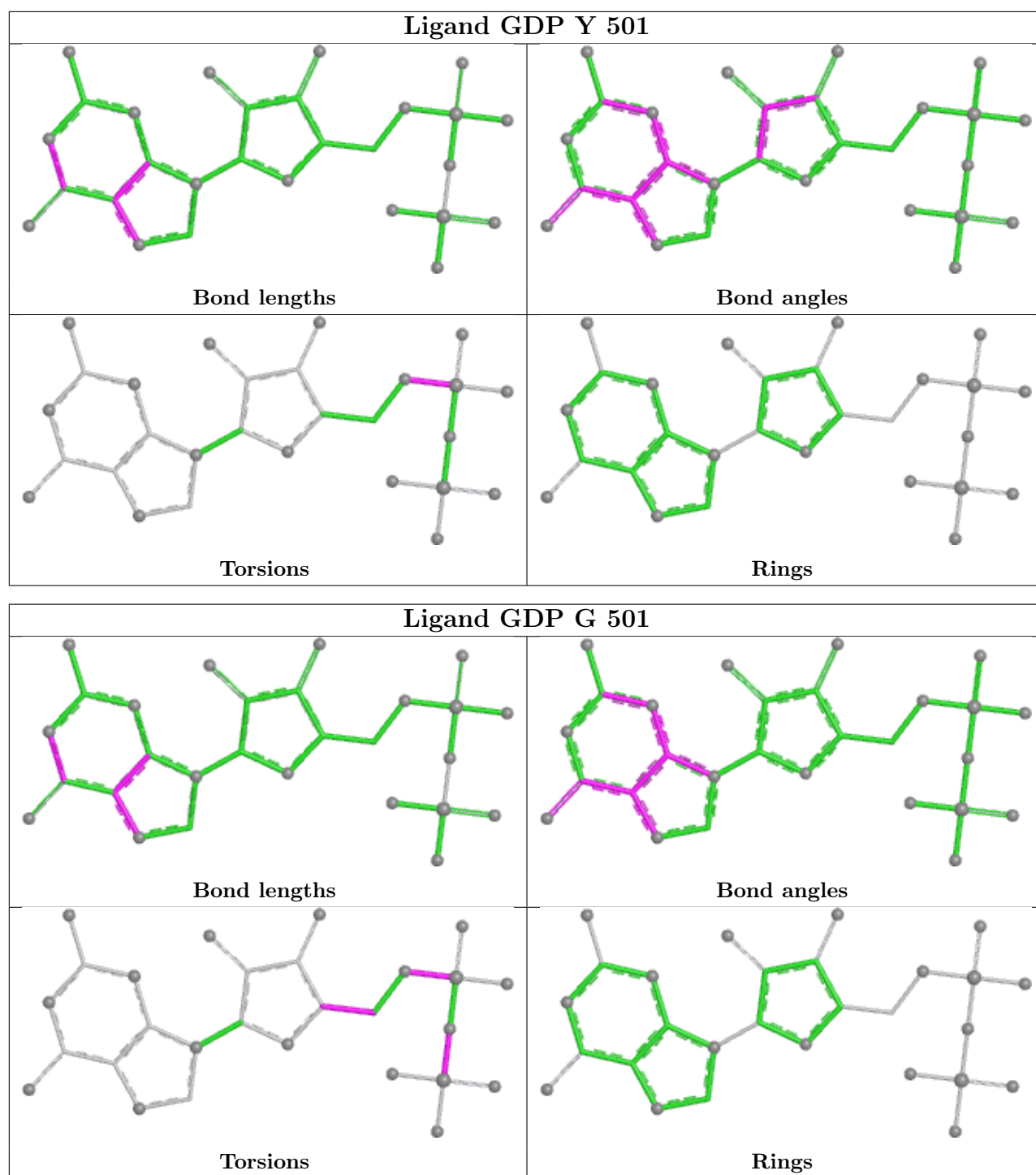
Ligand GTP Z 501



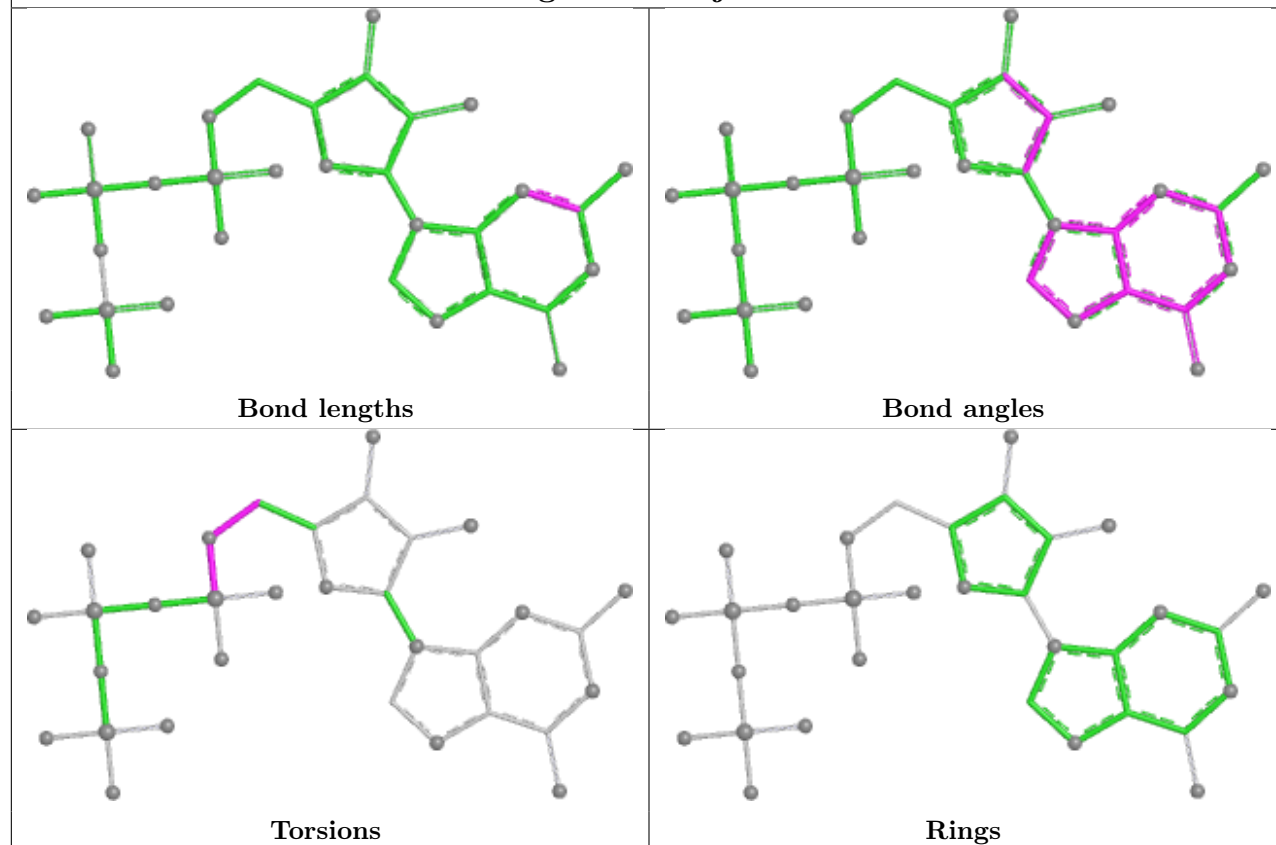
Ligand GTP 9 501



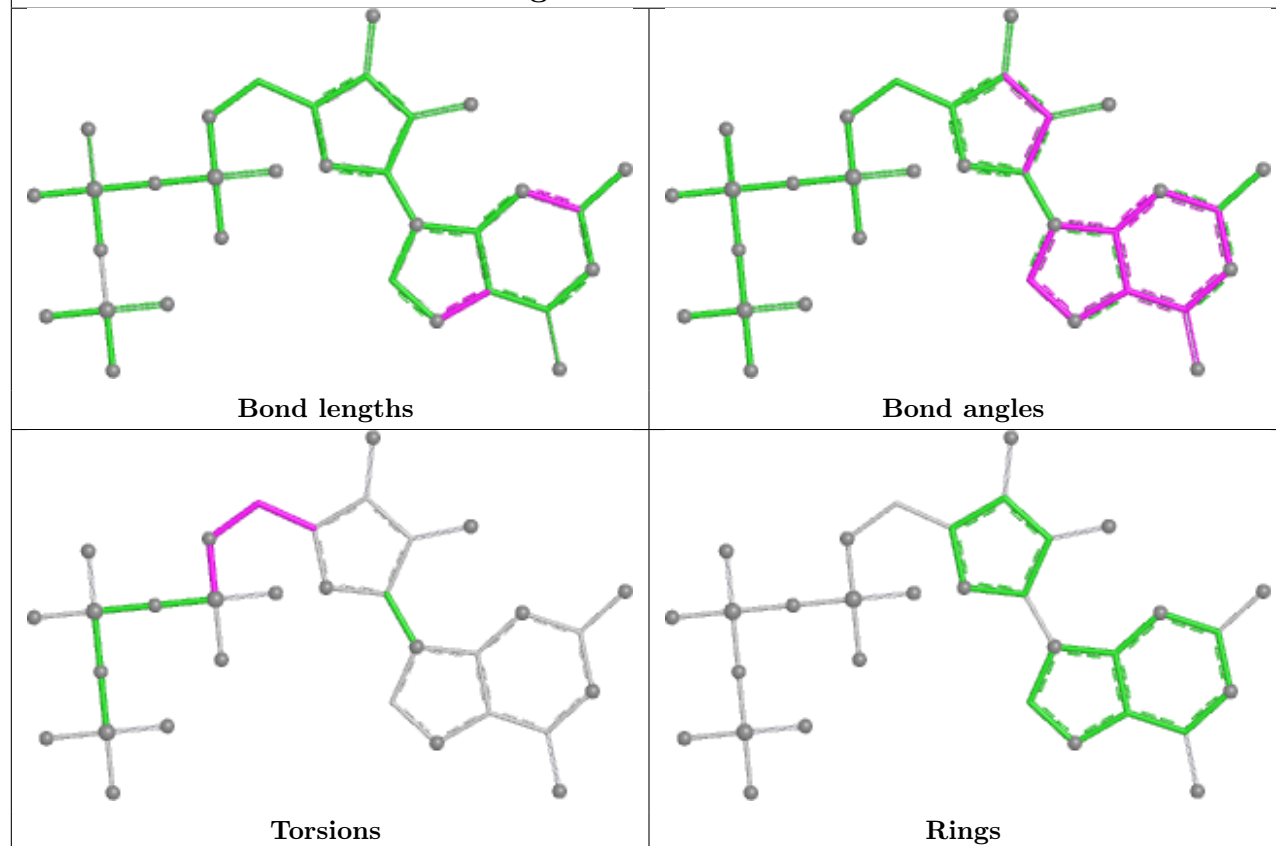


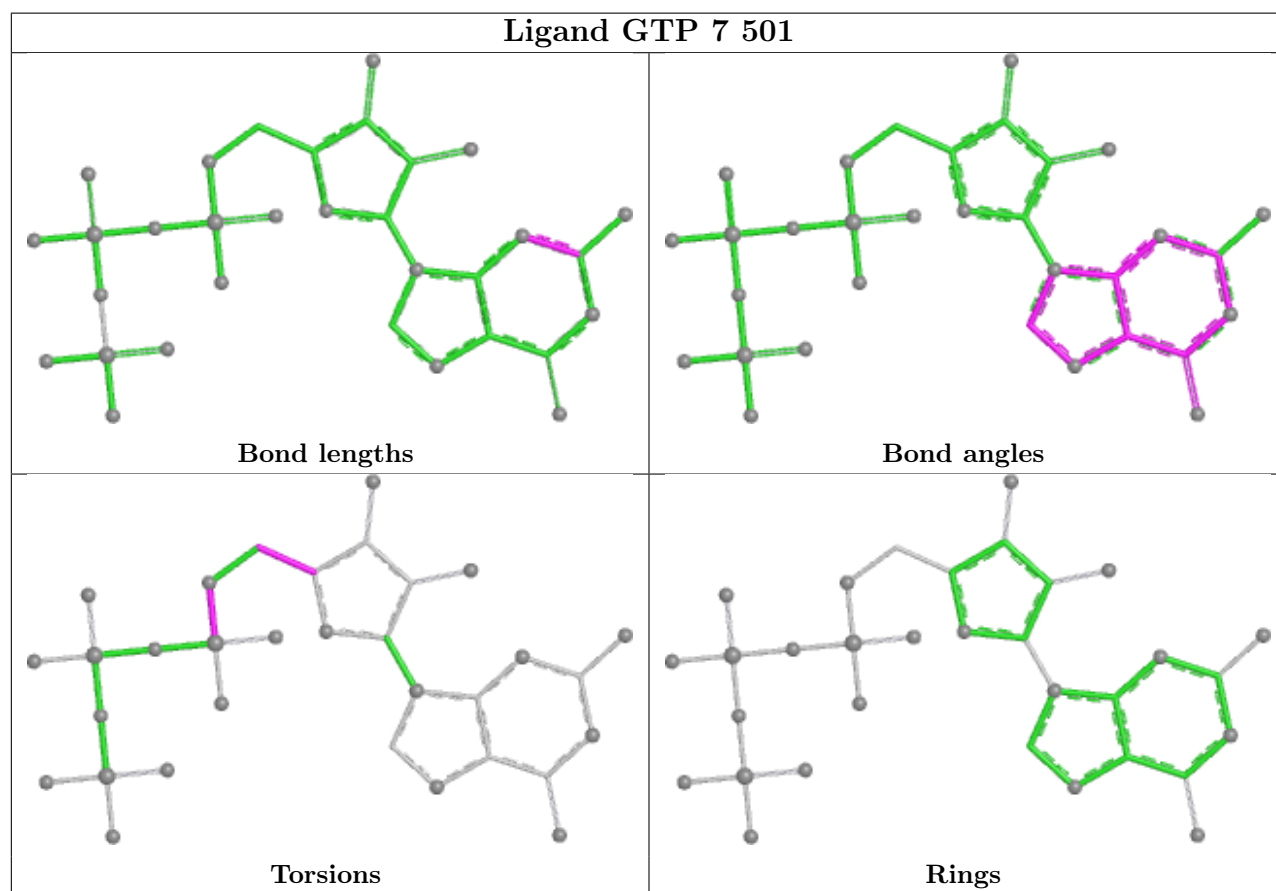
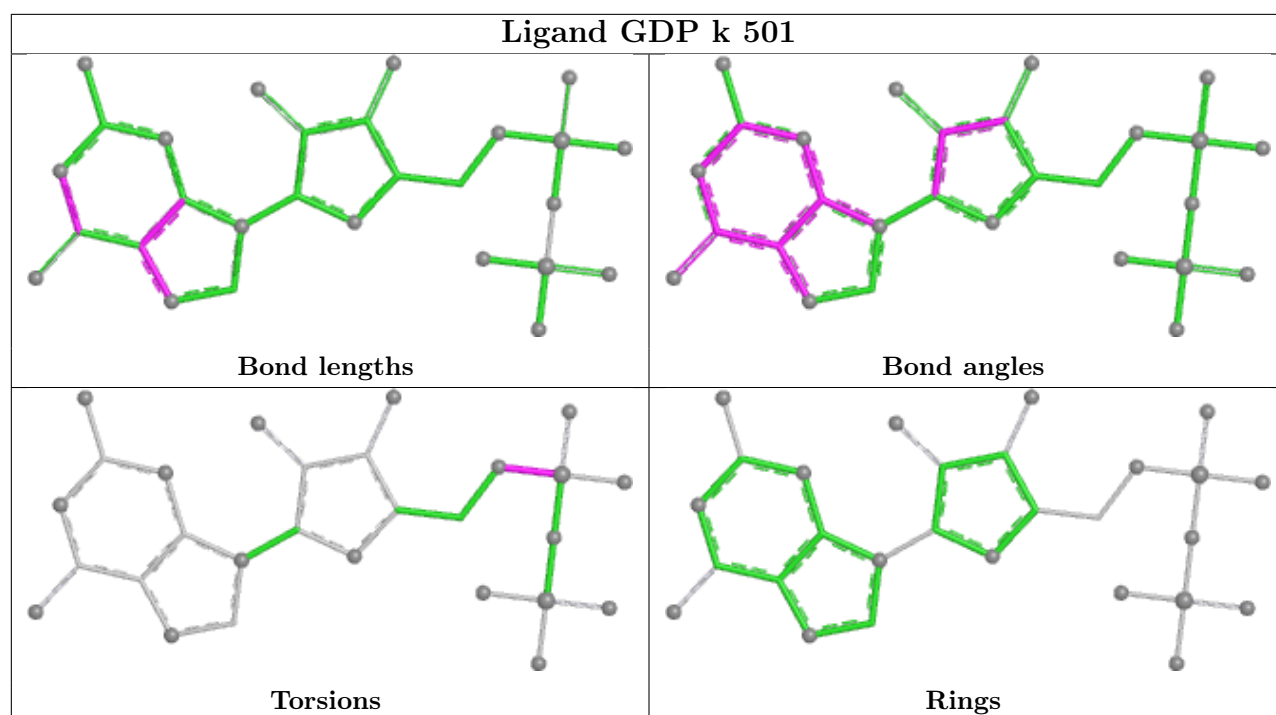


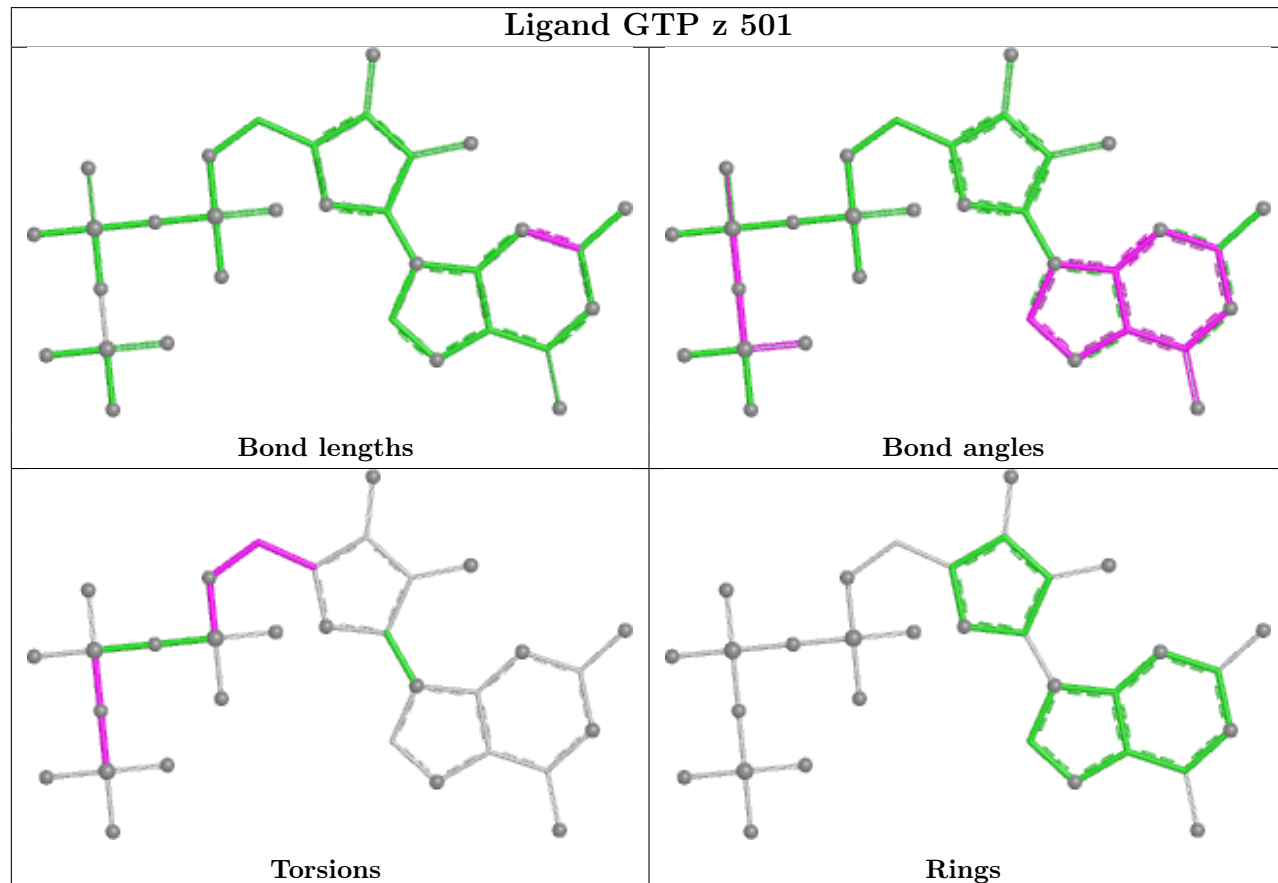
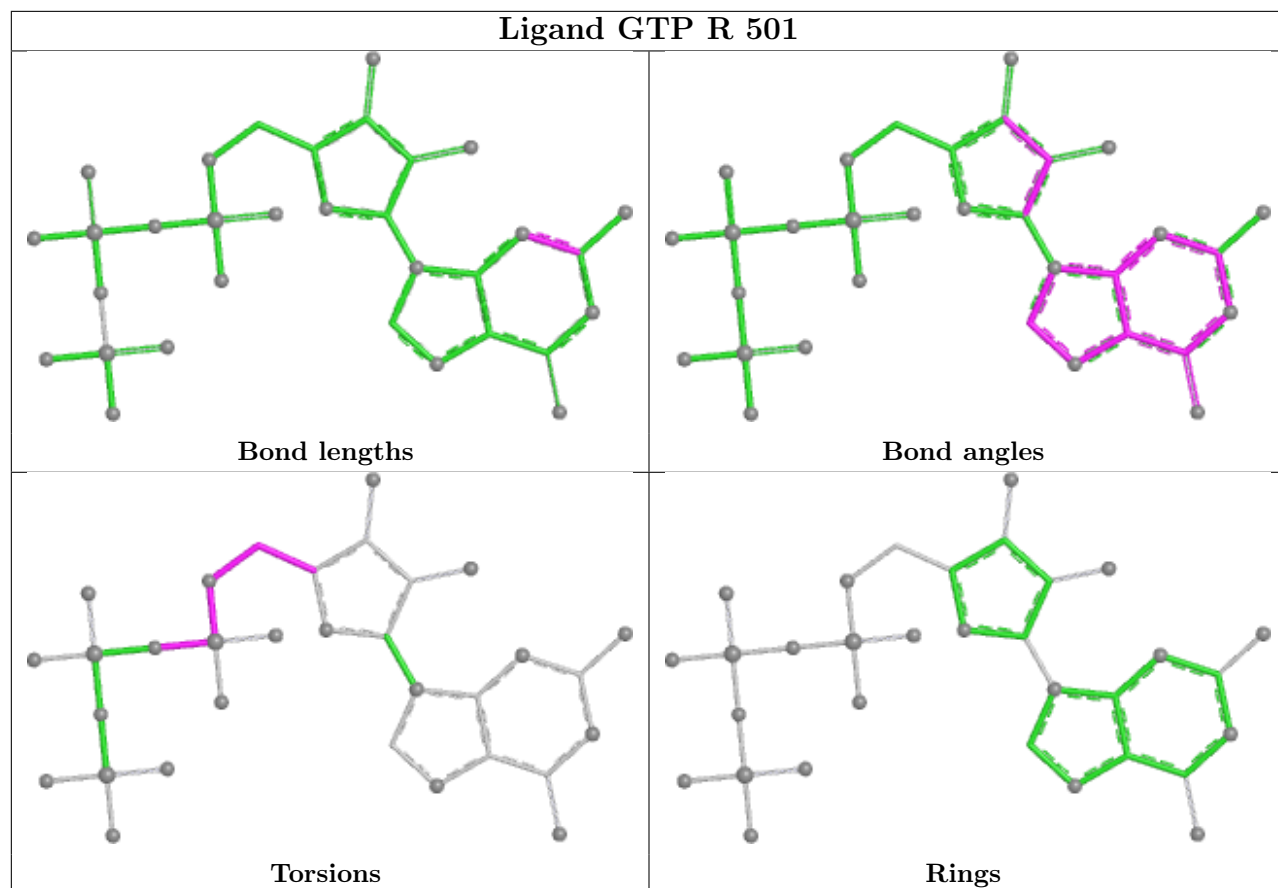
Ligand GTP j 501

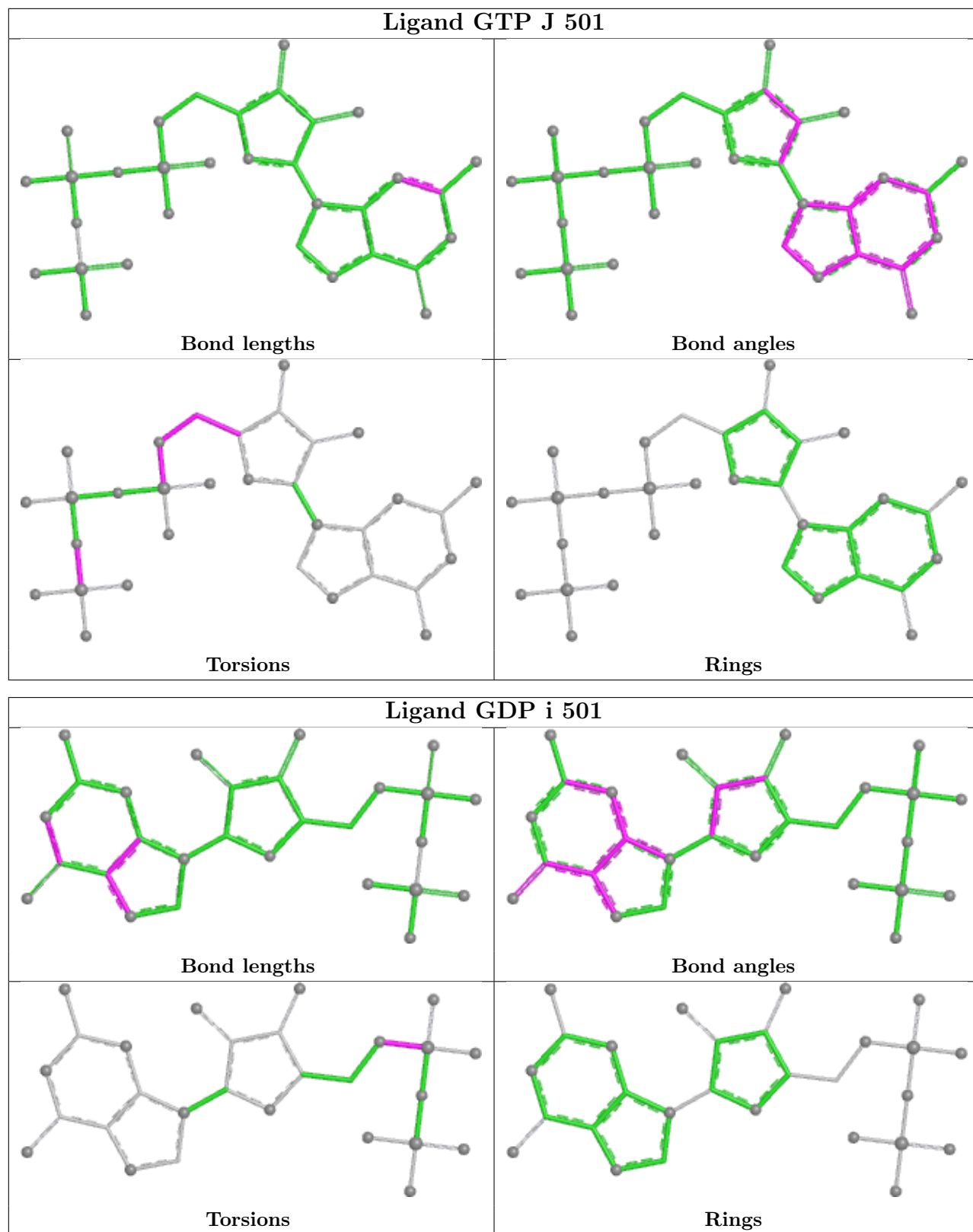


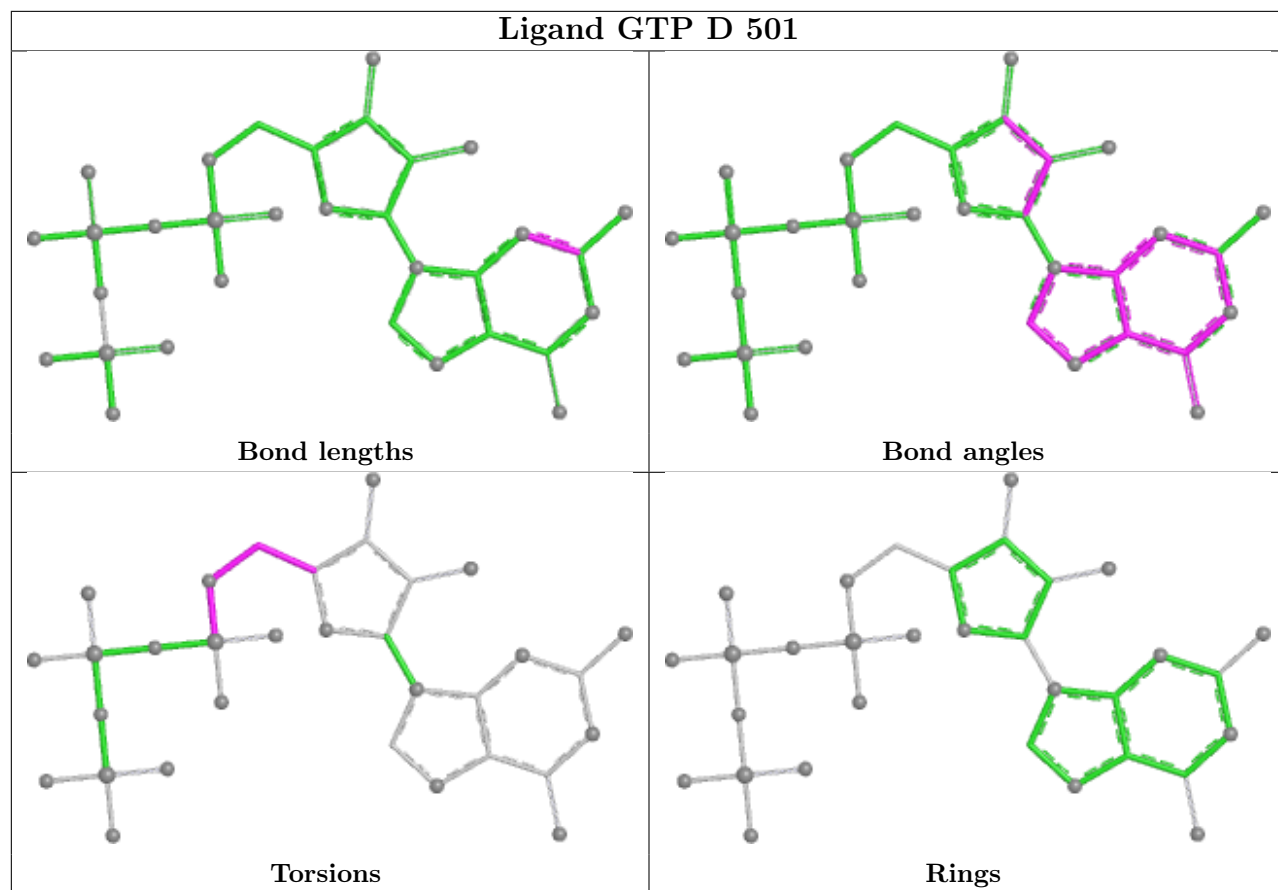
Ligand GTP X 501



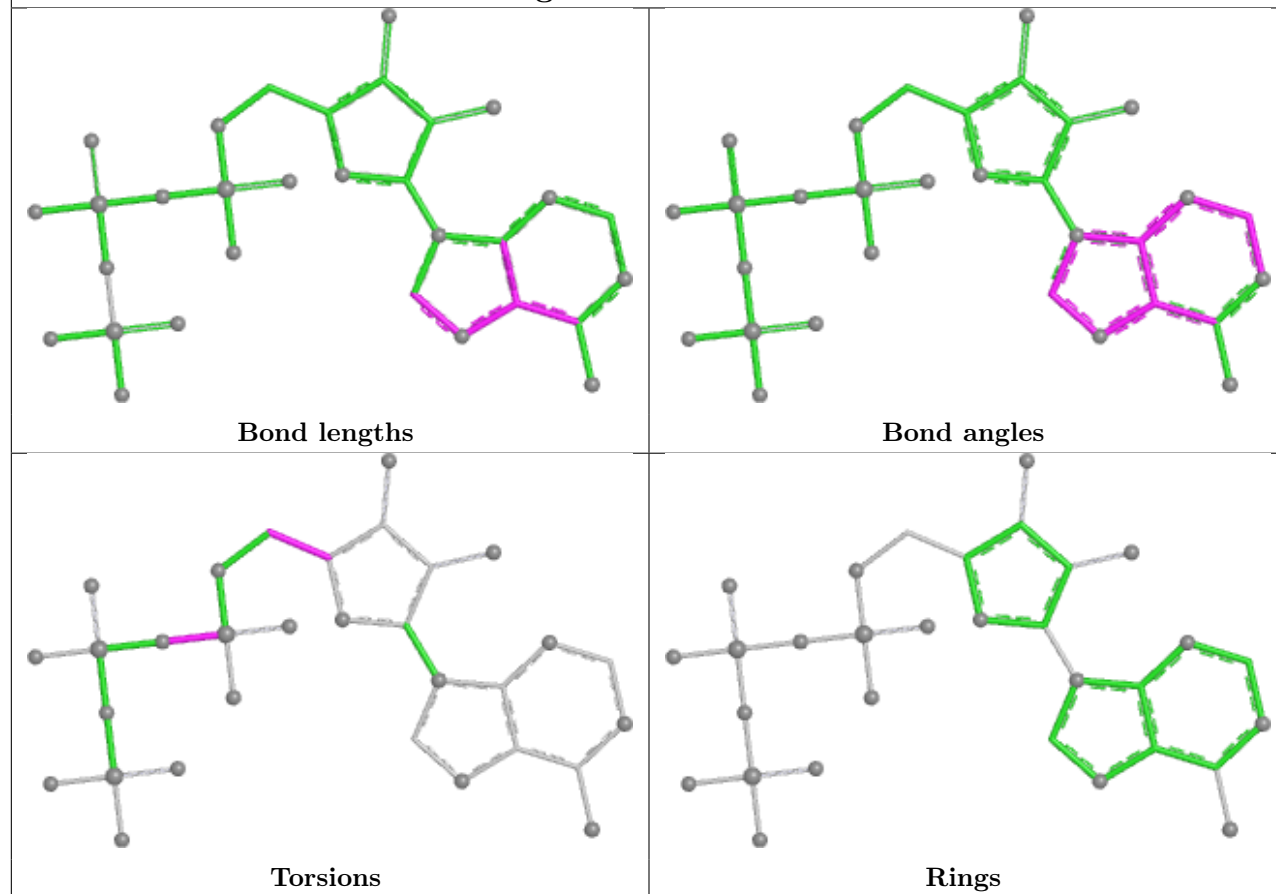




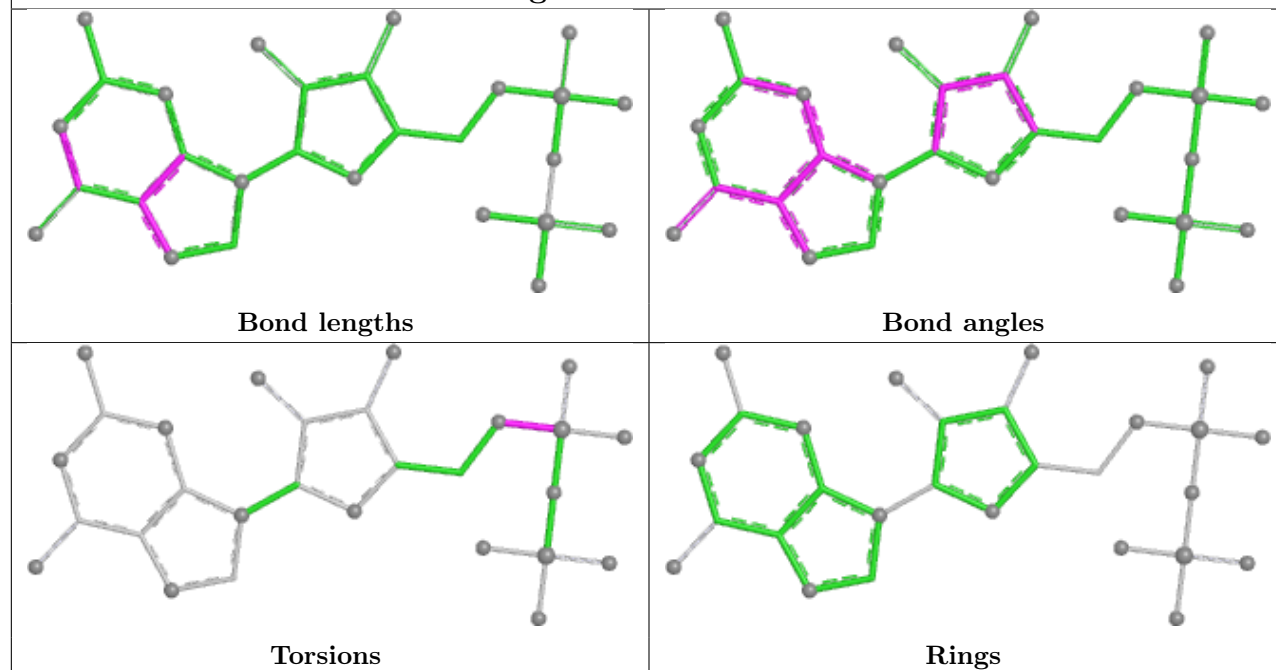


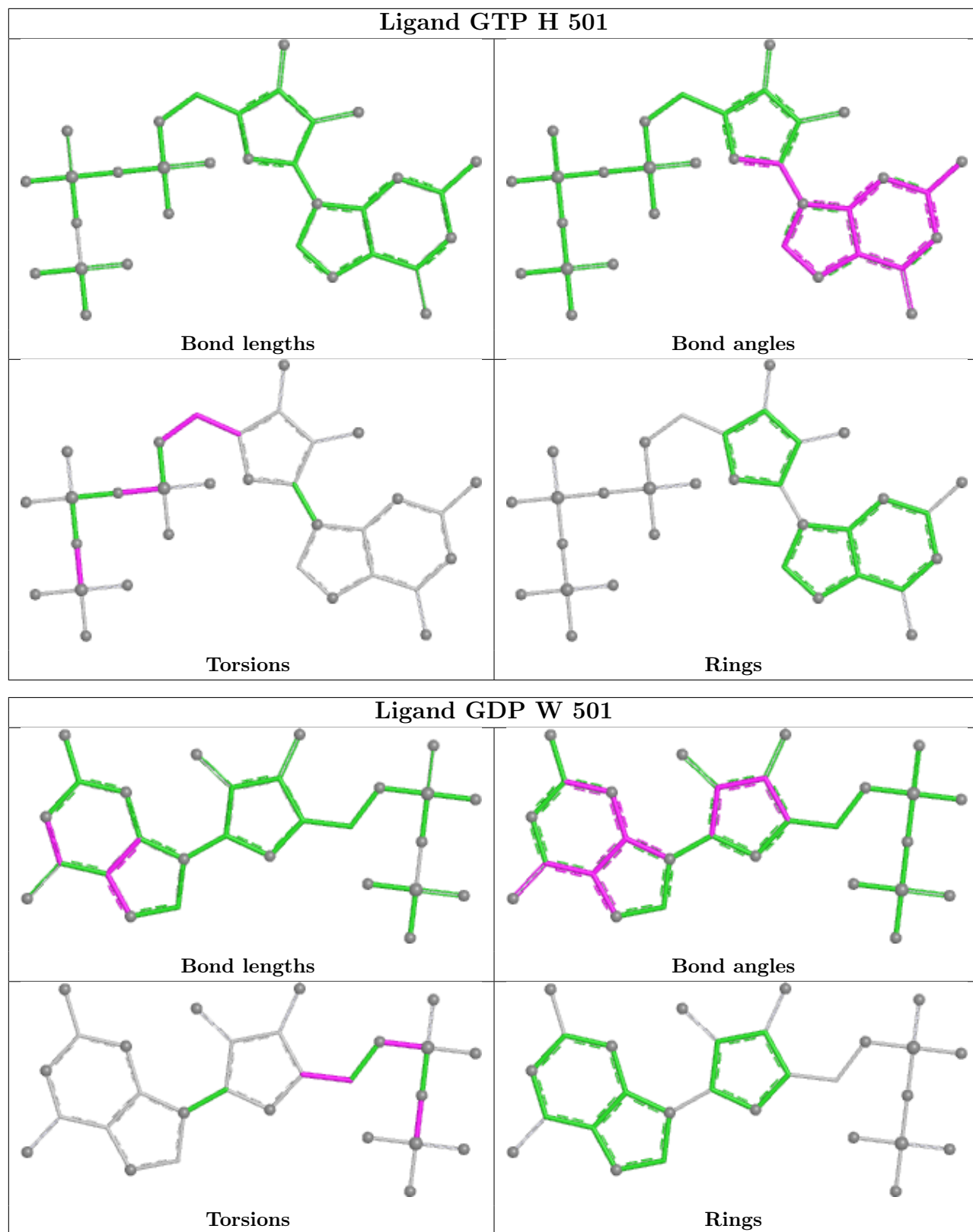


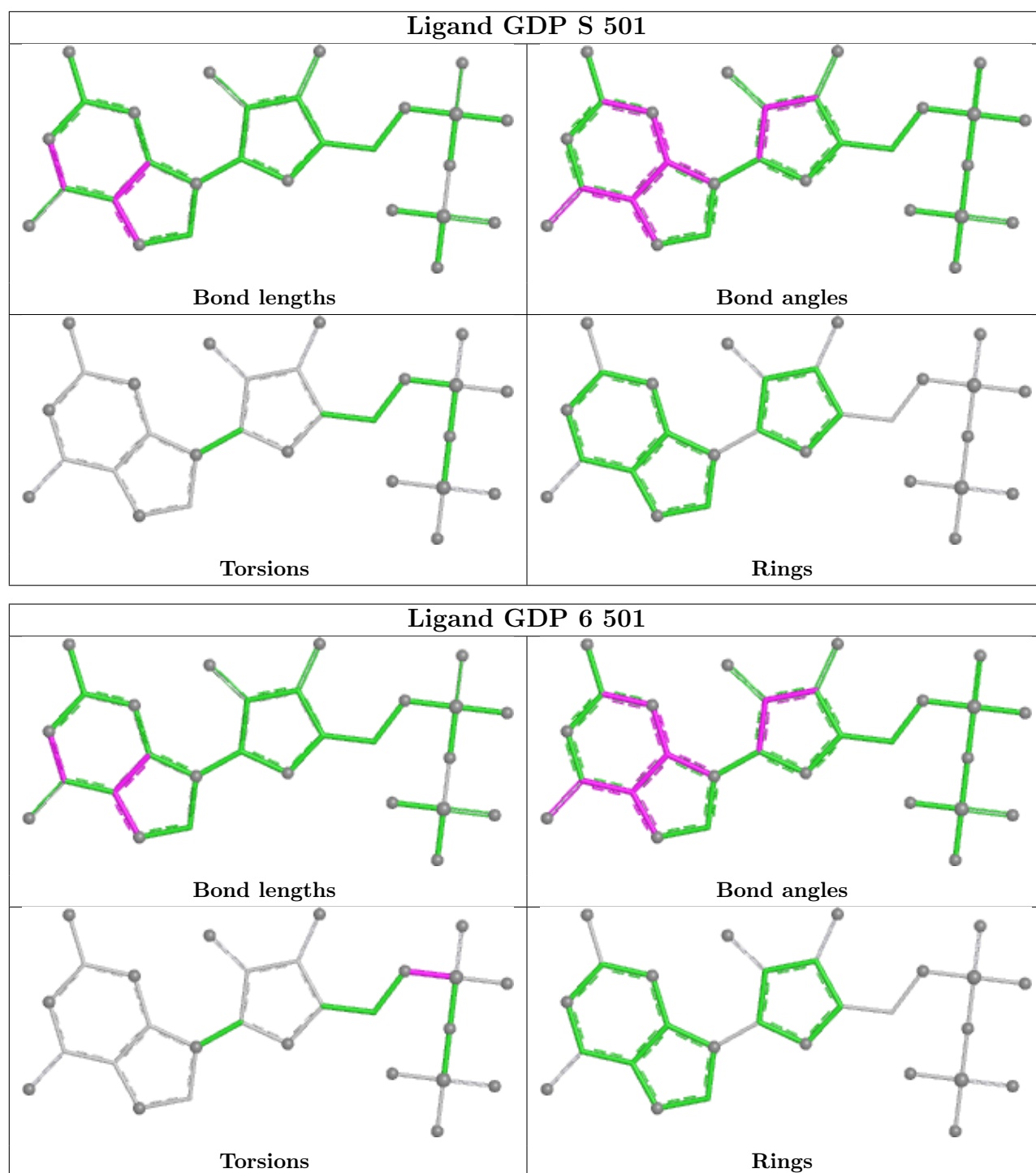
Ligand ATP u 401



Ligand GDP C 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.

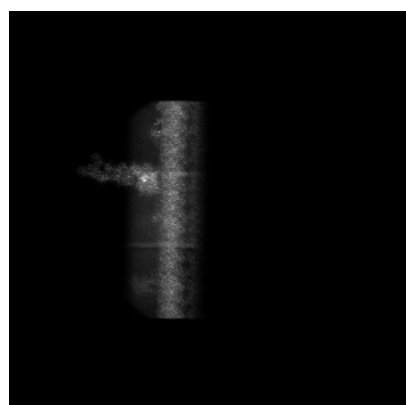
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22481. These allow visual inspection of the internal detail of the map and identification of artifacts.

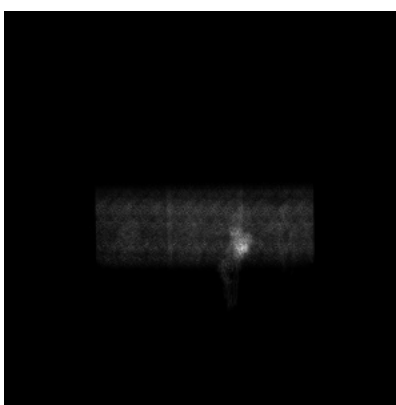
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

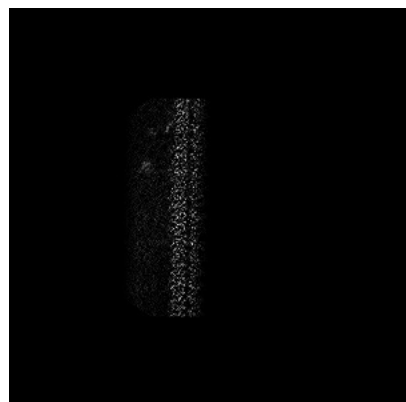


Z

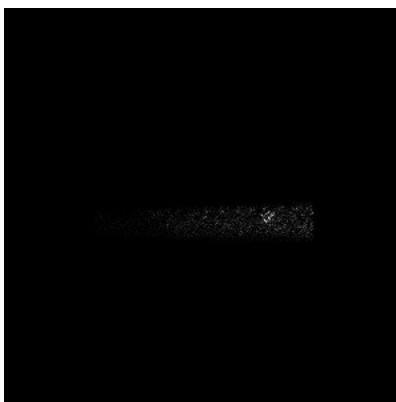
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

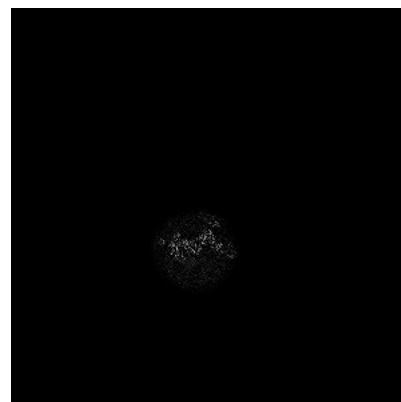
6.2.1 Primary map



X Index: 416



Y Index: 416

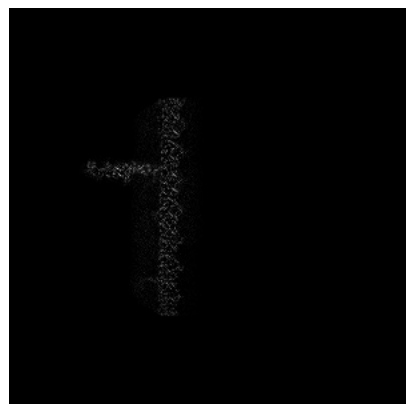


Z Index: 416

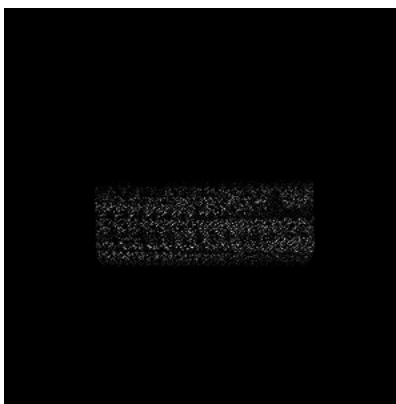
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

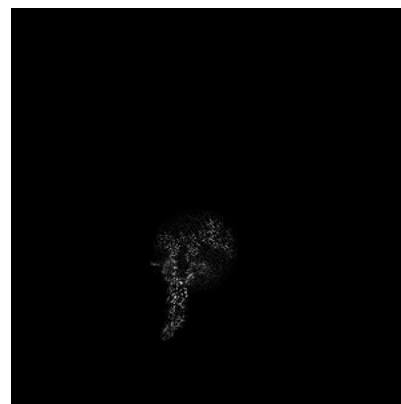
6.3.1 Primary map



X Index: 339



Y Index: 341

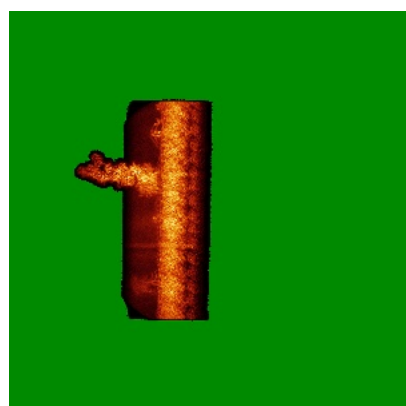


Z Index: 493

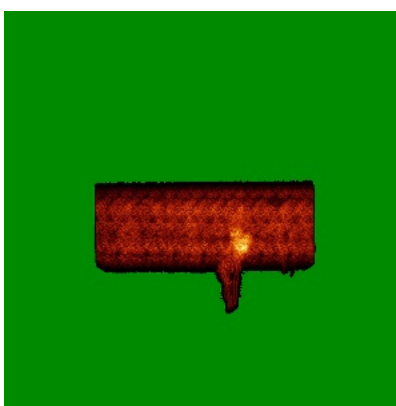
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

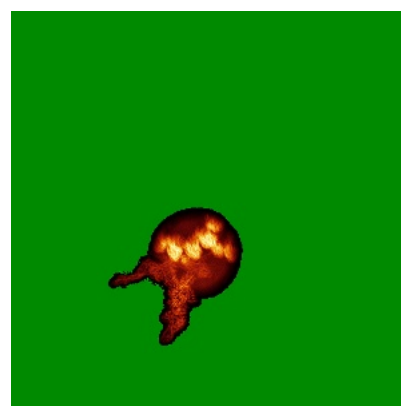
6.4.1 Primary map



X



Y

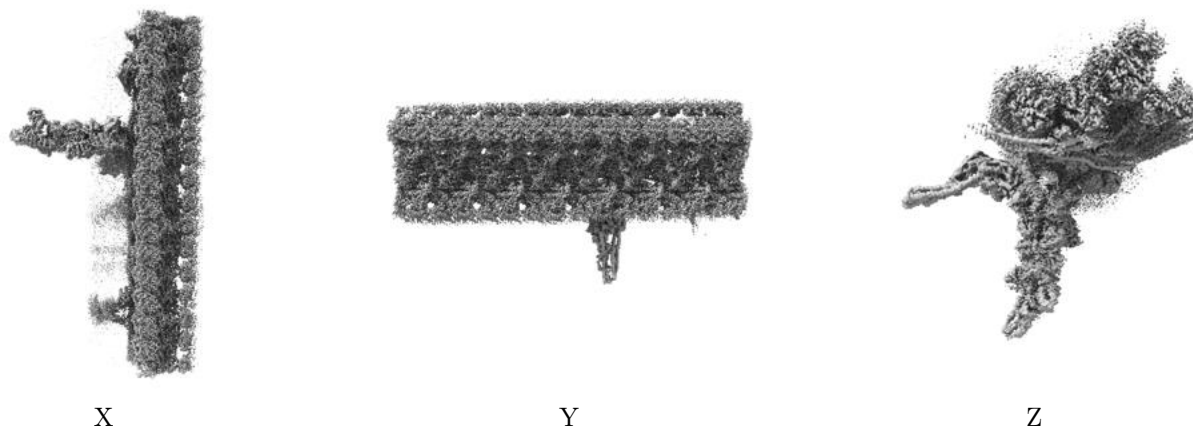


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

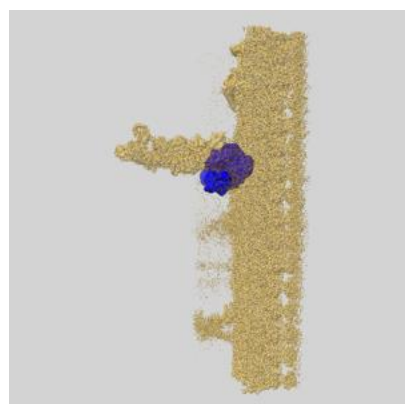
6.6 Mask visualisation [i](#)

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

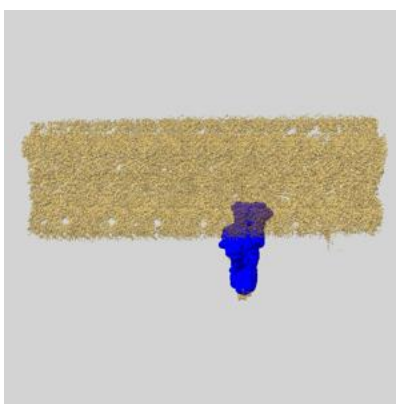
A mask typically either:

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

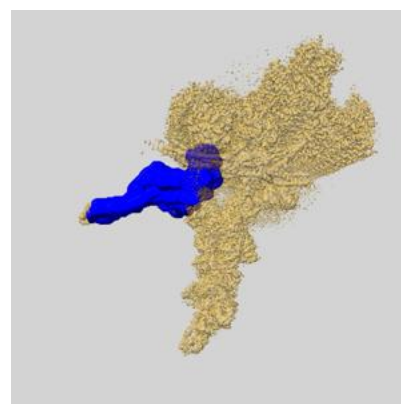
6.6.1 emd_22481_msk_2.map [i](#)



X

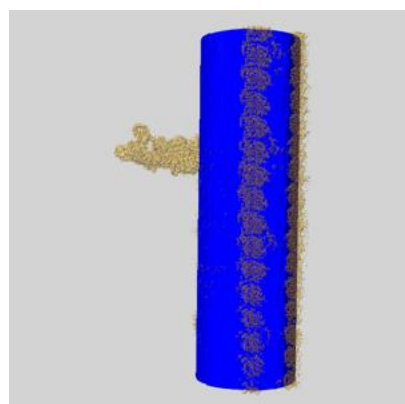


Y

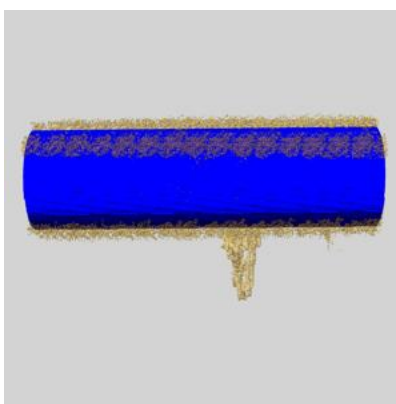


Z

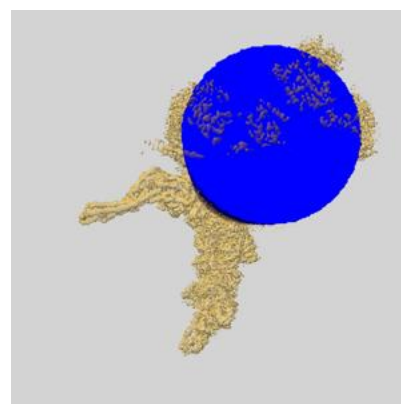
6.6.2 emd_22481_msk_3.map [i](#)



X

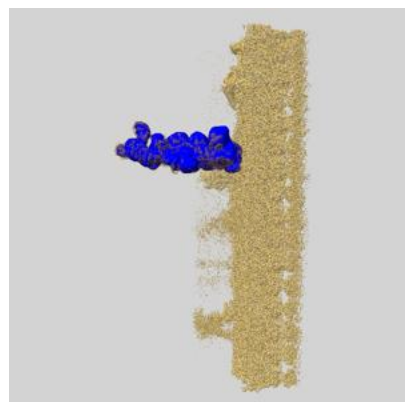


Y

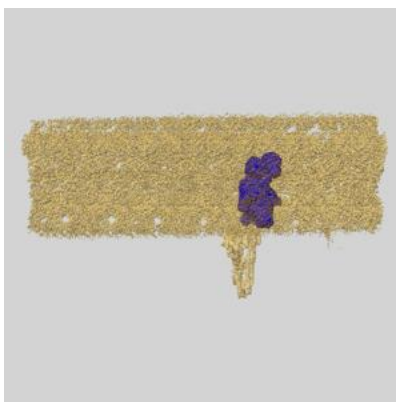


Z

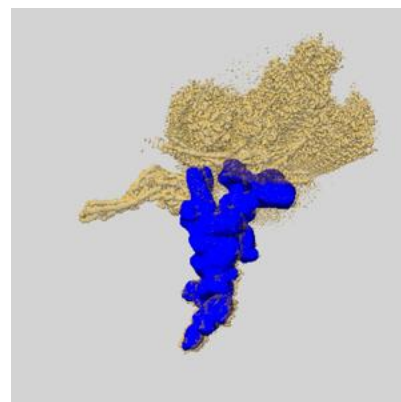
6.6.3 emd_22481_msk_4.map [i](#)



X

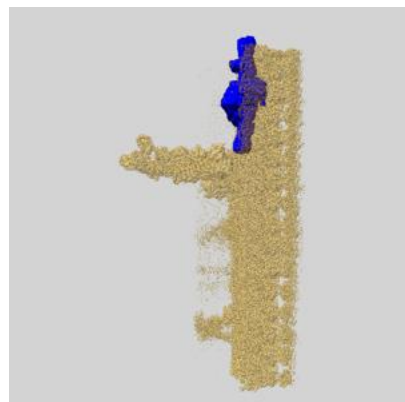


Y

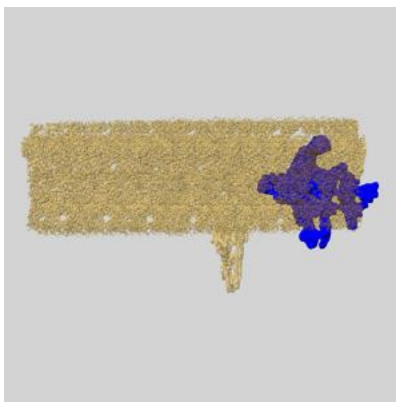


Z

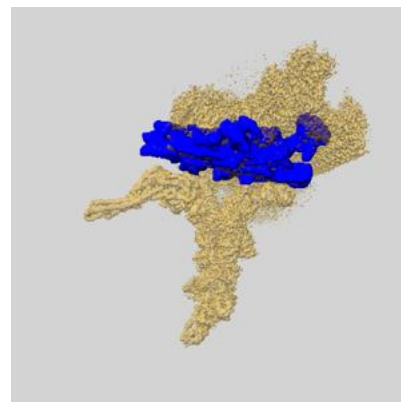
6.6.4 emd_22481_msk_1.map [i](#)



X



Y

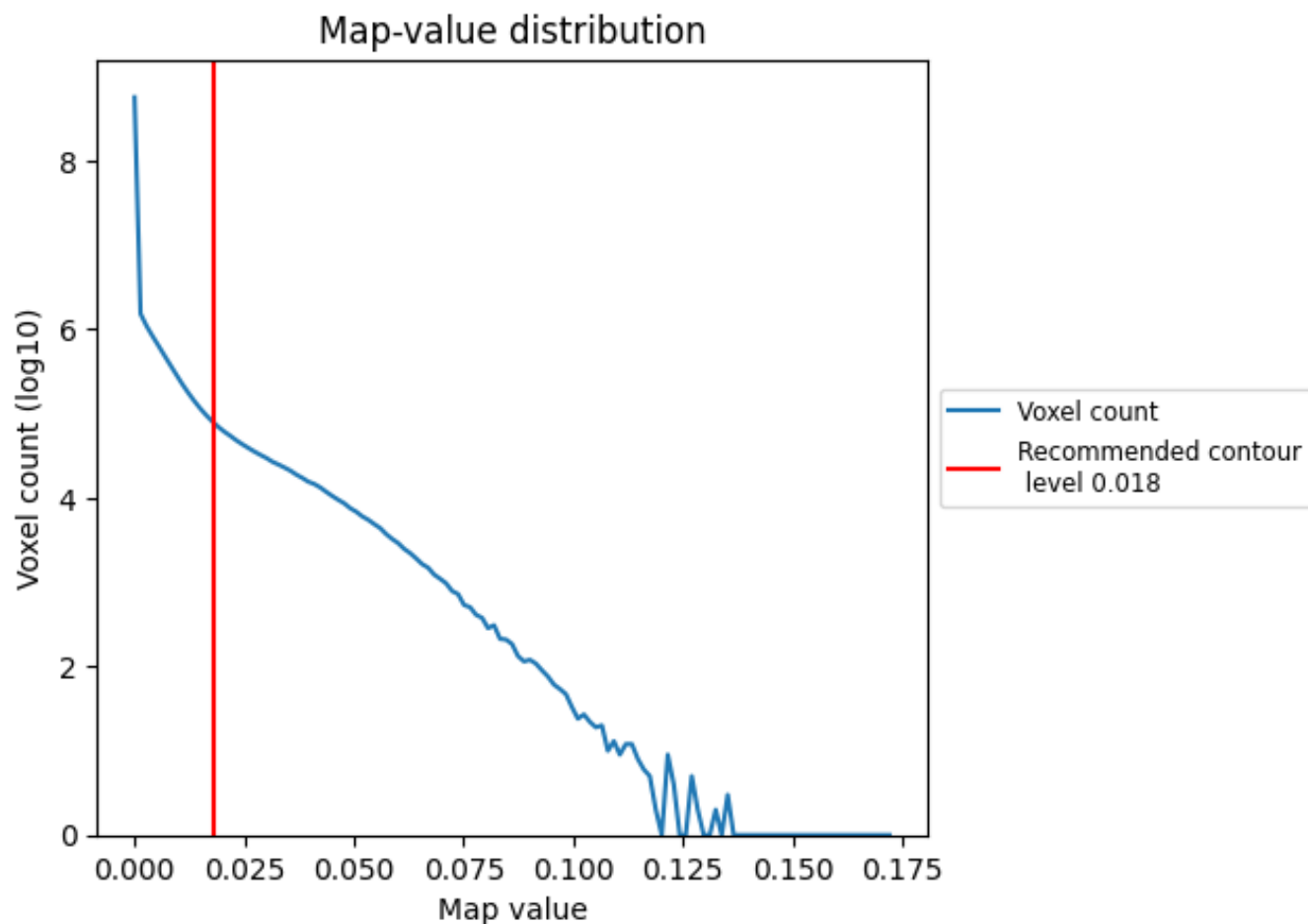


Z

7 Map analysis [i](#)

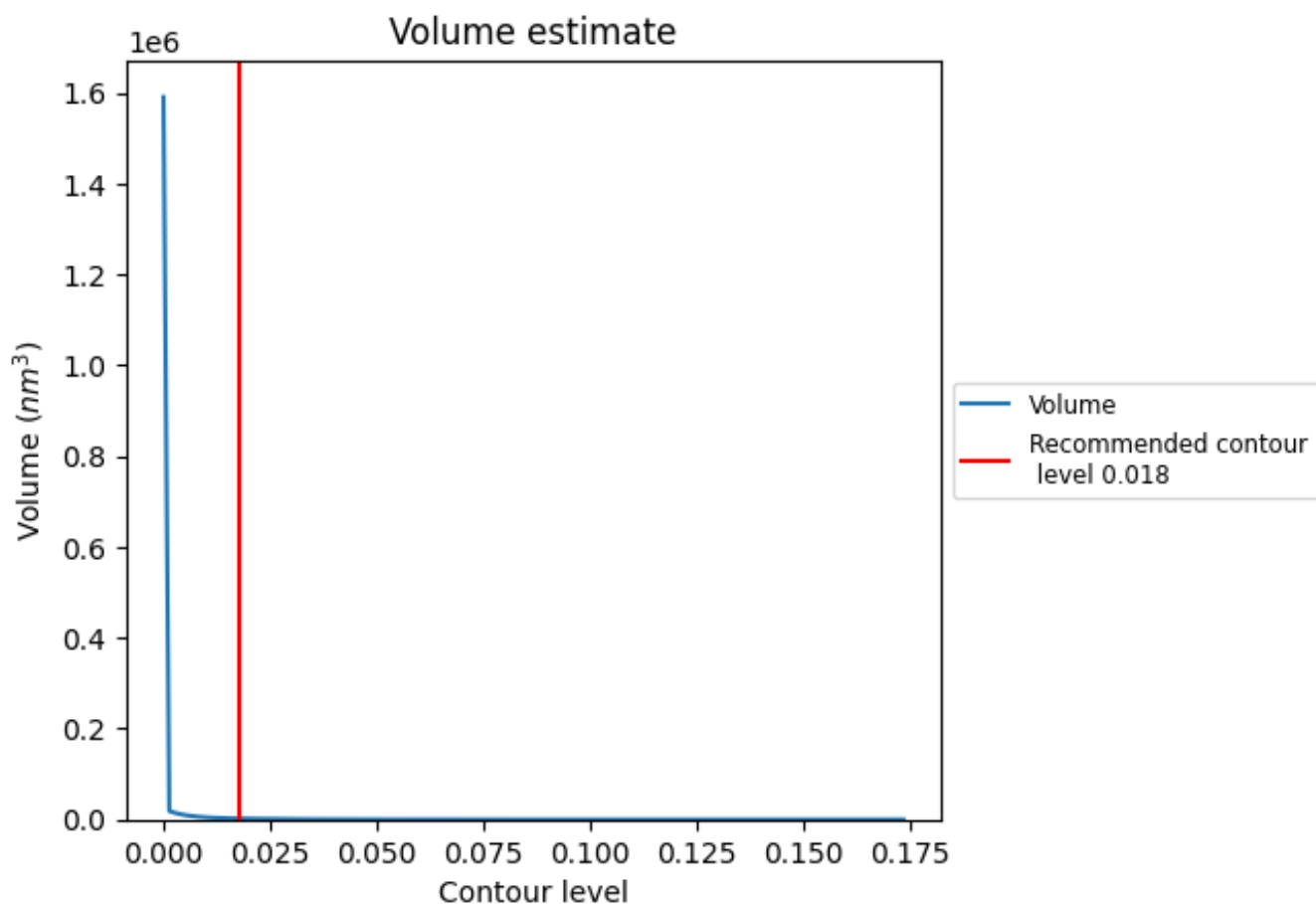
This section contains the results of statistical analysis of the map.

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.

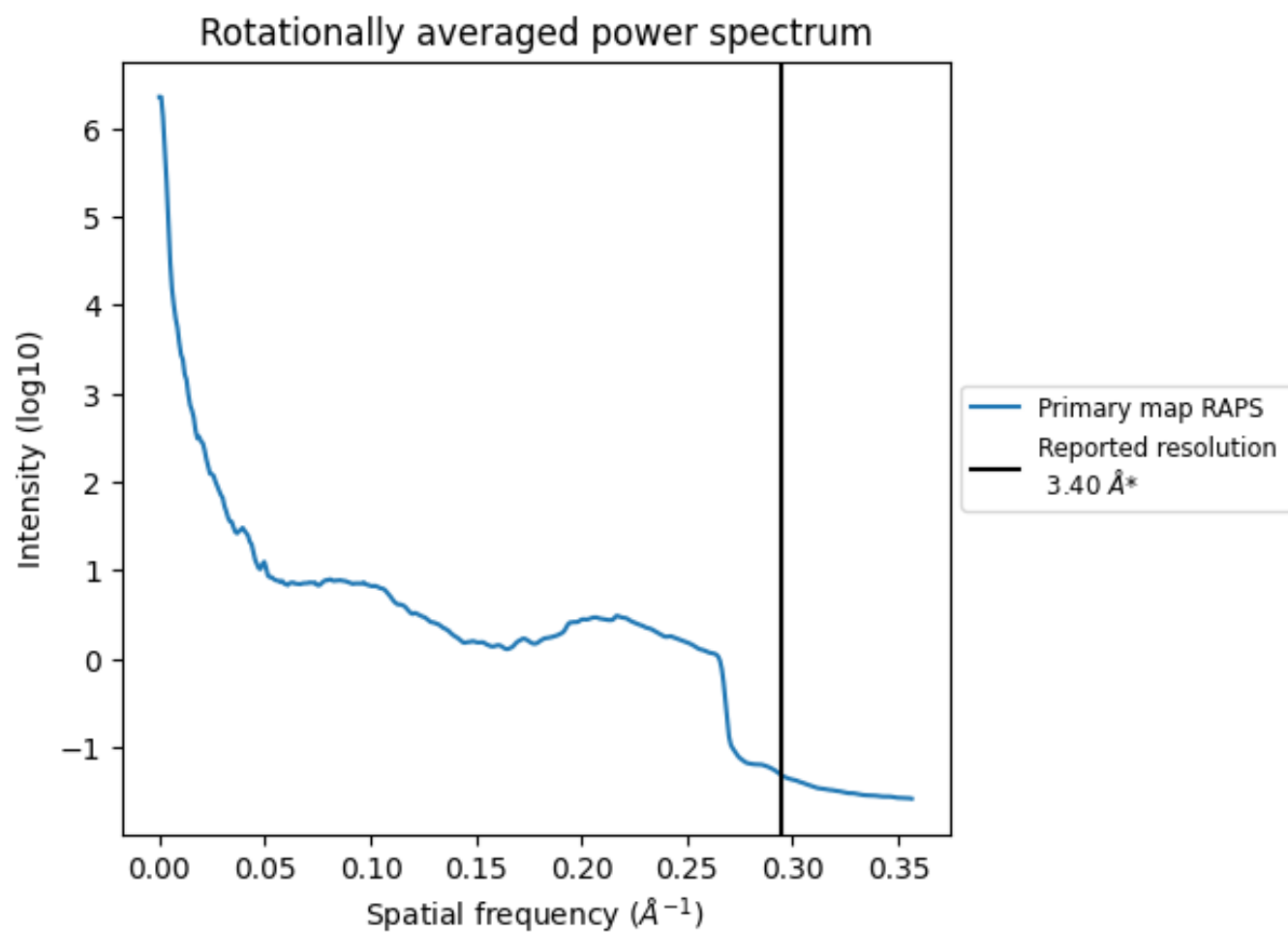
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2099 nm^3 ; this corresponds to an approximate mass of 1896 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 0.294 Å⁻¹

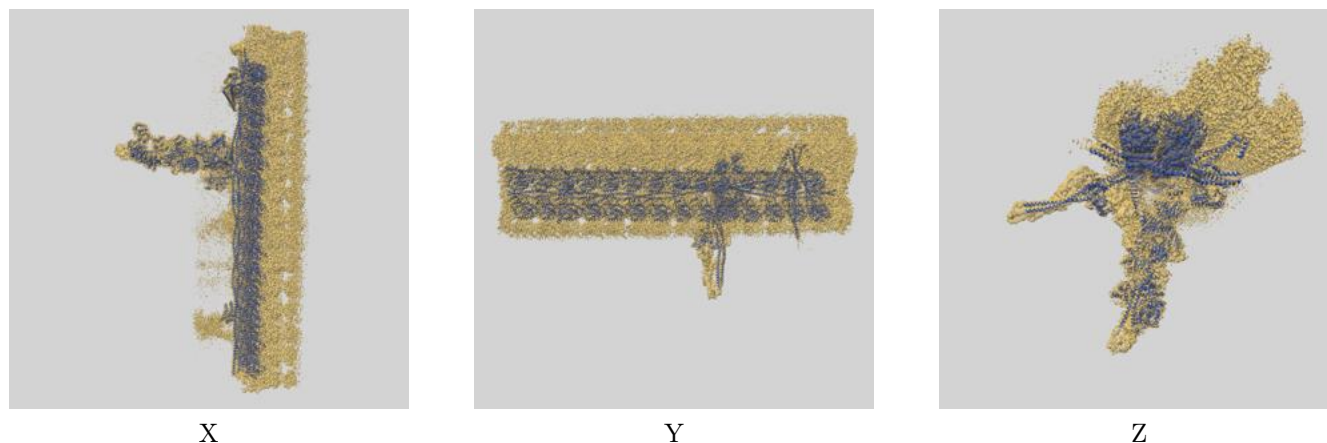
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

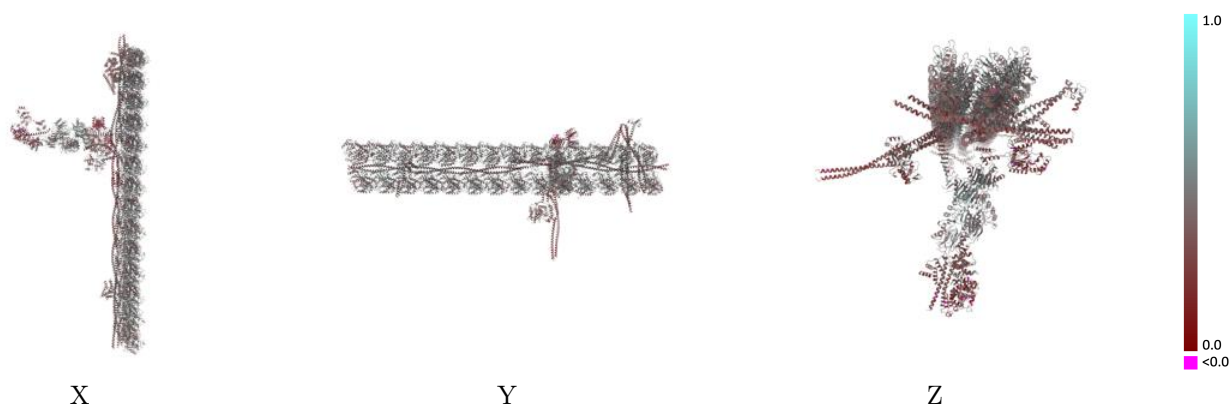
This section contains information regarding the fit between EMDB map EMD-22481 and PDB model 7JU4. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



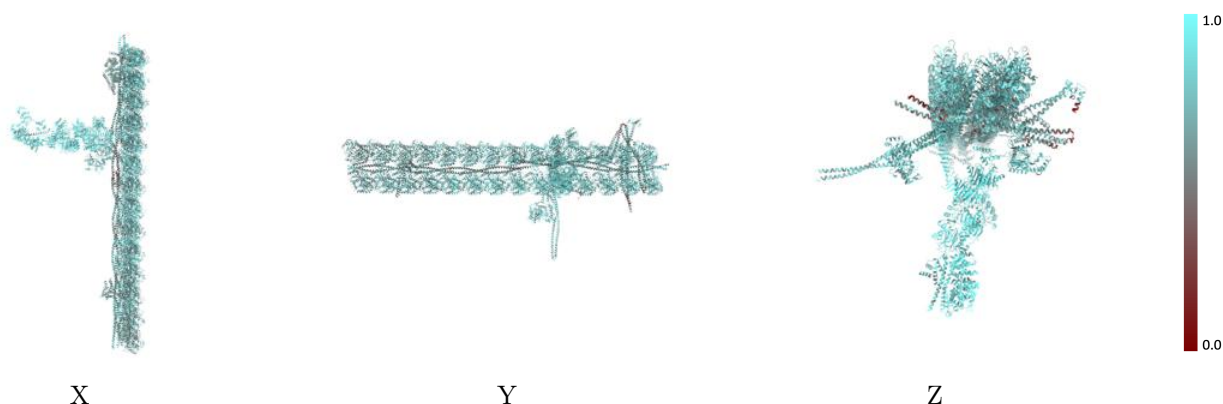
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



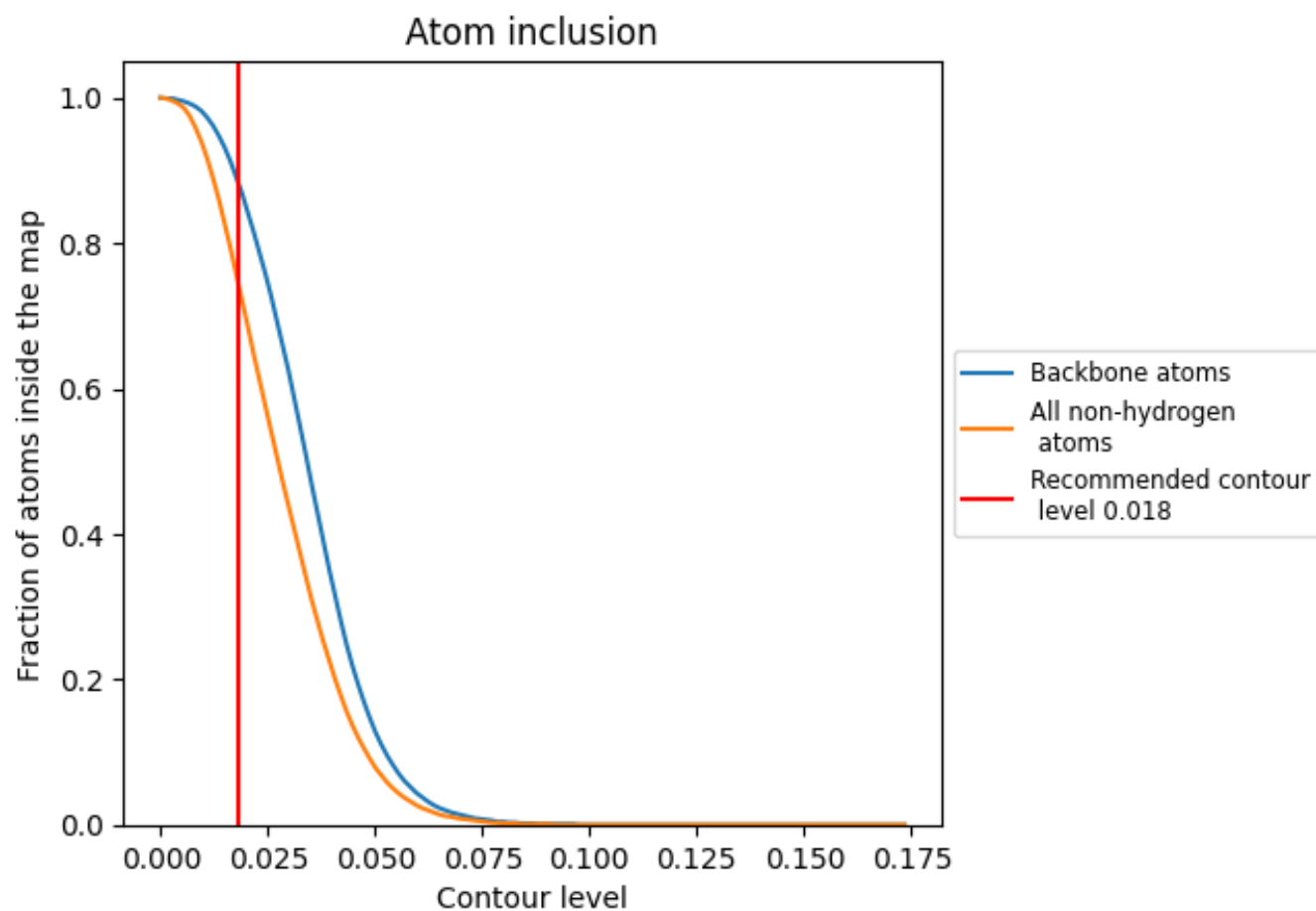
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 75% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7480	 0.4310
0	 0.5410	 0.3280
1	 0.6790	 0.3800
2	 0.6780	 0.3860
3	 0.9560	 0.4160
4	 0.5790	 0.3550
6	 0.7420	 0.4630
7	 0.7480	 0.4560
8	 0.7740	 0.4700
9	 0.7400	 0.4460
A	 0.6540	 0.3750
B	 0.6570	 0.3750
C	 0.6760	 0.4300
D	 0.7410	 0.4660
E	 0.8650	 0.3800
F	 0.8590	 0.3670
G	 0.7310	 0.4520
H	 0.7320	 0.4540
I	 0.7700	 0.4590
J	 0.7450	 0.4560
K	 0.7860	 0.4650
L	 0.7710	 0.4640
M	 0.7960	 0.3180
N	 0.8730	 0.3470
O	 0.7970	 0.4670
P	 0.7880	 0.4500
Q	 0.7640	 0.4640
R	 0.7560	 0.4540
S	 0.7640	 0.4510
T	 0.7310	 0.4300
U	 0.7900	 0.3230
V	 0.8940	 0.3330
W	 0.6210	 0.4210
X	 0.6740	 0.4510
Y	 0.6880	 0.4530



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Z	 0.6920	 0.4540
a	 0.9250	 0.4470
b	 0.9260	 0.4580
c	 0.8930	 0.4580
d	 0.9070	 0.4780
e	 0.9440	 0.4800
f	 0.9570	 0.4840
g	 0.9230	 0.4330
h	 0.9330	 0.4500
i	 0.7420	 0.4600
j	 0.7160	 0.4490
k	 0.7710	 0.4640
l	 0.8870	 0.4600
m	 0.8670	 0.3880
n	 0.8770	 0.3060
o	 0.8430	 0.2920
p	 0.7800	 0.2620
q	 0.7680	 0.2610
r	 0.7510	 0.2900
s	 0.6480	 0.3910
t	 0.7390	 0.4610
u	 0.7870	 0.3610
v	 0.7460	 0.3090
w	 0.7070	 0.2910
x	 0.6420	 0.3750
y	 0.7700	 0.4650
z	 0.7630	 0.4540