



wwPDB EM Validation Summary Report ⓘ

Dec 8, 2025 – 10:55 PM EST

PDB ID : 9YA3 / pdb_00009ya3
EMDB ID : EMD-72719
Title : Cryo-EM structure of the apical region of subpellicular microtubule (SPMT)
from Toxoplasma gondii (8-nm repeat)
Authors : Zeng, J.; Zhang, R.
Deposited on : 2025-09-15
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.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.47

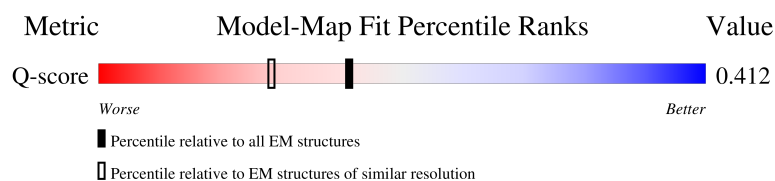
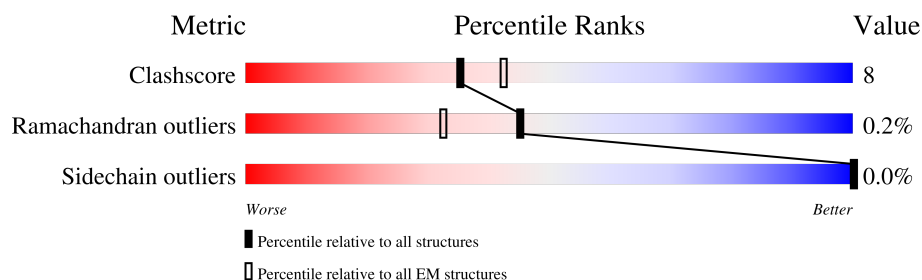
1 Overall quality at a glance

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.



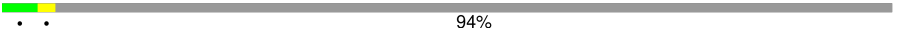

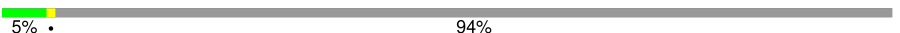


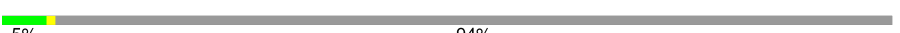









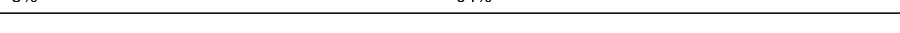
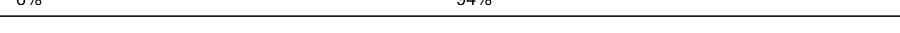
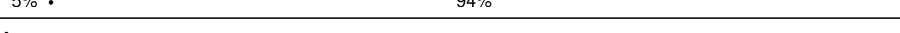
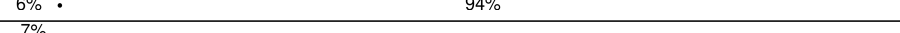






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	351	5% • 94%
1	1	351	5% • 94%
1	10	351	5% • 94%
1	11	351	5% • 94%

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Mol	Chain	Length	Quality of chain
1	12	351	 94%
1	13	351	 94%
1	14	351	 94%
1	15	351	 94%
1	16	351	 94%
1	17	351	 94%
1	18	351	 94%
1	19	351	 94%
1	2	351	 94%
1	22	351	 94%
1	23	351	 94%
1	3	351	 94%
1	4	351	 94%
1	5	351	 94%
1	6	351	 94%
1	7	351	 94%
1	8	351	 94%
1	9	351	 94%
2	A	583	 71%
2	B	583	 62%
2	C	583	 92%
3	A0	453	 76% 19% 6%
3	A2	453	 75% 20% 6%
3	A4	453	 83% 11% 6%
3	A6	453	 76% 19% 6%


























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Mol	Chain	Length	Quality of chain
3	A8	453	
3	B0	453	
3	B2	453	
3	B4	453	
3	B6	453	
3	B8	453	
3	C0	453	
3	C2	453	
3	C4	453	
3	C6	453	
3	C8	453	
3	D0	453	
3	D2	453	
3	D4	453	
3	D6	453	
3	D8	453	
3	E0	453	
3	E2	453	
3	E4	453	
3	E6	453	
3	E8	453	
3	F0	453	
4	A1	449	
4	A3	449	
4	A5	449	



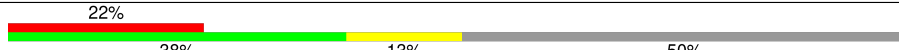
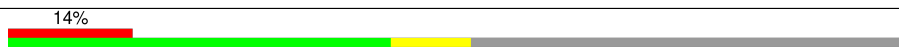
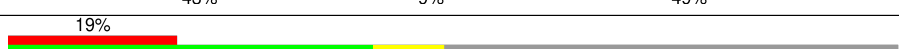
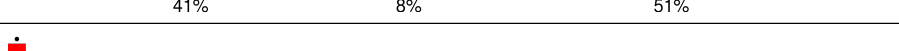
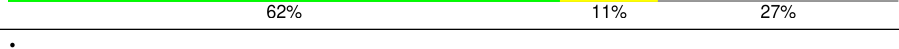





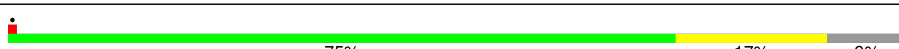


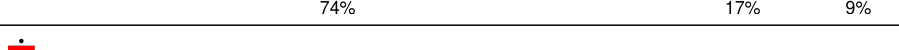








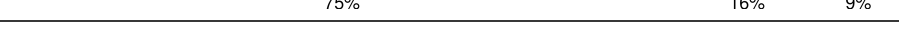
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Mol	Chain	Length	Quality of chain
4	A7	449	 73%21%5%
4	A9	449	 78%17%5%
4	B1	449	 77%18%5%
4	B3	449	 76%19%5%
4	B5	449	 77%18%5%
4	B7	449	 78%17%5%
4	B9	449	 75%20%5%
4	C1	449	 73%21%5%
4	C3	449	 67%27%5%
4	C5	449	 72%23%5%
4	C7	449	 78%16%5%
4	C9	449	 72%22%5%
4	D1	449	 73%21%5%
4	D3	449	 73%21%5%
4	D5	449	 78%17%5%
4	D7	449	 75%20%5%
4	D9	449	 79%16%5%
4	E1	449	 74%20%5%
4	E3	449	 77%17%5%
4	E5	449	 78%17%5%
4	E7	449	 75%20%5%
4	E9	449	 62%32%5%
4	F1	449	 74%21%5%
5	E	336	 23%74%3%
5	F	336	 24%74%2%

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Mol	Chain	Length	Quality of chain
5	G	336	
6	H	446	
6	I	446	
6	J	446	
6	K	446	
7	a	220	
7	b	220	
7	c	220	
7	d	220	
7	e	220	
7	f	220	
7	g	220	
7	h	220	
7	i	220	
7	j	220	
7	m	220	
7	n	220	
7	o	220	
7	p	220	
7	q	220	
7	r	220	
7	s	220	
7	t	220	
7	u	220	
7	v	220	

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Mol	Chain	Length	Quality of chain
7	w	220	<div><div><div></div><div></div><div></div></div><div>73%18%9%</div></div>
7	x	220	<div><div><div></div><div></div><div></div></div><div>77%14%9%</div></div>
8	k	189	<div><div><div></div><div></div><div></div></div><div>53%19%26%</div></div>
8	l	189	<div><div><div></div><div></div><div></div></div><div>5%55%17%26%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 228257 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 Microtubule associated protein SPM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	1	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	10	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	11	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	12	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	13	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	14	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	15	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	16	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	17	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	18	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	19	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	2	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	22	20	Total	C	N	O	S	0	0
			160	105	26	28	1		
1	23	20	Total	C	N	O	S	0	0
			160	105	26	28	1		
1	3	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	4	22	Total	C	N	O	S	0	0
			174	114	28	31	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	5	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	6	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	7	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	8	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	9	22	Total	C	N	O	S	0	0
			174	114	28	31	1		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	93	ARG	PRO	conflict	UNP A0A7J6K285
1	93	ARG	PRO	conflict	UNP A0A7J6K285
10	93	ARG	PRO	conflict	UNP A0A7J6K285
11	93	ARG	PRO	conflict	UNP A0A7J6K285
12	93	ARG	PRO	conflict	UNP A0A7J6K285
13	93	ARG	PRO	conflict	UNP A0A7J6K285
14	93	ARG	PRO	conflict	UNP A0A7J6K285
15	93	ARG	PRO	conflict	UNP A0A7J6K285
16	93	ARG	PRO	conflict	UNP A0A7J6K285
17	93	ARG	PRO	conflict	UNP A0A7J6K285
18	93	ARG	PRO	conflict	UNP A0A7J6K285
19	93	ARG	PRO	conflict	UNP A0A7J6K285
2	93	ARG	PRO	conflict	UNP A0A7J6K285
22	93	ARG	PRO	conflict	UNP A0A7J6K285
23	93	ARG	PRO	conflict	UNP A0A7J6K285
3	93	ARG	PRO	conflict	UNP A0A7J6K285
4	93	ARG	PRO	conflict	UNP A0A7J6K285
5	93	ARG	PRO	conflict	UNP A0A7J6K285
6	93	ARG	PRO	conflict	UNP A0A7J6K285
7	93	ARG	PRO	conflict	UNP A0A7J6K285
8	93	ARG	PRO	conflict	UNP A0A7J6K285
9	93	ARG	PRO	conflict	UNP A0A7J6K285

- Molecule 2 is a protein called TLAP3 (apical cap protein AC5), TGME49_235380.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	169	Total	C	N	O	S	0	0
			1338	829	252	255	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	220	Total	C	N	O	S	0	0
			1744	1084	329	329	2		
2	C	49	Total	C	N	O		0	0
			384	240	74	70			

- Molecule 3 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	A2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	A4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	A6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	A8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	B0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	B2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	B4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	B6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	B8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	C0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	C2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	C4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	C6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	C8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	D0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
3	D2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	D4	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	D6	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	D8	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	E0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	E2	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	E4	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	E6	428	Total 3325	C 2105	N 569	O 625	S 26	0	0
3	E8	428	Total 3319	C 2102	N 566	O 625	S 26	0	0
3	F0	428	Total 3325	C 2105	N 569	O 625	S 26	0	0

- Molecule 4 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	A3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	A5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	A7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	A9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	B1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	B3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	B5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	B7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	B9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	C1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	C3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	C5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	C7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	C9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	D1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	D3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	D5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	D7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	D9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	E1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	E3	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	E5	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	E7	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	E9	426	Total 3331	C 2094	N 569	O 641	S 27	0	0
4	F1	426	Total 3331	C 2094	N 569	O 641	S 27	0	0

- Molecule 5 is a protein called TLAP4 (thioredoxin-like associated protein), TGME49_201760.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	89	Total 740	C 459	N 141	O 139	S 1	0	0
5	F	89	Total 740	C 459	N 141	O 139	S 1	0	0
5	G	67	Total 558	C 347	N 103	O 108		0	0

- Molecule 6 is a protein called TLAP2 (thioredoxin-like associated protein), TGME49_232130.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	223	Total	C	N	O	S	0	0
			1817	1173	322	319	3		
6	I	224	Total	C	N	O	S	0	0
			1817	1170	323	321	3		
6	J	229	Total	C	N	O	S	0	0
			1870	1202	334	331	3		
6	K	220	Total	C	N	O	S	0	0
			1795	1158	319	315	3		

- Molecule 7 is a protein called TRXL1, TGME49_232410.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	161	Total	C	N	O	S	0	0
			1289	824	224	236	5		
7	b	161	Total	C	N	O	S	0	0
			1289	824	224	236	5		
7	c	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	d	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	e	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	f	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	g	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	h	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	i	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	j	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	m	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	n	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	o	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	p	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	q	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	r	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	s	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	t	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	u	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	v	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	w	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
7	x	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		

- Molecule 8 is a protein called TRXL2, TGME49_225790.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	139	Total	C	N	O	S	0	0
			1140	738	203	195	4		
8	l	139	Total	C	N	O	S	0	0
			1140	738	203	195	4		

There are 46 discrepancies between the modelled and reference sequences:

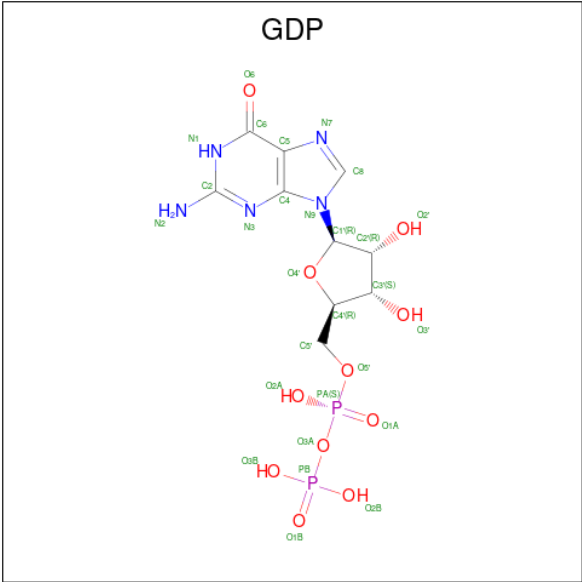
Chain	Residue	Modelled	Actual	Comment	Reference
k	167	SER	-	expression tag	UNP A0A7J6K232
k	168	ALA	-	expression tag	UNP A0A7J6K232
k	169	GLN	-	expression tag	UNP A0A7J6K232
k	170	ARG	-	expression tag	UNP A0A7J6K232
k	171	LEU	-	expression tag	UNP A0A7J6K232
k	172	ARG	-	expression tag	UNP A0A7J6K232
k	173	THR	-	expression tag	UNP A0A7J6K232
k	174	LEU	-	expression tag	UNP A0A7J6K232
k	175	ASN	-	expression tag	UNP A0A7J6K232
k	176	ASP	-	expression tag	UNP A0A7J6K232
k	177	ALA	-	expression tag	UNP A0A7J6K232
k	178	THR	-	expression tag	UNP A0A7J6K232
k	179	ASP	-	expression tag	UNP A0A7J6K232
k	180	PRO	-	expression tag	UNP A0A7J6K232
k	181	TRP	-	expression tag	UNP A0A7J6K232
k	182	LYS	-	expression tag	UNP A0A7J6K232

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Chain	Residue	Modelled	Actual	Comment	Reference
k	183	LYS	-	expression tag	UNP A0A7J6K232
k	184	ARG	-	expression tag	UNP A0A7J6K232
k	185	LEU	-	expression tag	UNP A0A7J6K232
k	186	PRO	-	expression tag	UNP A0A7J6K232
k	187	GLN	-	expression tag	UNP A0A7J6K232
k	188	ASN	-	expression tag	UNP A0A7J6K232
k	189	VAL	-	expression tag	UNP A0A7J6K232
l	167	SER	-	expression tag	UNP A0A7J6K232
l	168	ALA	-	expression tag	UNP A0A7J6K232
l	169	GLN	-	expression tag	UNP A0A7J6K232
l	170	ARG	-	expression tag	UNP A0A7J6K232
l	171	LEU	-	expression tag	UNP A0A7J6K232
l	172	ARG	-	expression tag	UNP A0A7J6K232
l	173	THR	-	expression tag	UNP A0A7J6K232
l	174	LEU	-	expression tag	UNP A0A7J6K232
l	175	ASN	-	expression tag	UNP A0A7J6K232
l	176	ASP	-	expression tag	UNP A0A7J6K232
l	177	ALA	-	expression tag	UNP A0A7J6K232
l	178	THR	-	expression tag	UNP A0A7J6K232
l	179	ASP	-	expression tag	UNP A0A7J6K232
l	180	PRO	-	expression tag	UNP A0A7J6K232
l	181	TRP	-	expression tag	UNP A0A7J6K232
l	182	LYS	-	expression tag	UNP A0A7J6K232
l	183	LYS	-	expression tag	UNP A0A7J6K232
l	184	ARG	-	expression tag	UNP A0A7J6K232
l	185	LEU	-	expression tag	UNP A0A7J6K232
l	186	PRO	-	expression tag	UNP A0A7J6K232
l	187	GLN	-	expression tag	UNP A0A7J6K232
l	188	ASN	-	expression tag	UNP A0A7J6K232
l	189	VAL	-	expression tag	UNP A0A7J6K232

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



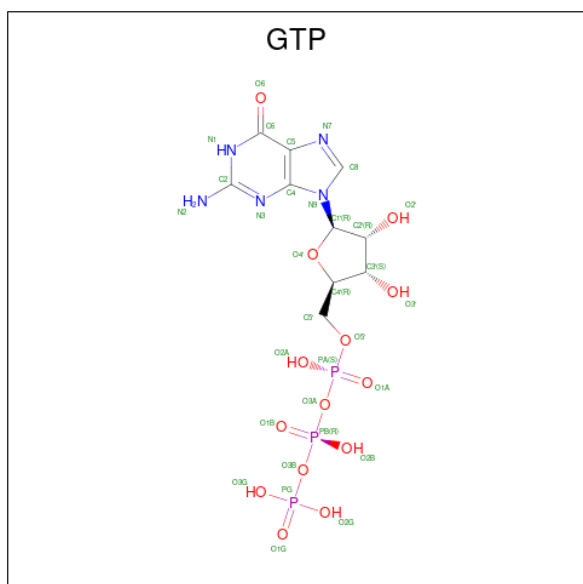
Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A1	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A3	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A5	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	A7	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	B3	1	Total	C	N	O	P	0
			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	
9	B9	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	C1	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	C3	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	C5	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	C7	1	Total	C	N	O	P	0
			28	10	5	11	2	

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Mol	Chain	Residues	Atoms					AltConf
9	C9	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	D1	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	D3	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	D5	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	D7	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	D9	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	E1	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	E3	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	E5	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	E7	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	E9	1	Total	C	N	O	P	0
			28	10	5	11	2	
9	F1	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 10 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	A0	1	Total 32	C 10	N 5	O 14	P 3	0
10	A2	1	Total 32	C 10	N 5	O 14	P 3	0
10	A4	1	Total 32	C 10	N 5	O 14	P 3	0
10	A6	1	Total 32	C 10	N 5	O 14	P 3	0
10	A8	1	Total 32	C 10	N 5	O 14	P 3	0
10	B0	1	Total 32	C 10	N 5	O 14	P 3	0
10	B2	1	Total 32	C 10	N 5	O 14	P 3	0
10	B4	1	Total 32	C 10	N 5	O 14	P 3	0
10	B6	1	Total 32	C 10	N 5	O 14	P 3	0
10	B8	1	Total 32	C 10	N 5	O 14	P 3	0
10	C0	1	Total 32	C 10	N 5	O 14	P 3	0
10	C2	1	Total 32	C 10	N 5	O 14	P 3	0
10	C4	1	Total 32	C 10	N 5	O 14	P 3	0
10	C6	1	Total 32	C 10	N 5	O 14	P 3	0
10	C8	1	Total 32	C 10	N 5	O 14	P 3	0
10	D0	1	Total 32	C 10	N 5	O 14	P 3	0
10	D2	1	Total 32	C 10	N 5	O 14	P 3	0
10	D4	1	Total 32	C 10	N 5	O 14	P 3	0
10	D6	1	Total 32	C 10	N 5	O 14	P 3	0
10	D8	1	Total 32	C 10	N 5	O 14	P 3	0
10	E0	1	Total 32	C 10	N 5	O 14	P 3	0
10	E2	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
10	E4	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	E6	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	E8	1	Total	C	N	O	P	0
			32	10	5	14	3	
10	F0	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	A0	1	Total	Mg	0
			1	1	
11	A3	1	Total	Mg	0
			1	1	
11	A4	1	Total	Mg	0
			1	1	
11	A6	1	Total	Mg	0
			1	1	
11	A8	1	Total	Mg	0
			1	1	
11	B0	1	Total	Mg	0
			1	1	
11	B2	1	Total	Mg	0
			1	1	
11	B4	1	Total	Mg	0
			1	1	
11	B6	1	Total	Mg	0
			1	1	
11	B8	1	Total	Mg	0
			1	1	
11	C0	1	Total	Mg	0
			1	1	
11	C2	1	Total	Mg	0
			1	1	
11	C4	1	Total	Mg	0
			1	1	
11	C6	1	Total	Mg	0
			1	1	
11	C8	1	Total	Mg	0
			1	1	

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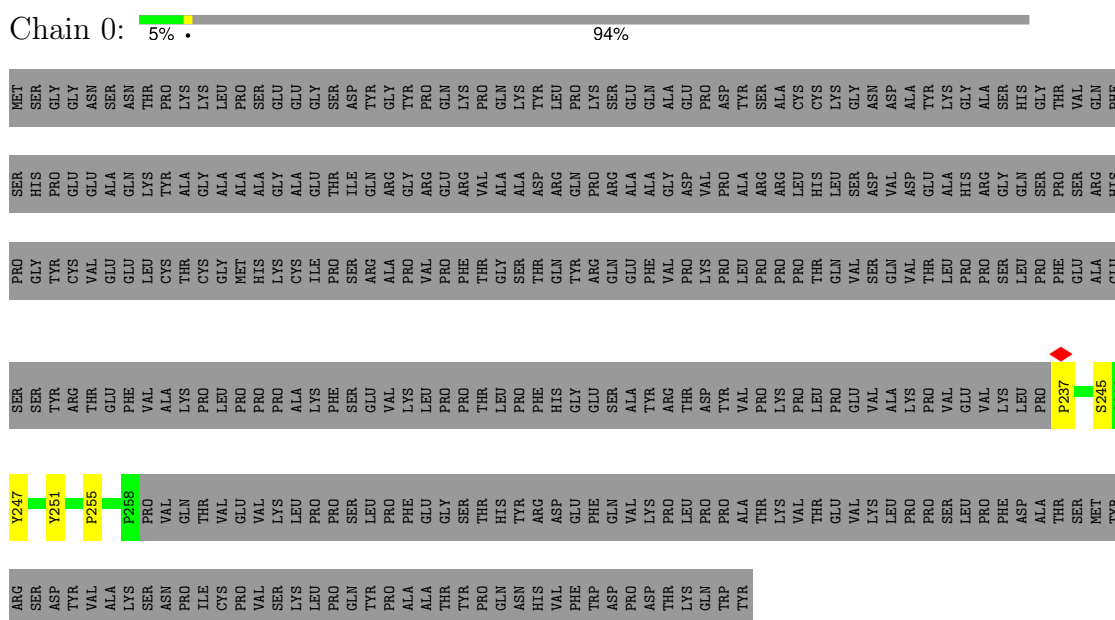
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Mol	Chain	Residues	Atoms		AltConf
11	D0	1	Total 1	Mg 1	0
11	D2	1	Total 1	Mg 1	0
11	D4	1	Total 1	Mg 1	0
11	D6	1	Total 1	Mg 1	0
11	D8	1	Total 1	Mg 1	0
11	E0	1	Total 1	Mg 1	0
11	E2	1	Total 1	Mg 1	0
11	E4	1	Total 1	Mg 1	0
11	E6	1	Total 1	Mg 1	0
11	E8	1	Total 1	Mg 1	0
11	F0	1	Total 1	Mg 1	0

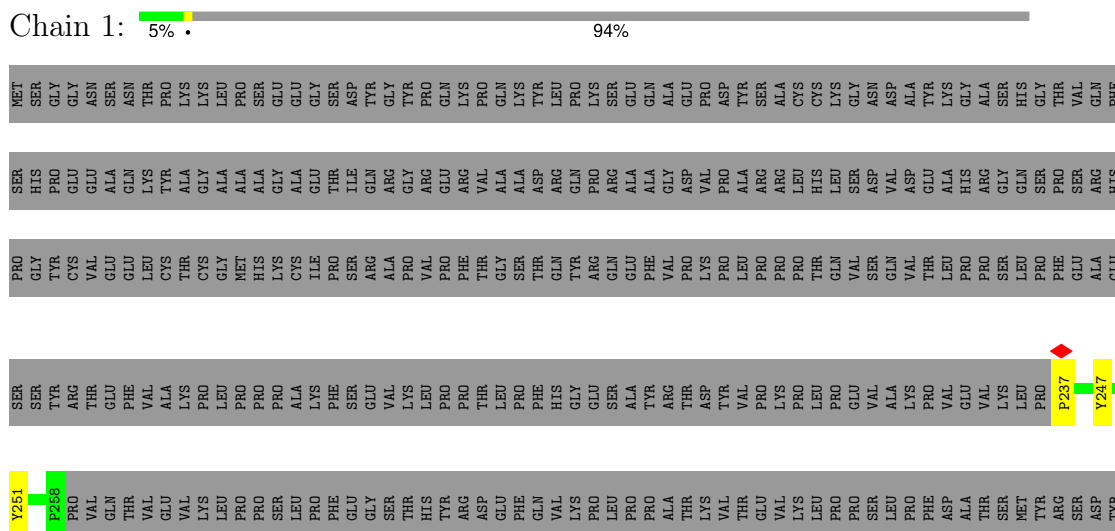
3 Residue-property plots

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: Microtubule associated protein SPM1



• Molecule 1: Microtubule associated protein SPM1



[illegible]

- Molecule 1: Microtubule associated protein SPM1

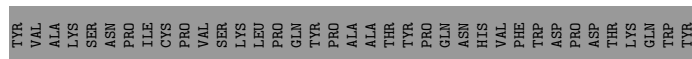
Chain 13:  6% 94%

[illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 14: 5% . 94%

[illegible]



Chain 18:  5% 94%



Chain 19: 5% 94%



[illegible][illegible][illegible]

LYS	SER	ASN	PRO	ILE	CYS	PRO	VAL	SER	LYS	LEU	PRO	GLN	TYR	PRO	ALA	ALA	THR	TYR	PRO	GLN	ASN	HIS	VAL	PHE	TRP	ASP	PRO	ASP	THR	LYS	GLN	TRP	TYR
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- Molecule 1: Microtubule associated protein SPM1

Chain 3: 5% • 94%

PRO	GLY	TYR	CYS	VAL	GLU	GLU	LEU	CYS	THR	THR	GLY	MET	HIS	LYS	CYS	ILE	PRO	ARG	ARG	ALA	VAL	PRO	PRO	PHE	THR	GLY	THR	SER	SER	GLN	TYR	ARG	GLN	GLU	PHE	VAL	PRO	PRO	LYS	PRO	PRO	LEU	PRO	PRO	THR	GLN	GLN	SER	SER	GLN	VAL	THR	LEU	PRO	PRO	PRO	THR	ALA	THR
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Y247 **Y251** **Y258**

ASP	TYR	VAL	ALA	LYS	SER	ASN	PRO	ILE	CYS	PRO	VAL	SER	LYS	LEU	PRO	GLN	TYR	PRO	ALA	ALA	THR	TYR	PRO	GLN	ASN	HIS	VAL	PHE	TRP	ASP	PRO	ASP	THR	LYS	GLN	TRP	TYR
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- Molecule 1: Microtubule associated protein SPM1

Chain 4: 5% • 94%

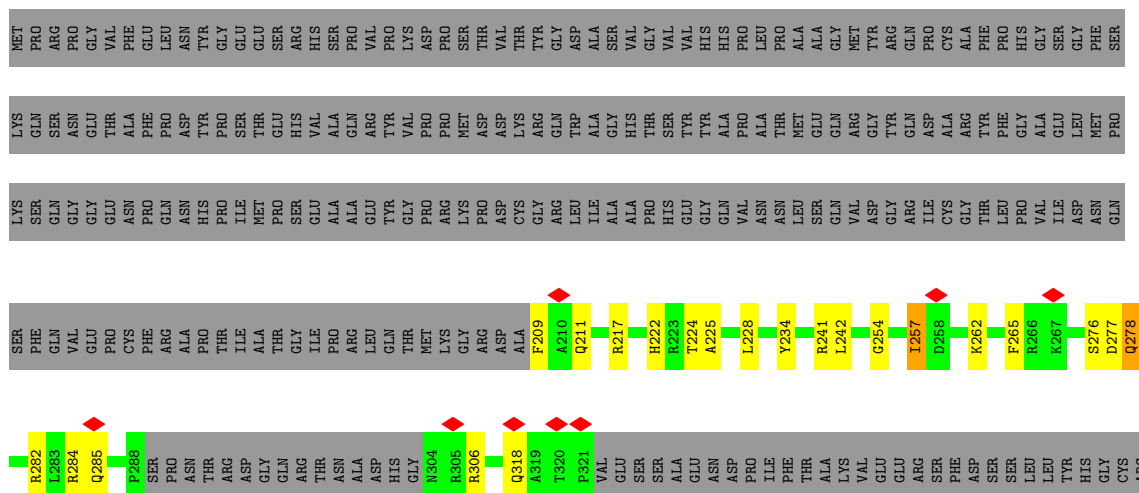
PRO	GLY	TYR	CYS	VAL	GLU	GLU	LEU	CYS	THR	CYS	GLY	MET	HIS	LYS	CYS	ILE	PRO	ARG	ARG	ALA	PRO	PRO	VAL	GLN	THR	GLY	THR	SER	SER	THR	GLN	TYR	ARG	GLN	GLU	PHE	VAL	PRO	PRO	LYS	PRO	LEU	LEU	PRO	PRO	PRO	PRO	THR	GLN	VAL	GLN	SER	SER	GLN	VAL	THR	LEU	THR	PRO	PRO	PRO	SER	PRO	PRO	PHE	GLU	GLU	ALA	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Y247 K254 L255 P257 P258 P259 VAL GLN VAL THR THR VAL VAL VAL LYS LEU LEU PRO PRO SER SER PRO PRO PHE PHE GLY GLU SER SER THR HIS TYR ARG ASP PHE PHE GLN VAL LYS LYS PRO LEU LEU PRO PRO PRO PRO ALA ALA THR LYS VAL VAL THR GLU THR LYS LEU LEU PRO PRO PRO ASP ASP ALA THR SER MET ASP

ARG	SER	ASP	TYR	VAL	ALA	LYS	SER	ASN	PRO	ILE	CYS	PRO	CYS	VAL	SER	LYS	LEU	PRO	GLN	TYR	PRO	ALA	ALA	THR	TYR	PRO	GLN	ASN	HIS	VAL	PHE	TRP	ASP	PRO	ASP	THR	LYS	GLN	TRP	TYR
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- Molecule 1: Microtubule associated protein SPM1

- Chain A: 7% 23% 6% 64%



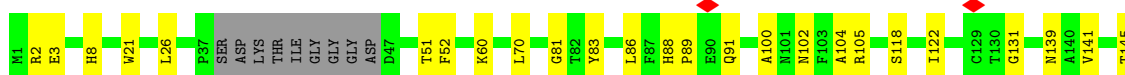
- Molecule 2: TLAP3 (apical cap protein AC5), TGME49 235380

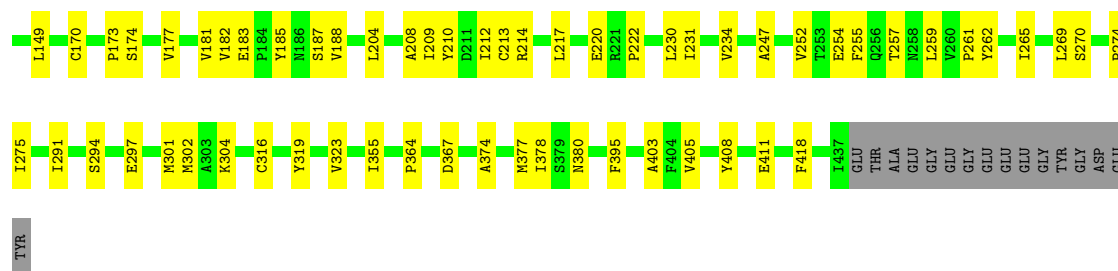
Chain C:  7% 92%



- Molecule 3: Tubulin alpha chain

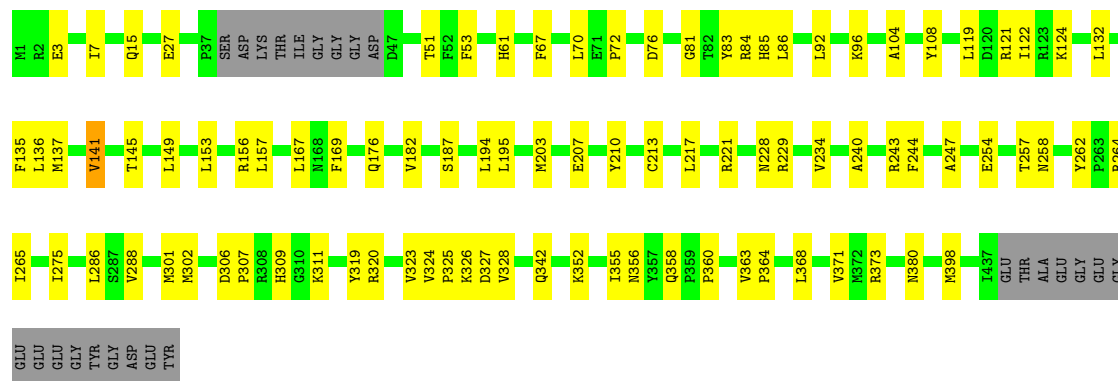
Chain A0: 76% 19% 6%





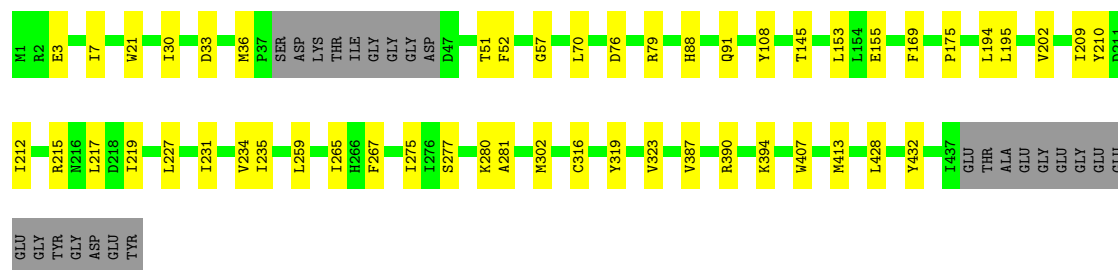
• Molecule 3: Tubulin alpha chain

Chain A2: 75% 20% 6%



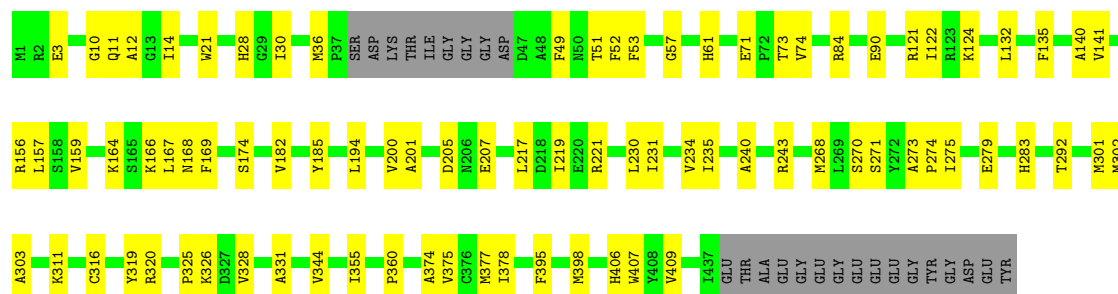
• Molecule 3: Tubulin alpha chain

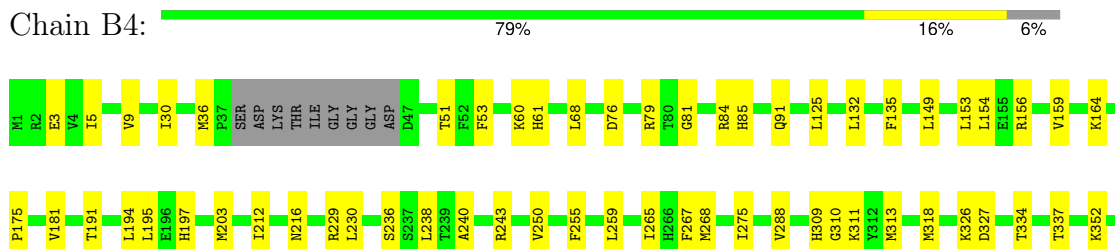
Chain A4: 83% 11% 6%



• Molecule 3: Tubulin alpha chain

Chain A6: 76% 19% 6%

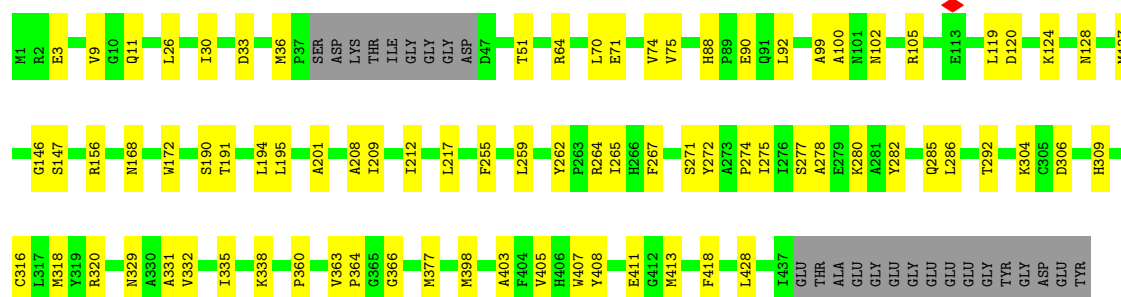






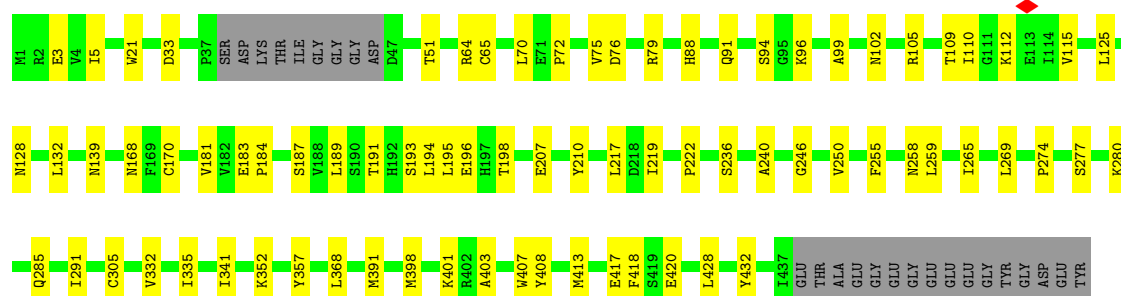
• Molecule 3: Tubulin alpha chain

Chain B6: 77% 18% 6%



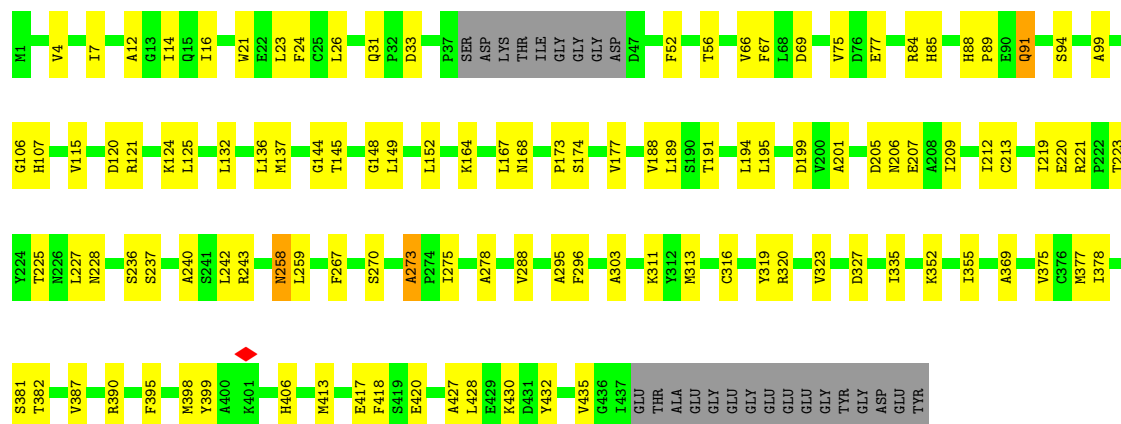
• Molecule 3: Tubulin alpha chain

Chain B8: 77% 17% 6%

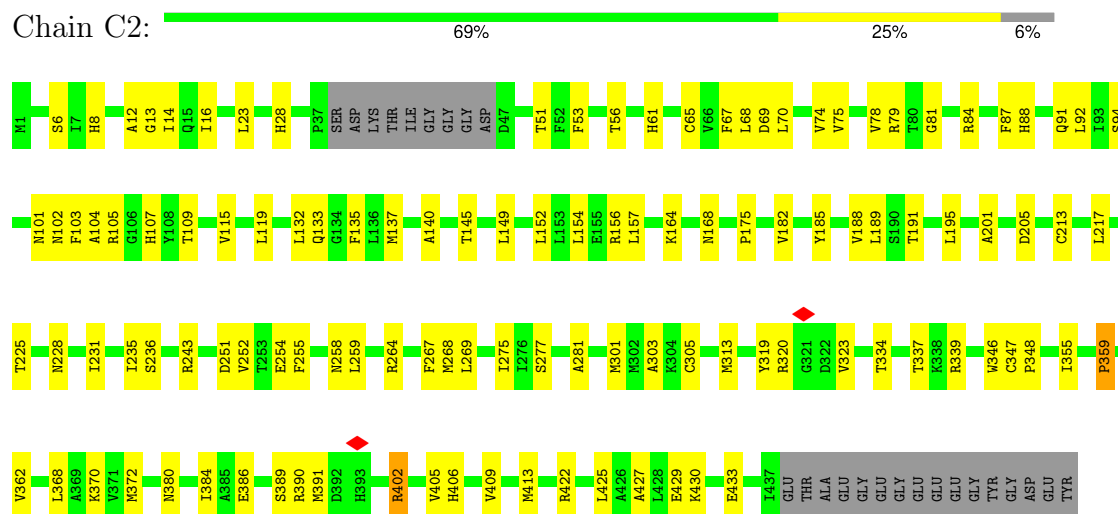


• Molecule 3: Tubulin alpha chain

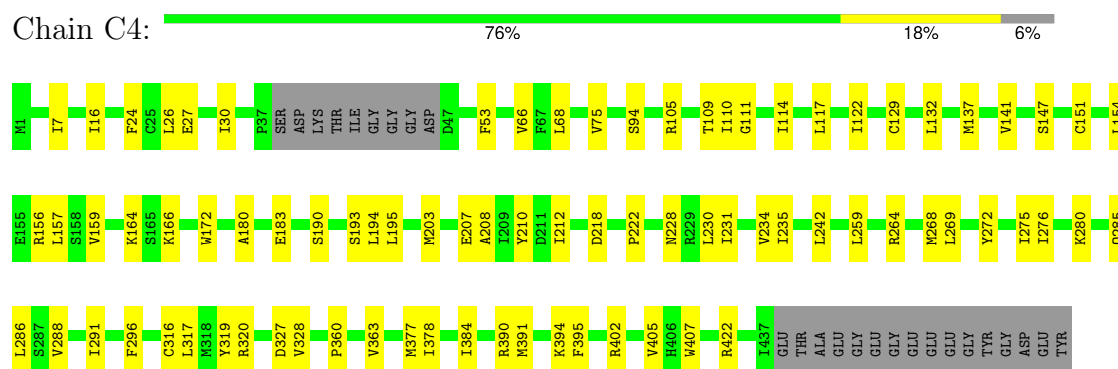
Chain C0: 70% 24% 6%



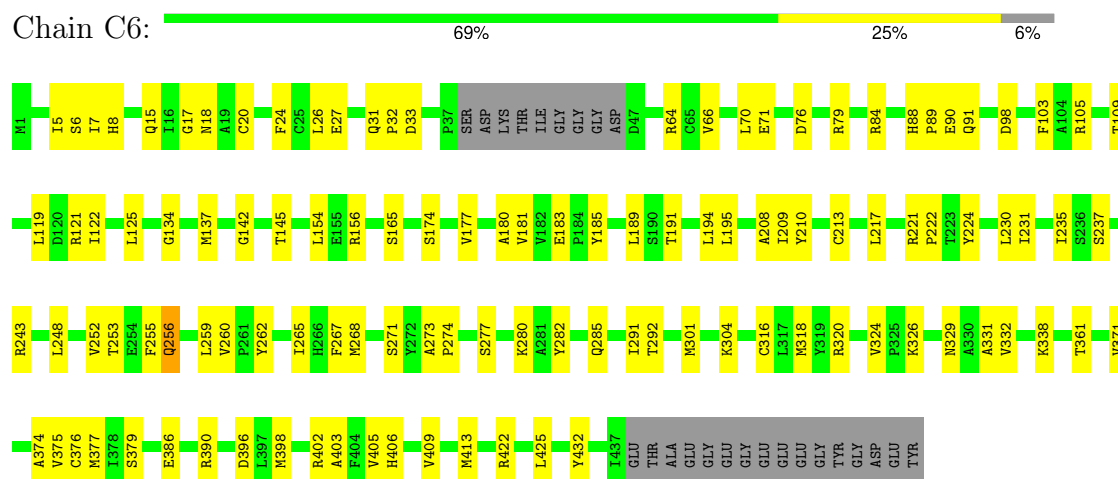
• Molecule 3: Tubulin alpha chain



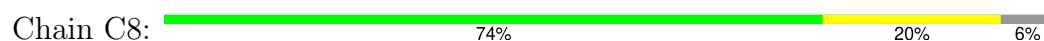
- Molecule 3: Tubulin alpha chain

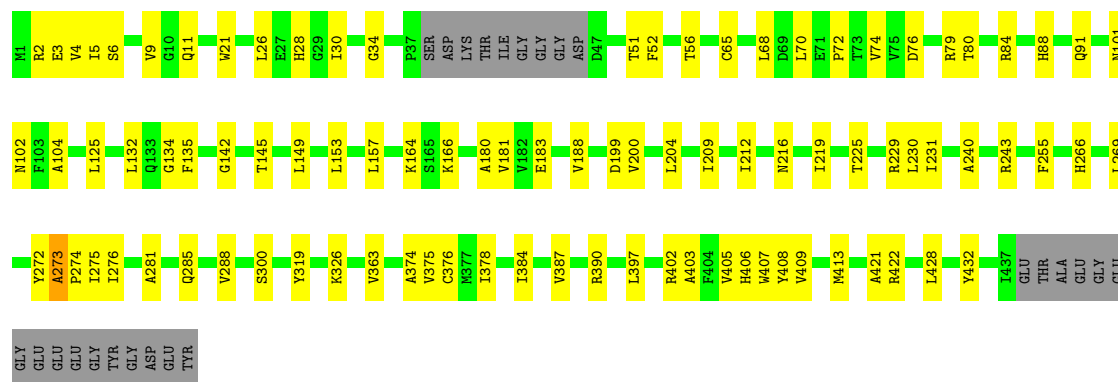


- Molecule 3: Tubulin alpha chain



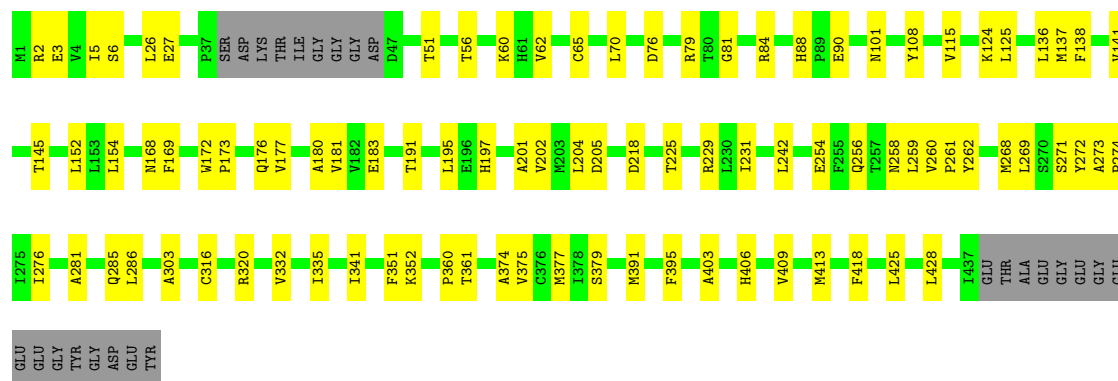
- Molecule 3: Tubulin alpha chain





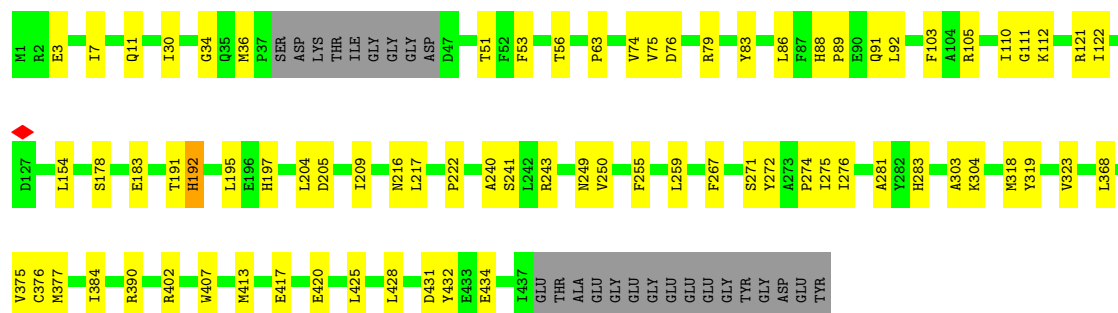
• Molecule 3: Tubulin alpha chain

Chain D0: 74% 20% 6%



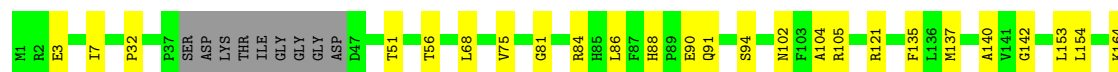
• Molecule 3: Tubulin alpha chain

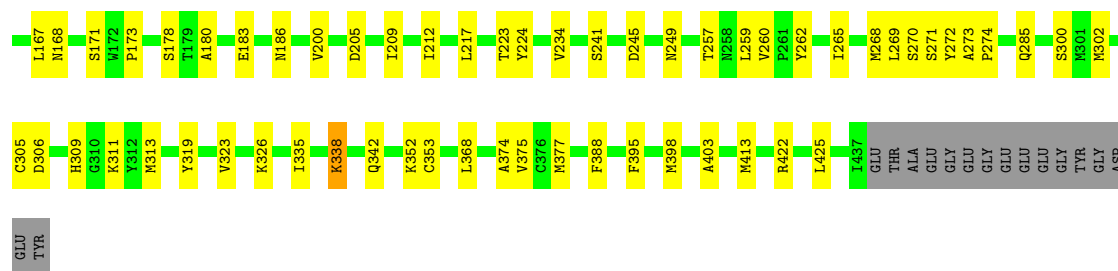
Chain D2: 78% 17% 6%



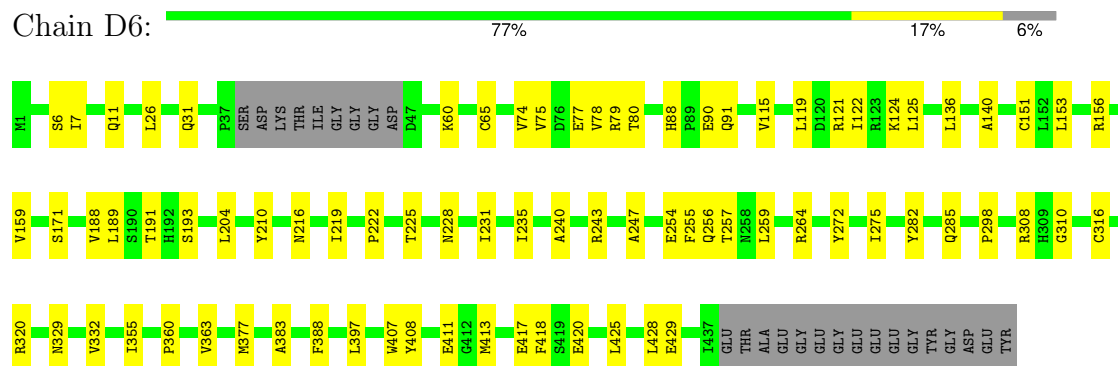
• Molecule 3: Tubulin alpha chain

Chain D4: 76% 18% 6%

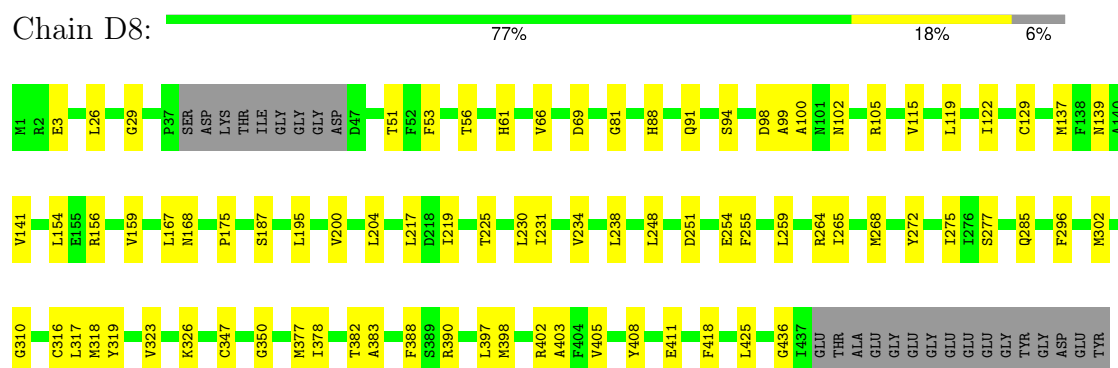




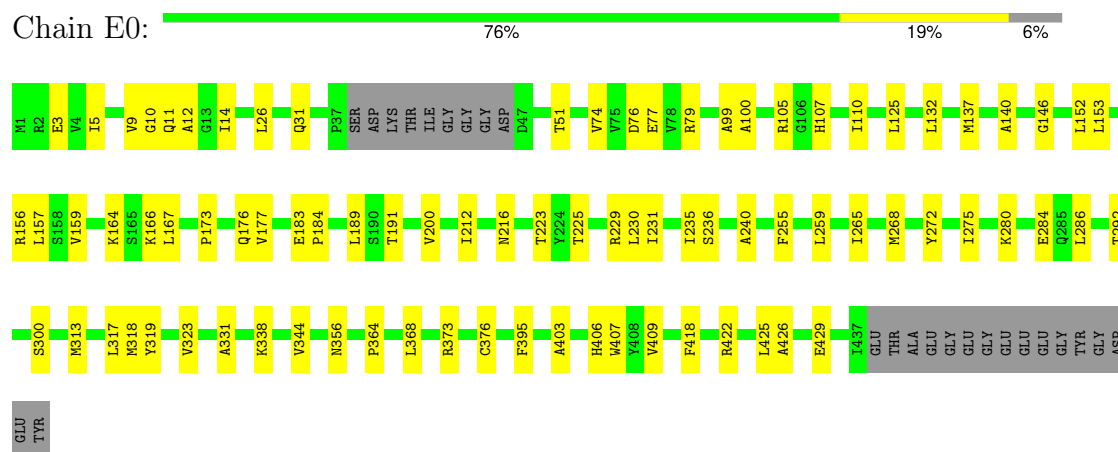
• Molecule 3: Tubulin alpha chain



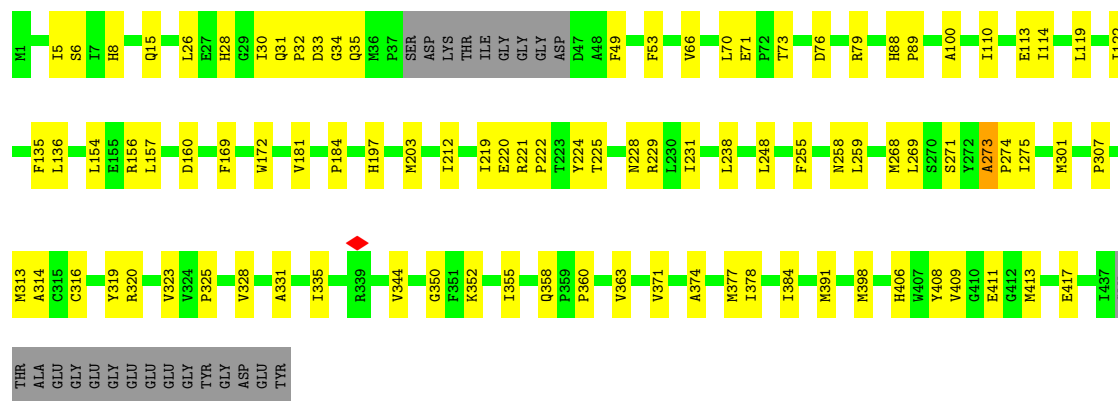
• Molecule 3: Tubulin alpha chain



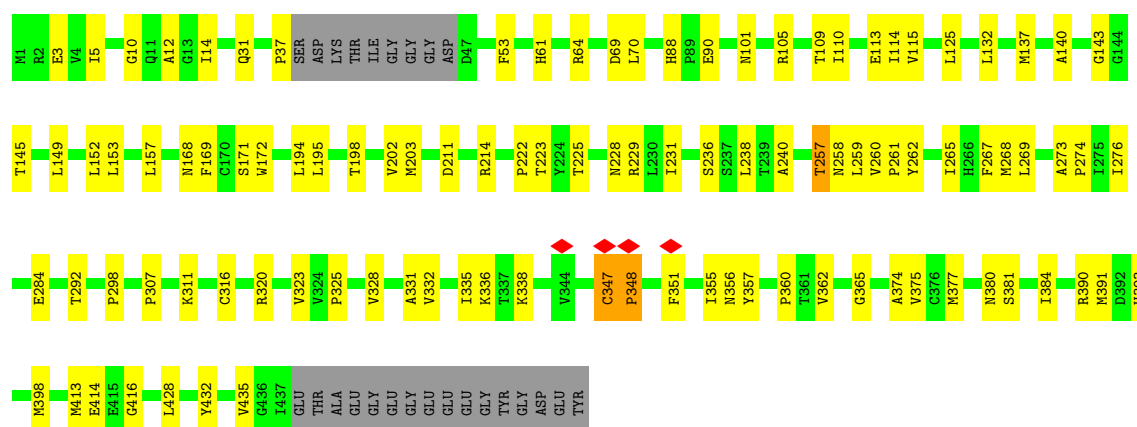
• Molecule 3: Tubulin alpha chain



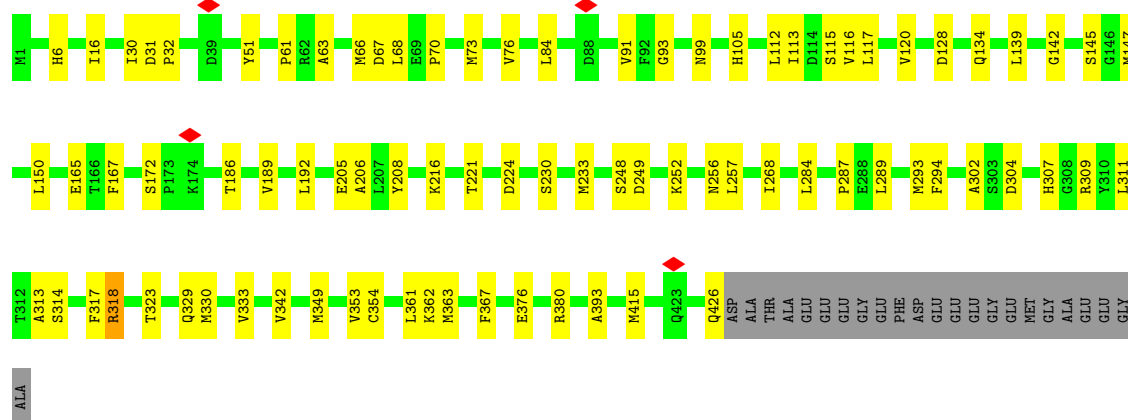
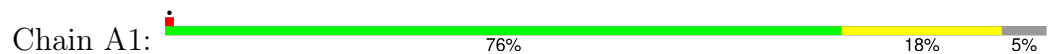




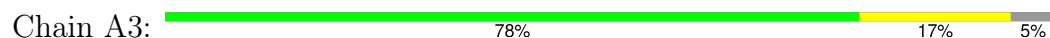
• Molecule 3: Tubulin alpha chain

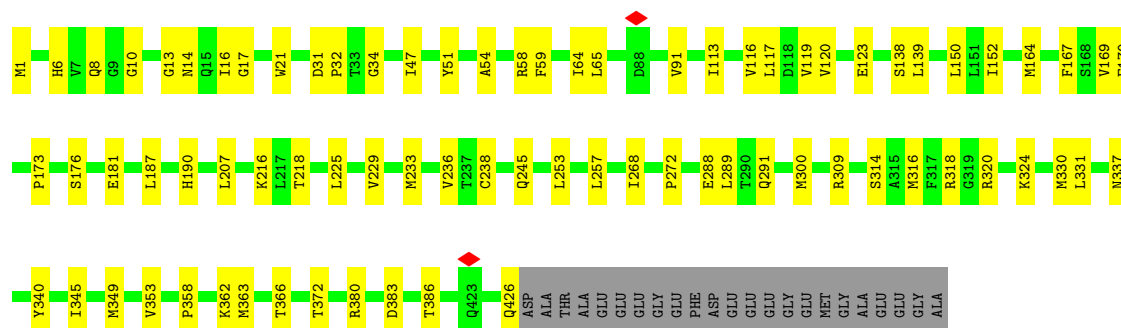


• Molecule 4: Tubulin beta chain



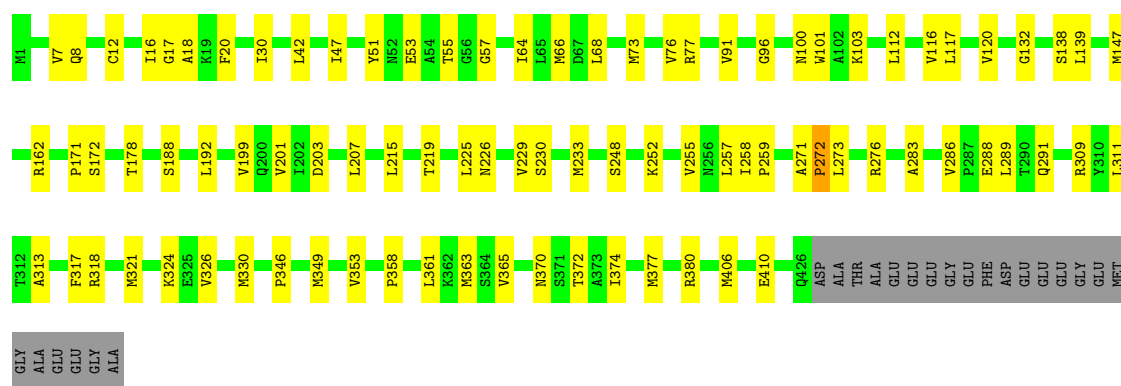
• Molecule 4: Tubulin beta chain





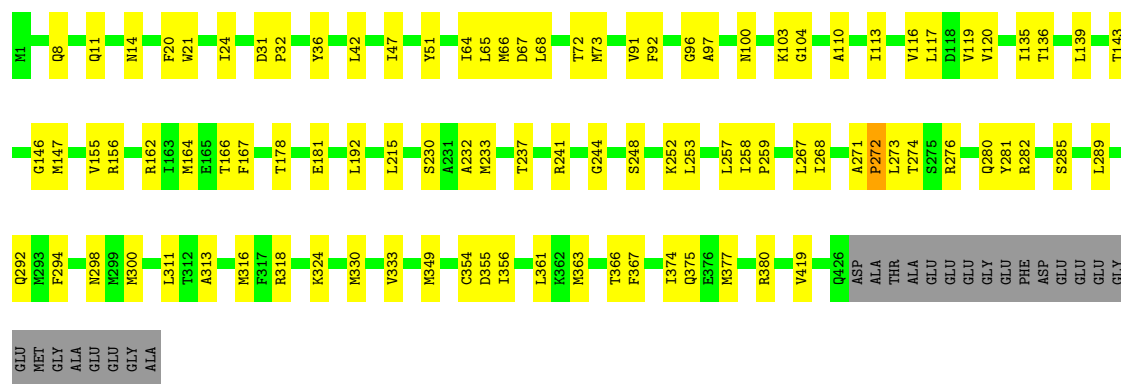
- Molecule 4: Tubulin beta chain

Chain A5: 75% 19% 5%



- Molecule 4: Tubulin beta chain

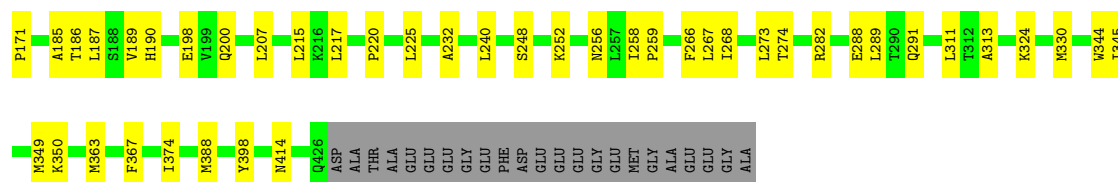
Chain A7: 73% 21% 5%



- Molecule 4: Tubulin beta chain

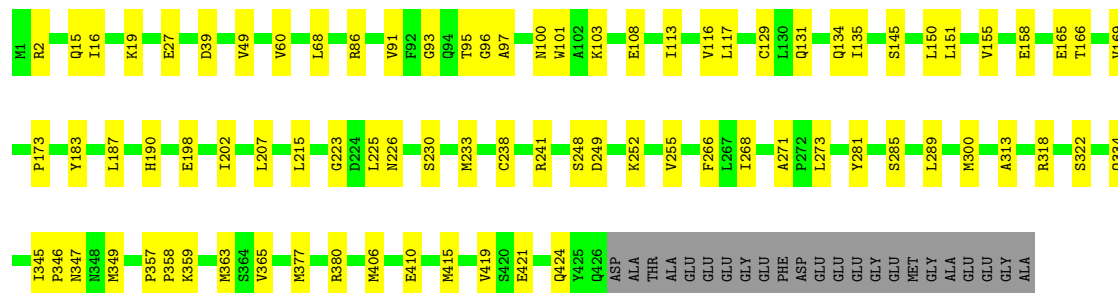
Chain A9: 78% 17% 5%





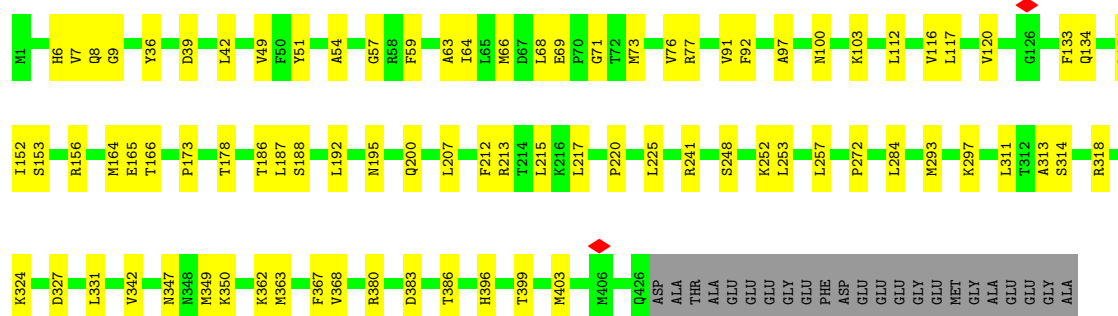
- Molecule 4: Tubulin beta chain

Chain B1: 77% 18% 5%



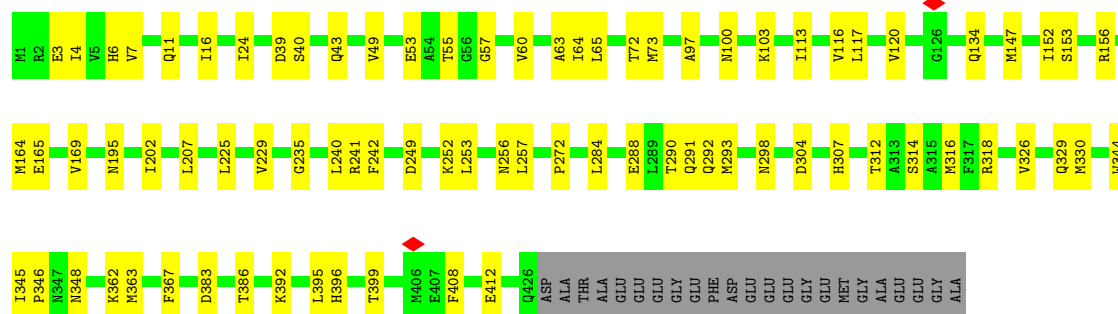
- Molecule 4: Tubulin beta chain

Chain B3: 76% 19% 5%




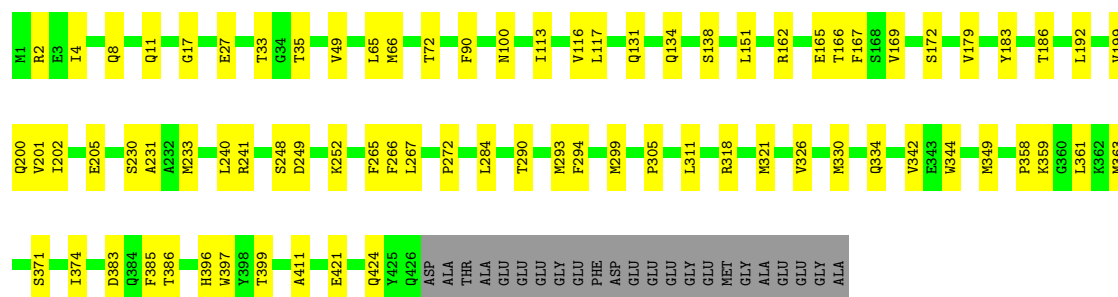
- Molecule 4: Tubulin beta chain

Chain B5: 77% 18% 5%




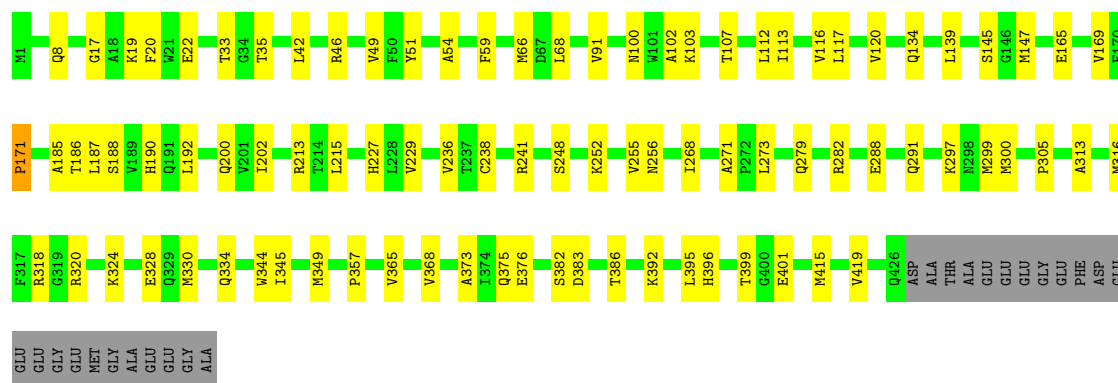
- Molecule 4: Tubulin beta chain

Chain B7:  78% 17% 5%



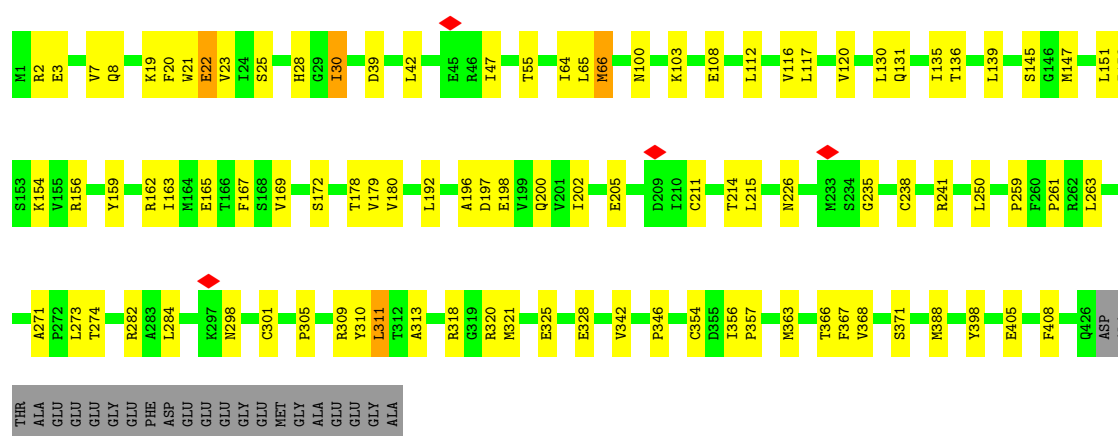
• Molecule 4: Tubulin beta chain

Chain B9:  75% 20% 5%



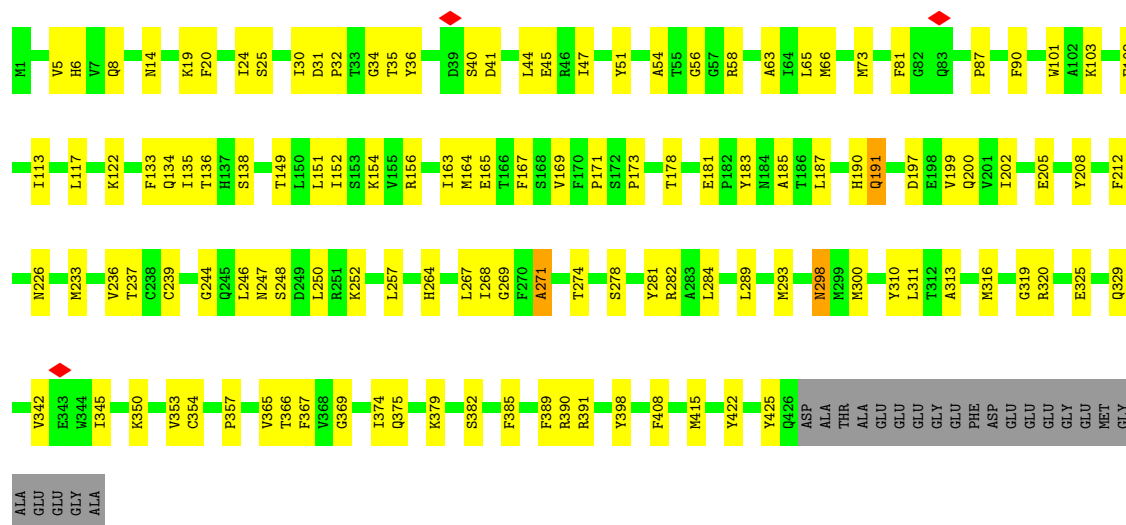
• Molecule 4: Tubulin beta chain

Chain C1:  73% 21% 5%



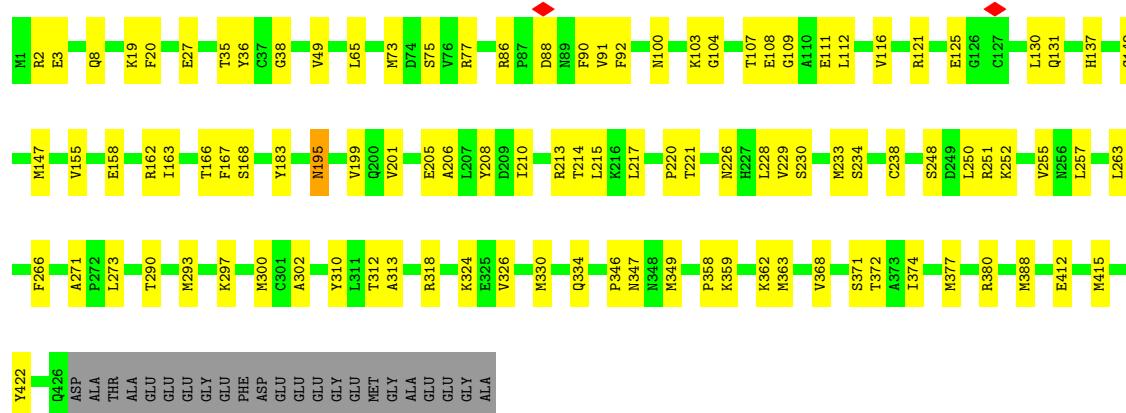
• Molecule 4: Tubulin beta chain

Chain C3:  67% 27% 5%



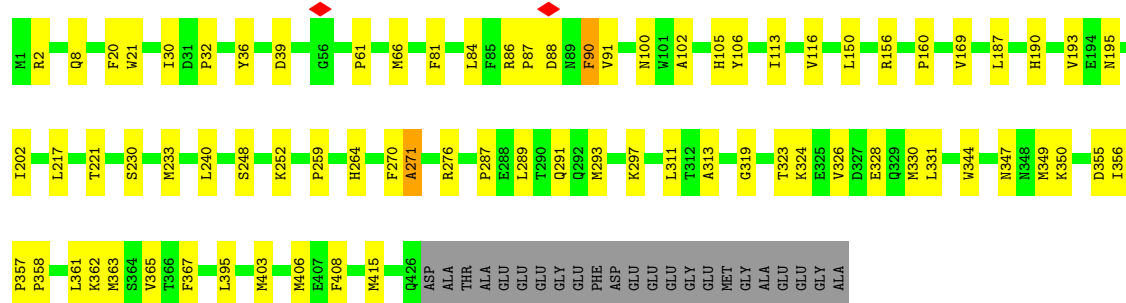
• Molecule 4: Tubulin beta chain

Chain C5: 72% 23% 5%



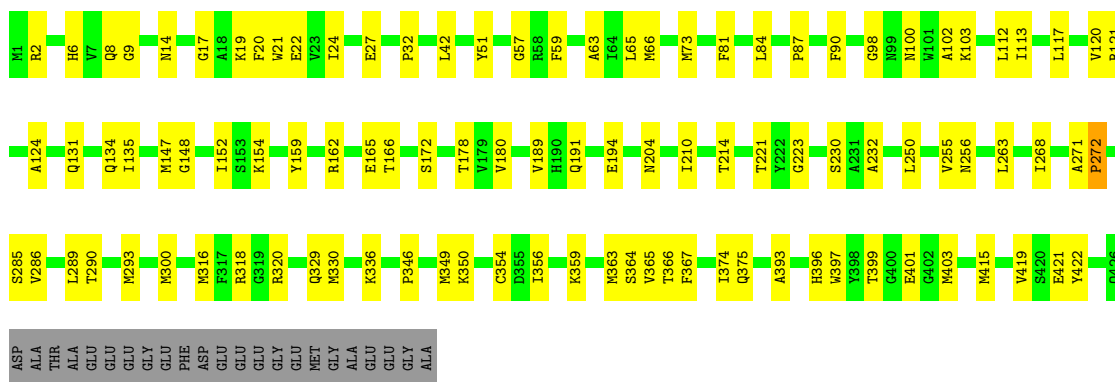
• Molecule 4: Tubulin beta chain

Chain C7: 78% 16% 5%



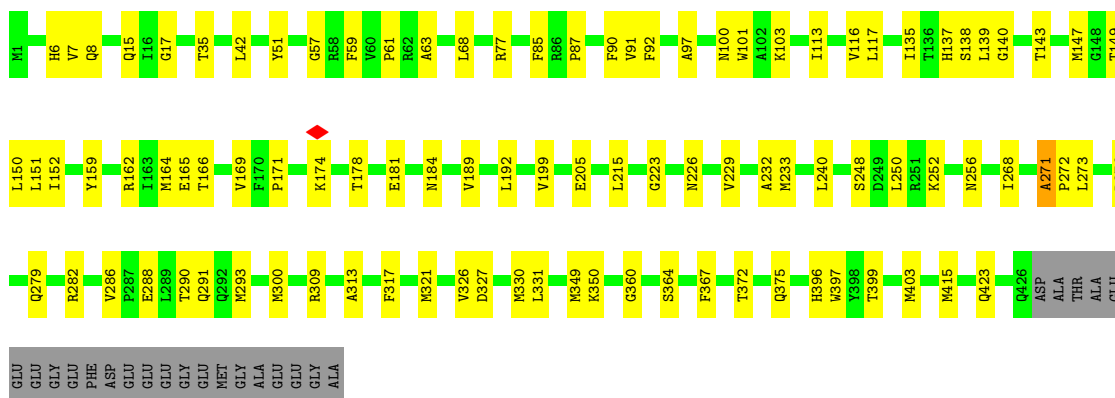
• Molecule 4: Tubulin beta chain

Chain C9: 72% 22% 5%



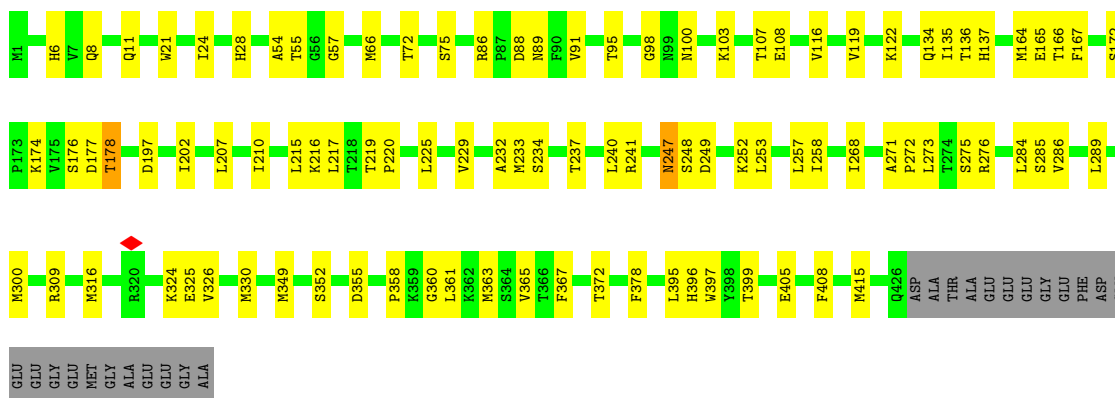
• Molecule 4: Tubulin beta chain

Chain D1: 73% 21% 5%



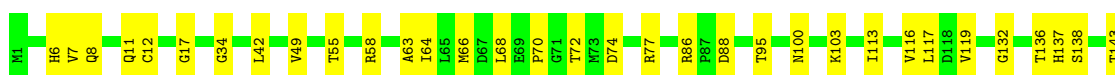
• Molecule 4: Tubulin beta chain

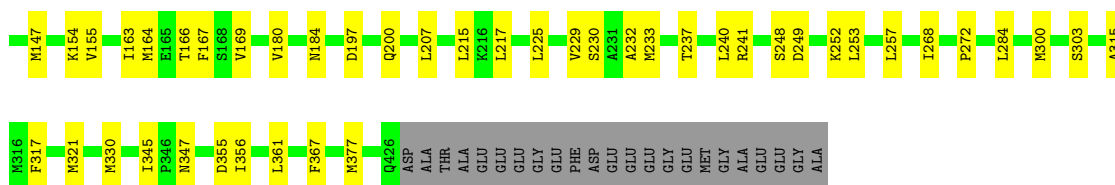
Chain D3: 73% 21% 5%



• Molecule 4: Tubulin beta chain

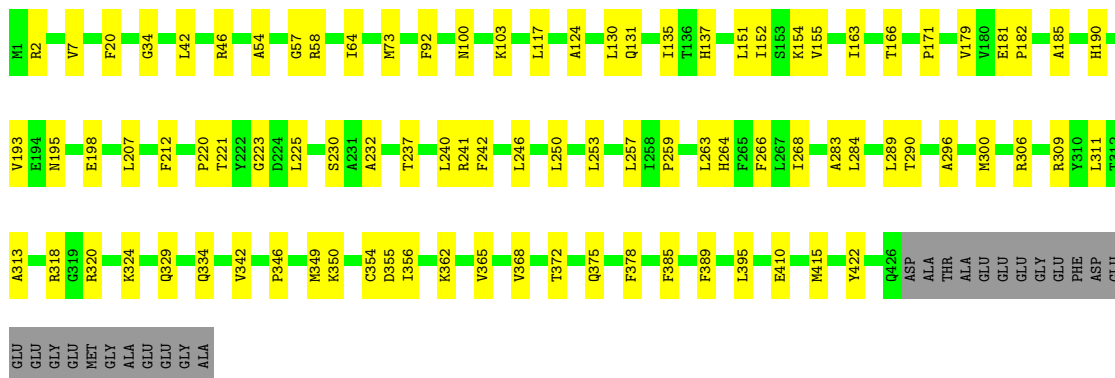
Chain D5: 78% 17% 5%





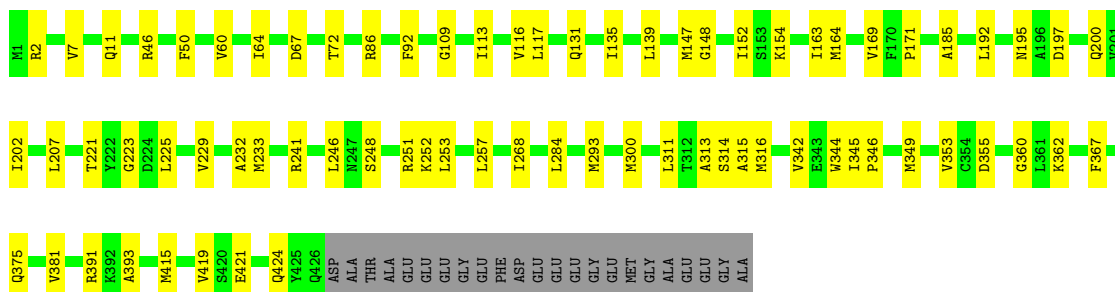
- Molecule 4: Tubulin beta chain

Chain D7: 75% 20% 5%



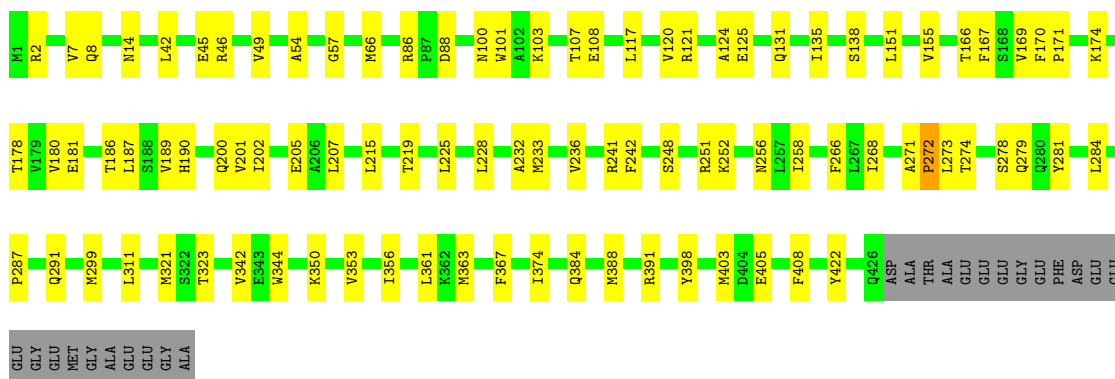
- Molecule 4: Tubulin beta chain

Chain D9: 79% 16% 5%

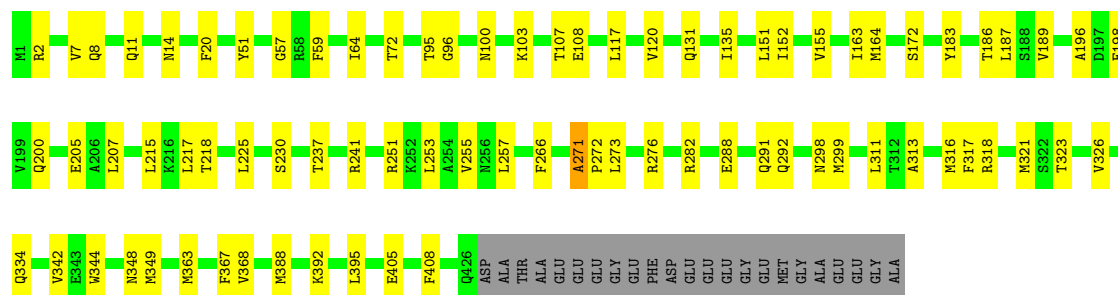



- Molecule 4: Tubulin beta chain

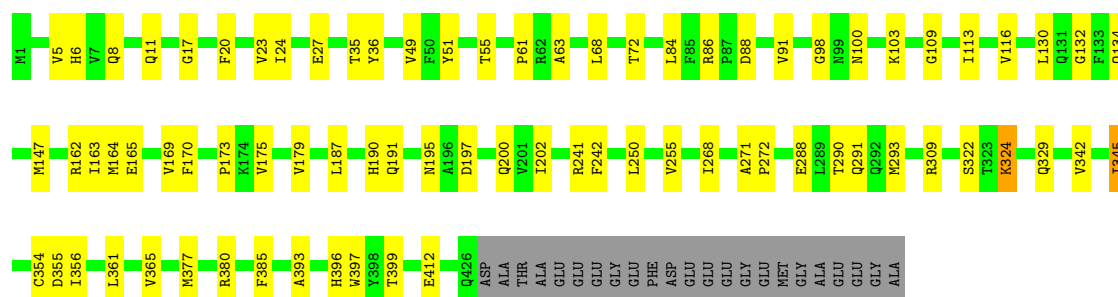

Chain E1: 74% 20% 5%



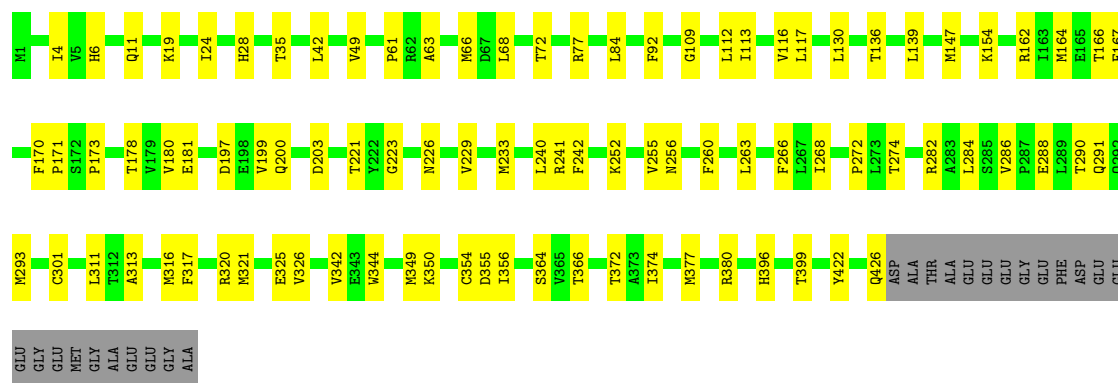

• Molecule 4: Tubulin beta chain

Chain E3: 

• Molecule 4: Tubulin beta chain

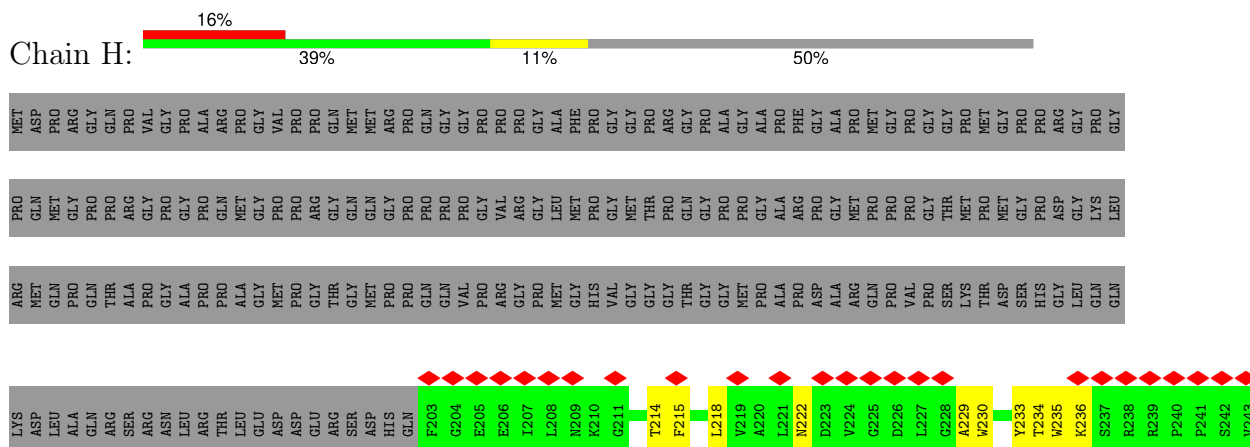
Chain E5: 

• Molecule 4: Tubulin beta chain

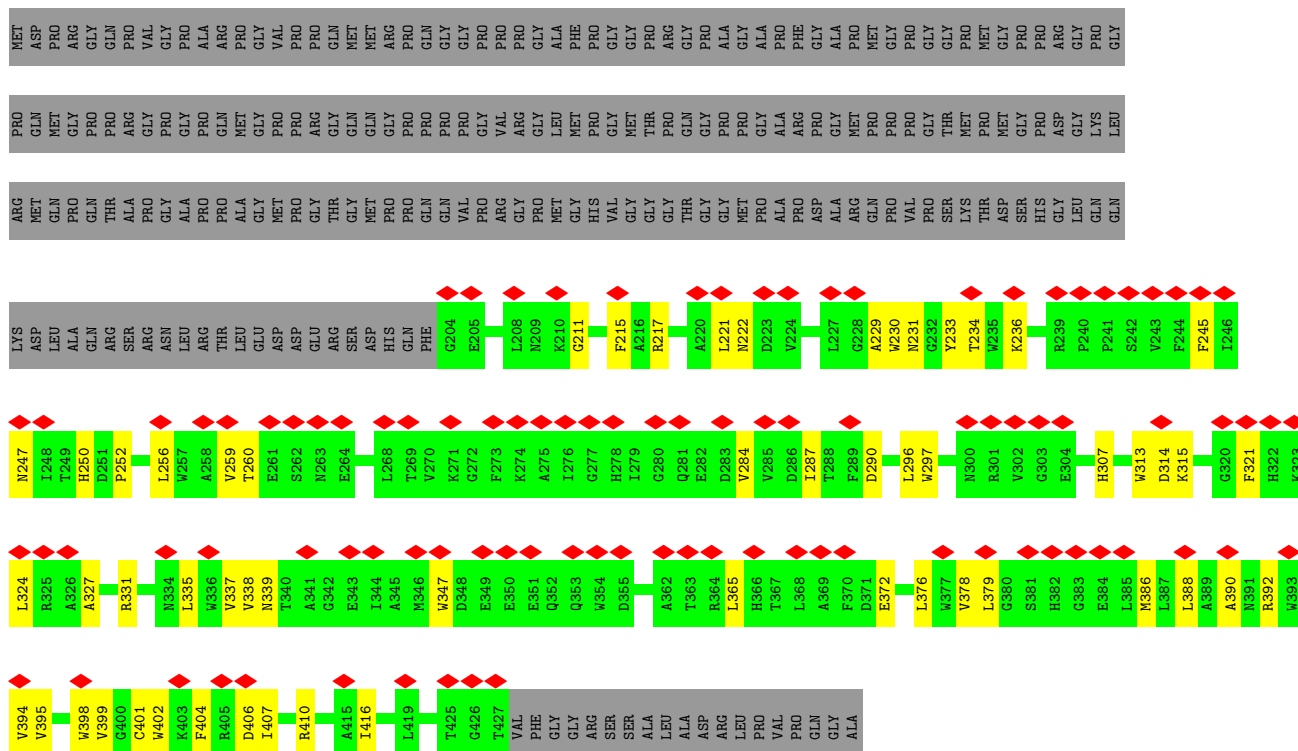
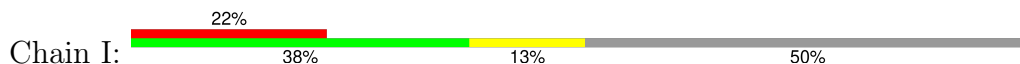
Chain E7: 

• Molecule 4: Tubulin beta chain

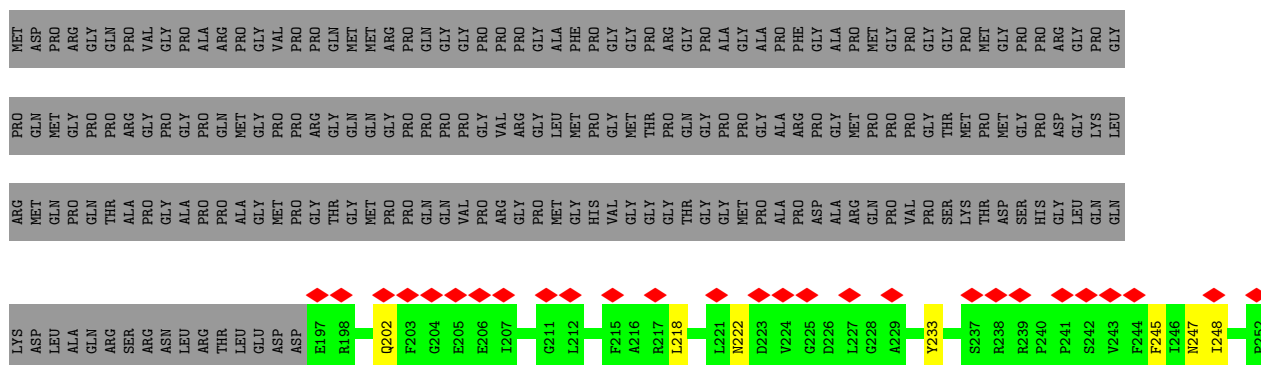
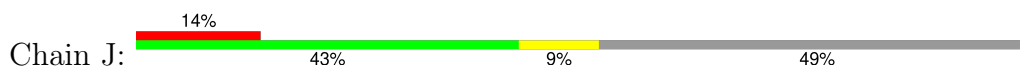
Chain E9: 



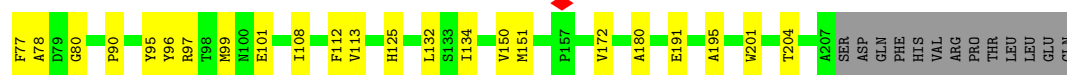
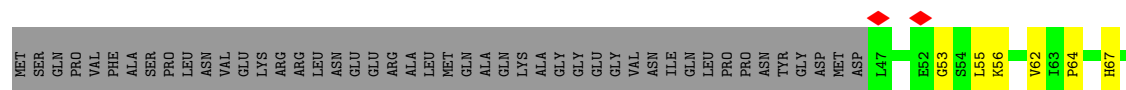
- Molecule 6: TLAP2 (thioredoxin-like associated protein), TGME49 232130



- Molecule 6: TLAP2 (thioredoxin-like associated protein), TGME49 232130







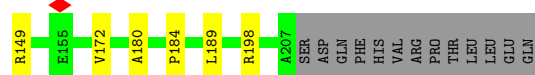
• Molecule 7: TRXL1, TGME49_232410

Chain c: 76% 15% 9%



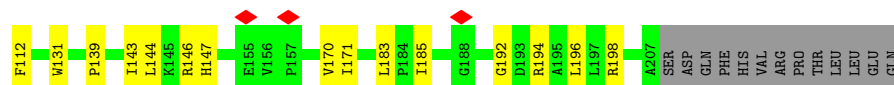
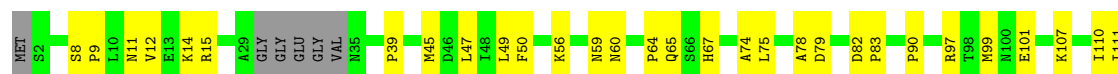
• Molecule 7: TRXL1, TGME49_232410

Chain d: 76% 15% 9%



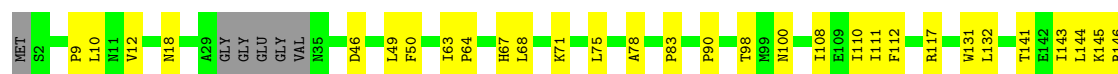
• Molecule 7: TRXL1, TGME49_232410

Chain e: 71% 20% 9%

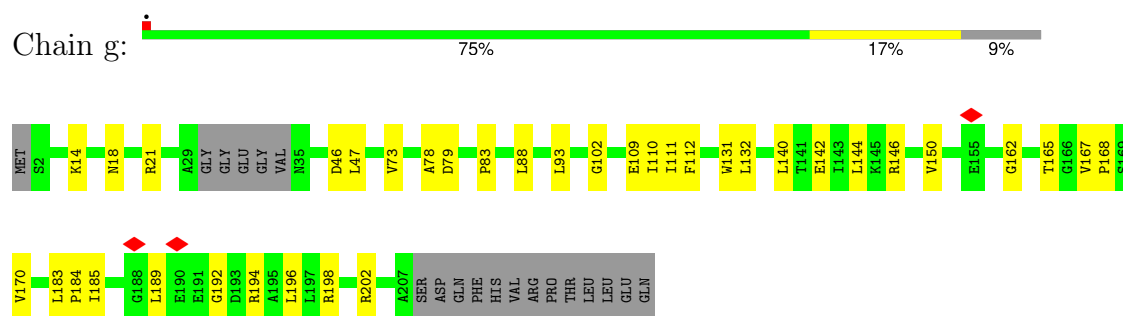


• Molecule 7: TRXL1, TGME49_232410

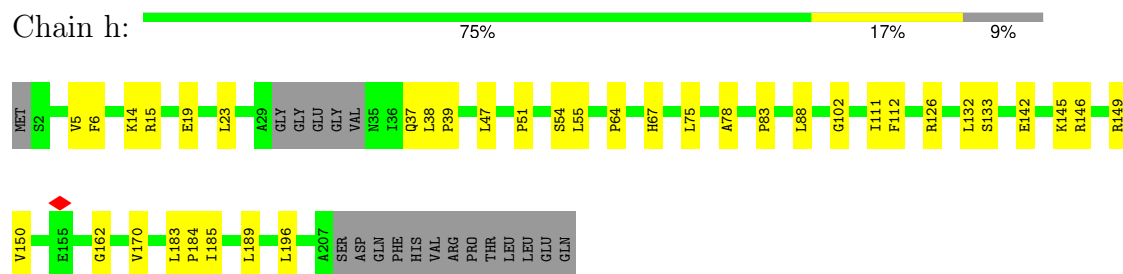
Chain f: 72% 20% 9%



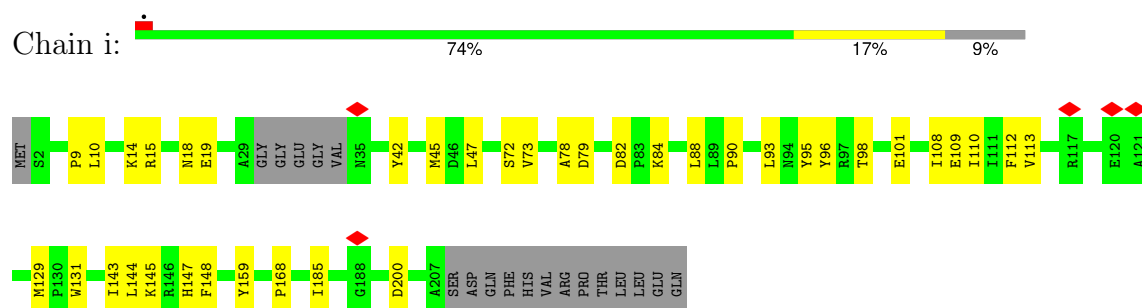
- Molecule 7: TRXL1, TGME49_232410



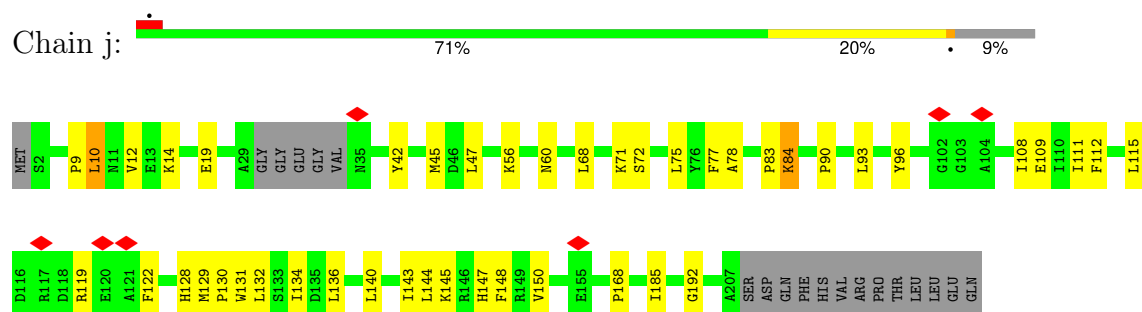
- Molecule 7: TRXL1, TGME49_232410



- Molecule 7: TRXL1, TGME49_232410

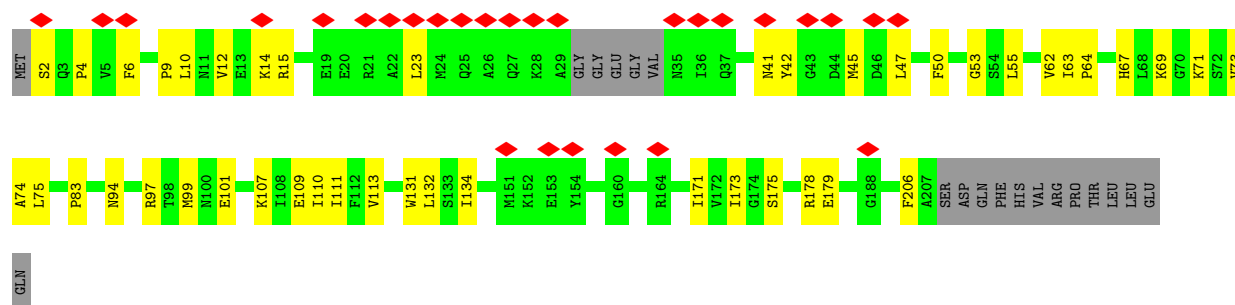


- Molecule 7: TRXL1, TGME49_232410

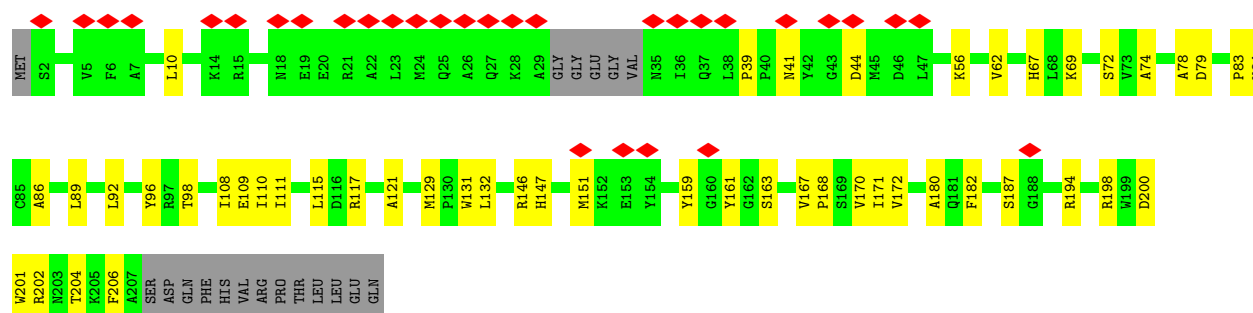


- Molecule 7: TRXL1, TGME49_232410

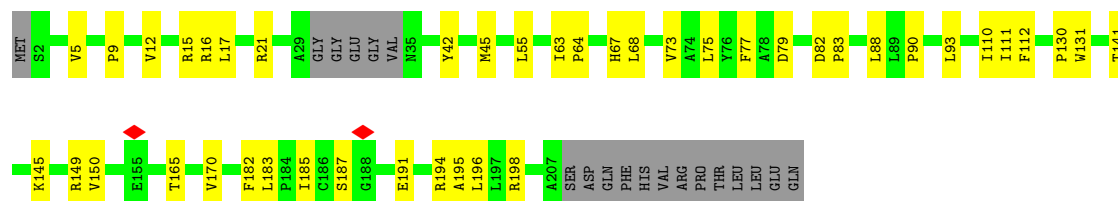




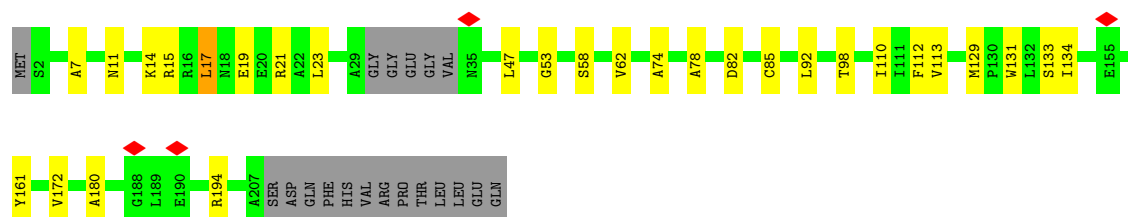
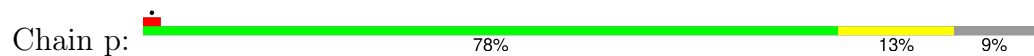
• Molecule 7: TRXL1, TGME49_232410



• Molecule 7: TRXL1, TGME49_232410

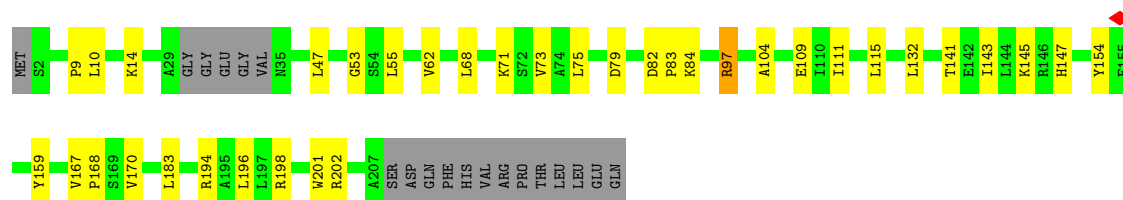


• Molecule 7: TRXL1, TGME49_232410

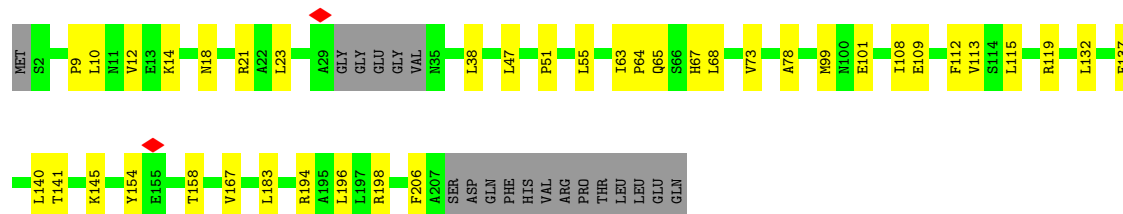


• Molecule 7: TRXL1, TGME49_232410

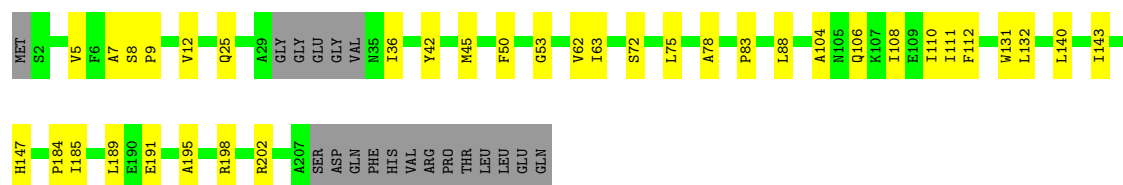




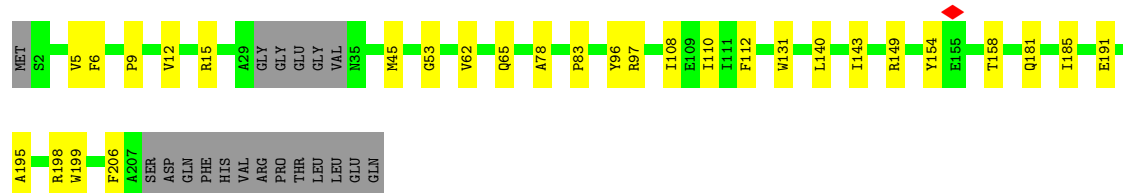
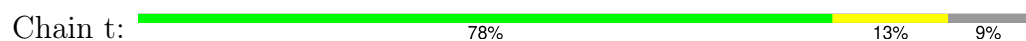
- Molecule 7: TRXL1, TGME49_232410



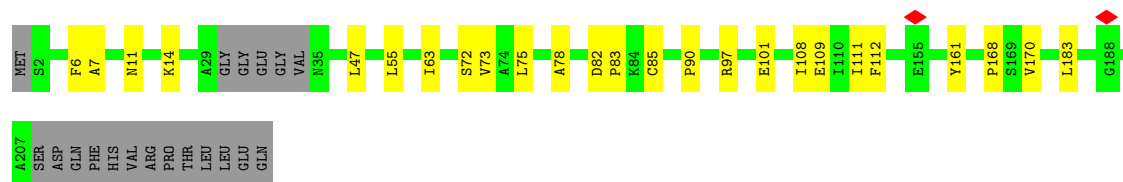
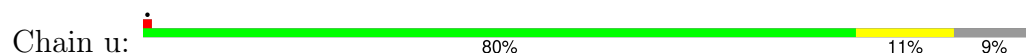
- Molecule 7: TRXL1, TGME49_232410



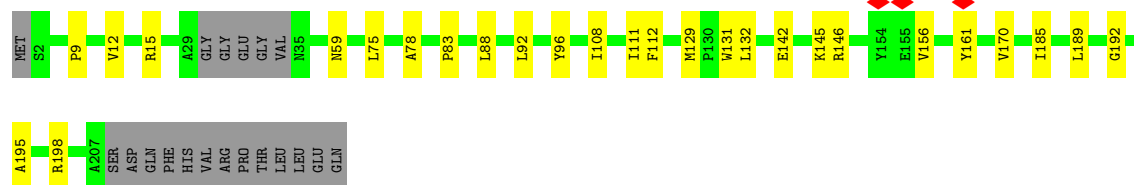
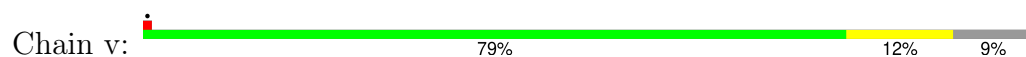
- Molecule 7: TRXL1, TGME49_232410



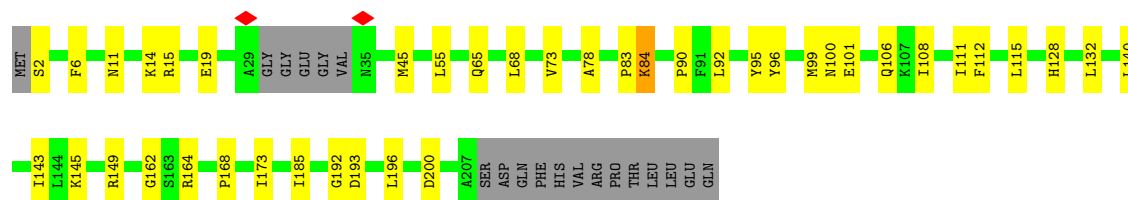
- Molecule 7: TRXL1, TGME49_232410



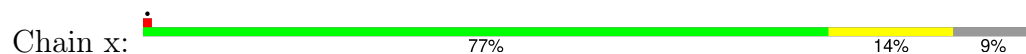
- Molecule 7: TRXL1, TGME49_232410



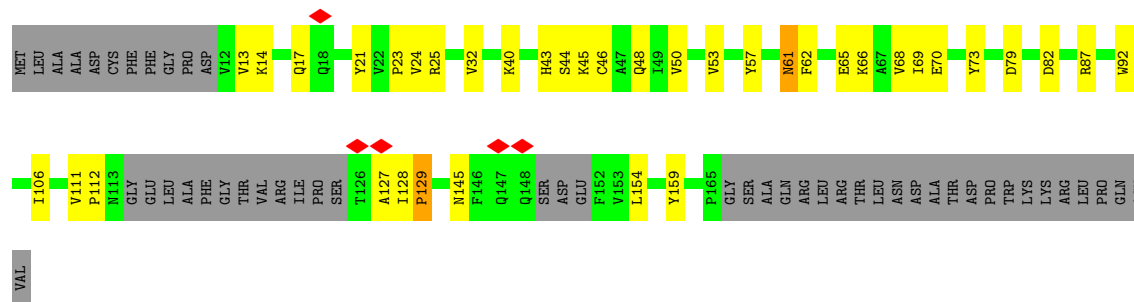
- Molecule 7: TRXL1, TGME49_232410



- Molecule 7: TRXL1, TGME49_232410

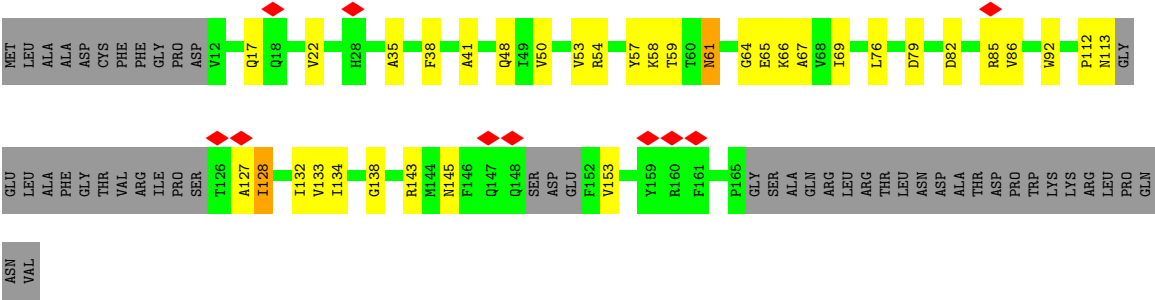


- Molecule 8: TRXL2, TGME49_225790



- Molecule 8: TRXL2, TGME49_225790





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	225207	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.187	Depositor
Minimum map value	0.000	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.067	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, 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	0	0.17	0/181	0.42	0/248
1	1	0.18	0/181	0.39	0/248
1	10	0.17	0/181	0.43	0/248
1	11	0.16	0/181	0.38	0/248
1	12	0.19	0/181	0.33	0/248
1	13	0.15	0/181	0.32	0/248
1	14	0.19	0/181	0.46	0/248
1	15	0.18	0/181	0.45	0/248
1	16	0.19	0/181	0.42	0/248
1	17	0.21	0/181	0.45	0/248
1	18	0.21	0/181	0.55	0/248
1	19	0.24	0/181	0.67	0/248
1	2	0.19	0/181	0.39	0/248
1	22	0.20	0/166	0.44	0/227
1	23	0.17	0/166	0.36	0/227
1	3	0.18	0/181	0.37	0/248
1	4	0.20	0/181	0.45	0/248
1	5	0.16	0/181	0.44	0/248
1	6	0.17	0/181	0.33	0/248
1	7	0.14	0/181	0.27	0/248
1	8	0.27	0/181	0.95	2/248 (0.8%)
1	9	0.23	0/181	0.79	0/248
2	A	0.26	0/1359	0.73	0/1837
2	B	0.27	0/1776	0.71	0/2403
2	C	0.30	0/392	0.75	0/529
3	A0	0.27	0/3398	0.63	1/4606 (0.0%)
3	A2	0.27	0/3398	0.68	2/4606 (0.0%)
3	A4	0.28	0/3398	0.61	1/4606 (0.0%)
3	A6	0.26	0/3398	0.61	0/4606
3	A8	0.25	0/3398	0.56	0/4606
3	B0	0.25	0/3398	0.59	0/4606
3	B2	0.25	0/3398	0.54	0/4606

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	B4	0.24	0/3398	0.53	0/4606
3	B6	0.23	0/3398	0.53	0/4606
3	B8	0.24	0/3398	0.53	0/4606
3	C0	0.29	0/3398	0.75	3/4606 (0.1%)
3	C2	0.31	0/3398	0.71	3/4606 (0.1%)
3	C4	0.25	0/3398	0.64	3/4606 (0.1%)
3	C6	0.29	0/3398	0.68	2/4606 (0.0%)
3	C8	0.27	0/3398	0.70	1/4606 (0.0%)
3	D0	0.26	0/3398	0.61	1/4606 (0.0%)
3	D2	0.25	0/3398	0.63	3/4606 (0.1%)
3	D4	0.27	0/3398	0.60	0/4606
3	D6	0.24	0/3398	0.57	0/4606
3	D8	0.25	0/3398	0.56	1/4606 (0.0%)
3	E0	0.28	1/3398 (0.0%)	0.63	3/4606 (0.1%)
3	E2	0.28	0/3398	0.59	0/4606
3	E4	0.26	0/3398	0.67	3/4606 (0.1%)
3	E6	0.27	0/3398	0.68	3/4606 (0.1%)
3	E8	0.28	0/3392	0.70	2/4599 (0.0%)
3	F0	0.32	0/3398	0.74	3/4606 (0.1%)
4	A1	0.26	0/3404	0.64	2/4606 (0.0%)
4	A3	0.24	0/3404	0.57	1/4606 (0.0%)
4	A5	0.29	0/3404	0.63	0/4606
4	A7	0.27	0/3404	0.61	0/4606
4	A9	0.27	0/3404	0.57	0/4606
4	B1	0.25	0/3404	0.60	0/4606
4	B3	0.26	0/3404	0.56	2/4606 (0.0%)
4	B5	0.24	0/3404	0.58	0/4606
4	B7	0.25	0/3404	0.57	0/4606
4	B9	0.25	0/3404	0.67	4/4606 (0.1%)
4	C1	0.27	0/3404	0.69	3/4606 (0.1%)
4	C3	0.27	0/3404	0.64	0/4606
4	C5	0.28	0/3404	0.66	0/4606
4	C7	0.29	0/3404	0.72	4/4606 (0.1%)
4	C9	0.26	0/3404	0.63	1/4606 (0.0%)
4	D1	0.27	0/3404	0.61	0/4606
4	D3	0.26	0/3404	0.65	3/4606 (0.1%)
4	D5	0.26	0/3404	0.61	0/4606
4	D7	0.25	0/3404	0.59	0/4606
4	D9	0.26	0/3404	0.55	1/4606 (0.0%)
4	E1	0.29	0/3404	0.68	0/4606
4	E3	0.27	0/3404	0.62	0/4606
4	E5	0.29	0/3404	0.68	4/4606 (0.1%)
4	E7	0.27	0/3404	0.58	2/4606 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	E9	0.35	0/3404	0.92	7/4606 (0.2%)
4	F1	0.29	0/3404	0.69	1/4606 (0.0%)
5	E	0.26	0/761	0.58	0/1031
5	F	0.24	0/761	0.58	0/1031
5	G	0.25	0/575	0.59	0/780
6	H	0.22	0/1871	0.61	2/2541 (0.1%)
6	I	0.23	0/1870	0.56	0/2540
6	J	0.18	0/1925	0.47	0/2613
6	K	0.19	0/1848	0.50	0/2510
7	a	0.25	0/1321	0.61	0/1788
7	b	0.29	0/1321	0.66	1/1788 (0.1%)
7	c	0.25	0/1645	0.60	0/2225
7	d	0.23	0/1645	0.53	0/2225
7	e	0.24	0/1645	0.51	2/2225 (0.1%)
7	f	0.25	0/1645	0.54	0/2225
7	g	0.21	0/1645	0.49	0/2225
7	h	0.22	0/1645	0.54	0/2225
7	i	0.24	0/1645	0.55	0/2225
7	j	0.24	0/1645	0.64	4/2225 (0.2%)
7	m	0.25	0/1645	0.60	0/2225
7	n	0.25	0/1645	0.59	0/2225
7	o	0.24	0/1645	0.57	0/2225
7	p	0.23	0/1645	0.55	3/2225 (0.1%)
7	q	0.26	0/1645	0.61	0/2225
7	r	0.23	0/1645	0.49	0/2225
7	s	0.21	0/1645	0.48	0/2225
7	t	0.23	0/1645	0.51	0/2225
7	u	0.21	0/1645	0.48	0/2225
7	v	0.24	0/1645	0.54	0/2225
7	w	0.27	0/1645	0.79	3/2225 (0.1%)
7	x	0.22	0/1645	0.55	0/2225
8	k	0.27	0/1168	0.72	2/1578 (0.1%)
8	l	0.27	0/1168	0.71	0/1578
All	All	0.26	1/231814 (0.0%)	0.62	89/313966 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	A0	0	1
3	A6	0	1
3	B2	0	1
3	B6	0	1
3	C0	0	2
3	C2	0	1
3	C6	0	1
3	C8	0	1
3	D0	0	2
3	D2	0	2
3	D4	0	1
3	D6	0	1
3	D8	0	1
3	E4	0	2
3	E6	0	3
3	E8	0	1
3	F0	0	3
4	A5	0	2
4	A7	0	1
4	C1	0	3
4	C3	0	2
4	C5	0	1
4	C7	0	2
4	C9	0	1
4	D1	0	3
4	D3	0	2
4	D5	0	1
4	D9	0	1
4	E1	0	1
4	E3	0	1
4	E5	0	1
4	E9	0	2
4	F1	0	2
7	q	0	1
8	k	0	1
8	l	0	1
All	All	0	56

All (1) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E0	173	PRO	C-N	-7.07	1.23	1.33

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B9	171	PRO	CA-C-N	14.91	149.28	120.94
4	B9	171	PRO	C-N-CA	14.91	149.28	120.94
7	w	128	HIS	CA-C-N	14.51	142.73	120.68
7	w	128	HIS	C-N-CA	14.51	142.73	120.68
3	E0	173	PRO	CA-C-N	8.85	134.13	120.68

There are no chirality outliers.

5 of 56 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	276	SER	Peptide
3	A0	262	TYR	Peptide
4	A5	271	ALA	Peptide
4	A5	272	PRO	Peptide
3	A6	273	ALA	Peptide

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	174	0	171	4	0
1	1	174	0	171	2	0
1	10	174	0	171	5	0
1	11	174	0	171	3	0
1	12	174	0	171	4	0
1	13	174	0	171	3	0
1	14	174	0	171	5	0
1	15	174	0	171	6	0
1	16	174	0	171	3	0
1	17	174	0	171	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	18	174	0	171	5	0
1	19	174	0	171	7	0
1	2	174	0	171	2	0
1	22	160	0	156	1	0
1	23	160	0	156	1	0
1	3	174	0	171	4	0
1	4	174	0	171	4	0
1	5	174	0	171	2	0
1	6	174	0	171	2	0
1	7	174	0	171	1	0
1	8	174	0	171	2	0
1	9	174	0	171	1	0
2	A	1338	0	1341	28	0
2	B	1744	0	1734	41	0
2	C	384	0	379	10	0
3	A0	3325	0	3252	52	0
3	A2	3325	0	3252	55	0
3	A4	3325	0	3252	34	0
3	A6	3325	0	3252	51	0
3	A8	3325	0	3252	33	0
3	B0	3325	0	3252	48	0
3	B2	3325	0	3252	45	0
3	B4	3325	0	3252	45	0
3	B6	3325	0	3252	51	0
3	B8	3325	0	3252	48	0
3	C0	3325	0	3252	69	0
3	C2	3325	0	3251	76	0
3	C4	3325	0	3252	54	0
3	C6	3325	0	3252	79	0
3	C8	3325	0	3252	59	0
3	D0	3325	0	3252	62	0
3	D2	3325	0	3252	44	0
3	D4	3325	0	3252	55	0
3	D6	3325	0	3252	51	0
3	D8	3325	0	3252	53	0
3	E0	3325	0	3252	52	0
3	E2	3325	0	3252	51	0
3	E4	3325	0	3252	63	0
3	E6	3325	0	3252	64	0
3	E8	3319	0	3241	65	0
3	F0	3325	0	3252	68	0
4	A1	3331	0	3207	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A3	3331	0	3208	53	0
4	A5	3331	0	3207	55	0
4	A7	3331	0	3207	62	0
4	A9	3331	0	3207	52	0
4	B1	3331	0	3209	56	0
4	B3	3331	0	3207	53	0
4	B5	3331	0	3207	51	0
4	B7	3331	0	3209	53	0
4	B9	3331	0	3209	63	0
4	C1	3331	0	3209	60	0
4	C3	3331	0	3209	88	0
4	C5	3331	0	3209	61	0
4	C7	3331	0	3209	56	0
4	C9	3331	0	3209	63	0
4	D1	3331	0	3209	60	0
4	D3	3331	0	3207	62	0
4	D5	3331	0	3207	43	0
4	D7	3331	0	3207	59	0
4	D9	3331	0	3207	42	0
4	E1	3331	0	3207	61	0
4	E3	3331	0	3209	48	0
4	E5	3331	0	3207	54	0
4	E7	3331	0	3207	59	0
4	E9	3331	0	3207	113	0
4	F1	3331	0	3207	56	0
5	E	740	0	690	12	0
5	F	740	0	690	8	0
5	G	558	0	507	13	0
6	H	1817	0	1768	32	0
6	I	1817	0	1769	38	0
6	J	1870	0	1811	26	0
6	K	1795	0	1749	27	0
7	a	1289	0	1274	14	0
7	b	1289	0	1274	18	0
7	c	1608	0	1590	22	0
7	d	1608	0	1590	26	0
7	e	1608	0	1590	26	0
7	f	1608	0	1590	29	0
7	g	1608	0	1590	23	0
7	h	1608	0	1590	25	0
7	i	1608	0	1590	24	0
7	j	1608	0	1590	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	m	1608	0	1590	30	0
7	n	1608	0	1590	33	0
7	o	1608	0	1590	28	0
7	p	1608	0	1590	21	0
7	q	1608	0	1590	26	0
7	r	1608	0	1590	26	0
7	s	1608	0	1590	24	0
7	t	1608	0	1590	18	0
7	u	1608	0	1590	15	0
7	v	1608	0	1590	18	0
7	w	1608	0	1590	24	0
7	x	1608	0	1590	22	0
8	k	1140	0	1143	24	0
8	l	1140	0	1143	27	0
9	A	28	0	12	0	0
9	A1	28	0	12	0	0
9	A3	28	0	12	0	0
9	A5	28	0	12	0	0
9	A7	28	0	12	0	0
9	B	28	0	12	0	0
9	B3	28	0	12	0	0
9	B5	28	0	12	0	0
9	B7	28	0	12	0	0
9	B9	28	0	12	0	0
9	C1	28	0	12	0	0
9	C3	28	0	12	0	0
9	C5	28	0	12	0	0
9	C7	28	0	12	0	0
9	C9	28	0	12	0	0
9	D1	28	0	12	0	0
9	D3	28	0	12	0	0
9	D5	28	0	12	0	0
9	D7	28	0	12	0	0
9	D9	28	0	12	0	0
9	E1	28	0	12	0	0
9	E3	28	0	12	0	0
9	E5	28	0	12	0	0
9	E7	28	0	12	0	0
9	E9	28	0	12	3	0
9	F1	28	0	12	0	0
10	A0	32	0	12	0	0
10	A2	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	A4	32	0	12	0	0
10	A6	32	0	12	0	0
10	A8	32	0	12	0	0
10	B0	32	0	12	0	0
10	B2	32	0	12	0	0
10	B4	32	0	12	0	0
10	B6	32	0	12	0	0
10	B8	32	0	12	0	0
10	C0	32	0	11	1	0
10	C2	32	0	12	0	0
10	C4	32	0	12	0	0
10	C6	32	0	12	0	0
10	C8	32	0	12	0	0
10	D0	32	0	12	0	0
10	D2	32	0	12	0	0
10	D4	32	0	12	0	0
10	D6	32	0	12	0	0
10	D8	32	0	12	0	0
10	E0	32	0	12	0	0
10	E2	32	0	12	0	0
10	E4	32	0	12	0	0
10	E6	32	0	12	0	0
10	E8	32	0	12	0	0
10	F0	32	0	12	0	0
11	A0	1	0	0	0	0
11	A3	1	0	0	0	0
11	A4	1	0	0	0	0
11	A6	1	0	0	0	0
11	A8	1	0	0	0	0
11	B0	1	0	0	0	0
11	B2	1	0	0	0	0
11	B4	1	0	0	0	0
11	B6	1	0	0	0	0
11	B8	1	0	0	0	0
11	C0	1	0	0	0	0
11	C2	1	0	0	0	0
11	C4	1	0	0	0	0
11	C6	1	0	0	0	0
11	C8	1	0	0	0	0
11	D0	1	0	0	0	0
11	D2	1	0	0	0	0
11	D4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	D6	1	0	0	0	0
11	D8	1	0	0	0	0
11	E0	1	0	0	0	0
11	E2	1	0	0	0	0
11	E4	1	0	0	0	0
11	E6	1	0	0	0	0
11	E8	1	0	0	0	0
11	F0	1	0	0	0	0
All	All	228257	0	221370	3461	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 8.

The worst 5 of 3461 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)
3:E2:212:ILE:O	3:E2:216:ASN:HB2	1.69	0.92
4:E9:183:TYR:O	4:E9:187:LEU:HB2	1.71	0.90
1:12:247:TYR:O	1:12:251:TYR:HB2	1.72	0.89
4:C3:289:LEU:O	4:C3:293:MET:HB2	1.74	0.87
4:C1:8:GLN:O	4:C1:66:MET:HB2	1.74	0.86

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	0	20/351 (6%)	20 (100%)	0	0	100	100
1	1	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	10	20/351 (6%)	20 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	11	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	12	20/351 (6%)	20 (100%)	0	0	100	100
1	13	20/351 (6%)	20 (100%)	0	0	100	100
1	14	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	15	20/351 (6%)	20 (100%)	0	0	100	100
1	16	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	17	20/351 (6%)	20 (100%)	0	0	100	100
1	18	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	19	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	2	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	22	18/351 (5%)	15 (83%)	3 (17%)	0	100	100
1	23	18/351 (5%)	16 (89%)	2 (11%)	0	100	100
1	3	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	4	20/351 (6%)	20 (100%)	0	0	100	100
1	5	20/351 (6%)	20 (100%)	0	0	100	100
1	6	20/351 (6%)	20 (100%)	0	0	100	100
1	7	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	8	20/351 (6%)	17 (85%)	2 (10%)	1 (5%)	1	12
1	9	20/351 (6%)	14 (70%)	5 (25%)	1 (5%)	1	12
2	A	159/583 (27%)	132 (83%)	22 (14%)	5 (3%)	3	21
2	B	210/583 (36%)	173 (82%)	30 (14%)	7 (3%)	3	19
2	C	47/583 (8%)	41 (87%)	5 (11%)	1 (2%)	5	27
3	A0	424/453 (94%)	389 (92%)	33 (8%)	2 (0%)	25	56
3	A2	424/453 (94%)	393 (93%)	31 (7%)	0	100	100
3	A4	424/453 (94%)	400 (94%)	24 (6%)	0	100	100
3	A6	424/453 (94%)	391 (92%)	33 (8%)	0	100	100
3	A8	424/453 (94%)	411 (97%)	13 (3%)	0	100	100
3	B0	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
3	B2	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
3	B4	424/453 (94%)	406 (96%)	18 (4%)	0	100	100
3	B6	424/453 (94%)	405 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B8	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
3	C0	424/453 (94%)	353 (83%)	69 (16%)	2 (0%)	25	56
3	C2	424/453 (94%)	364 (86%)	60 (14%)	0	100	100
3	C4	424/453 (94%)	377 (89%)	46 (11%)	1 (0%)	44	71
3	C6	424/453 (94%)	384 (91%)	38 (9%)	2 (0%)	25	56
3	C8	424/453 (94%)	376 (89%)	47 (11%)	1 (0%)	44	71
3	D0	424/453 (94%)	383 (90%)	40 (9%)	1 (0%)	44	71
3	D2	424/453 (94%)	384 (91%)	40 (9%)	0	100	100
3	D4	424/453 (94%)	394 (93%)	28 (7%)	2 (0%)	25	56
3	D6	424/453 (94%)	396 (93%)	28 (7%)	0	100	100
3	D8	424/453 (94%)	393 (93%)	31 (7%)	0	100	100
3	E0	424/453 (94%)	396 (93%)	28 (7%)	0	100	100
3	E2	424/453 (94%)	385 (91%)	38 (9%)	1 (0%)	44	71
3	E4	424/453 (94%)	386 (91%)	36 (8%)	2 (0%)	25	56
3	E6	424/453 (94%)	367 (87%)	56 (13%)	1 (0%)	44	71
3	E8	424/453 (94%)	388 (92%)	36 (8%)	0	100	100
3	F0	424/453 (94%)	372 (88%)	51 (12%)	1 (0%)	44	71
4	A1	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
4	A3	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
4	A5	424/449 (94%)	398 (94%)	24 (6%)	2 (0%)	25	56
4	A7	424/449 (94%)	399 (94%)	24 (6%)	1 (0%)	44	71
4	A9	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
4	B1	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
4	B3	424/449 (94%)	408 (96%)	15 (4%)	1 (0%)	44	71
4	B5	424/449 (94%)	406 (96%)	18 (4%)	0	100	100
4	B7	424/449 (94%)	396 (93%)	28 (7%)	0	100	100
4	B9	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
4	C1	424/449 (94%)	368 (87%)	54 (13%)	2 (0%)	25	56
4	C3	424/449 (94%)	386 (91%)	38 (9%)	0	100	100
4	C5	424/449 (94%)	381 (90%)	41 (10%)	2 (0%)	25	56
4	C7	424/449 (94%)	378 (89%)	43 (10%)	3 (1%)	19	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C9	424/449 (94%)	378 (89%)	44 (10%)	2 (0%)	25	56
4	D1	424/449 (94%)	386 (91%)	37 (9%)	1 (0%)	44	71
4	D3	424/449 (94%)	375 (88%)	44 (10%)	5 (1%)	11	38
4	D5	424/449 (94%)	384 (91%)	37 (9%)	3 (1%)	19	50
4	D7	424/449 (94%)	402 (95%)	21 (5%)	1 (0%)	44	71
4	D9	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
4	E1	424/449 (94%)	382 (90%)	40 (9%)	2 (0%)	25	56
4	E3	424/449 (94%)	390 (92%)	32 (8%)	2 (0%)	25	56
4	E5	424/449 (94%)	392 (92%)	31 (7%)	1 (0%)	44	71
4	E7	424/449 (94%)	396 (93%)	27 (6%)	1 (0%)	44	71
4	E9	424/449 (94%)	342 (81%)	79 (19%)	3 (1%)	19	50
4	F1	424/449 (94%)	377 (89%)	46 (11%)	1 (0%)	44	71
5	E	85/336 (25%)	68 (80%)	17 (20%)	0	100	100
5	F	85/336 (25%)	66 (78%)	19 (22%)	0	100	100
5	G	65/336 (19%)	53 (82%)	12 (18%)	0	100	100
6	H	221/446 (50%)	199 (90%)	22 (10%)	0	100	100
6	I	222/446 (50%)	206 (93%)	15 (7%)	1 (0%)	25	56
6	J	227/446 (51%)	206 (91%)	21 (9%)	0	100	100
6	K	218/446 (49%)	204 (94%)	14 (6%)	0	100	100
7	a	159/220 (72%)	144 (91%)	15 (9%)	0	100	100
7	b	159/220 (72%)	139 (87%)	20 (13%)	0	100	100
7	c	197/220 (90%)	185 (94%)	11 (6%)	1 (0%)	25	56
7	d	197/220 (90%)	188 (95%)	9 (5%)	0	100	100
7	e	197/220 (90%)	188 (95%)	9 (5%)	0	100	100
7	f	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
7	g	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
7	h	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
7	i	197/220 (90%)	190 (96%)	7 (4%)	0	100	100
7	j	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
7	m	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
7	n	197/220 (90%)	185 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	o	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
7	p	197/220 (90%)	189 (96%)	8 (4%)	0	100	100
7	q	197/220 (90%)	189 (96%)	8 (4%)	0	100	100
7	r	197/220 (90%)	191 (97%)	6 (3%)	0	100	100
7	s	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
7	t	197/220 (90%)	190 (96%)	7 (4%)	0	100	100
7	u	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
7	v	197/220 (90%)	183 (93%)	14 (7%)	0	100	100
7	w	197/220 (90%)	179 (91%)	18 (9%)	0	100	100
7	x	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
8	k	133/189 (70%)	115 (86%)	15 (11%)	3 (2%)	5	26
8	l	133/189 (70%)	109 (82%)	23 (17%)	1 (1%)	16	46
All	All	28547/40933 (70%)	26241 (92%)	2236 (8%)	70 (0%)	45	71

5 of 70 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	277	ASP
2	B	277	ASP
2	B	468	ASN
3	C4	218	ASP
3	C6	243	ARG

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	20/305 (7%)	20 (100%)	0	100	100
1	1	20/305 (7%)	20 (100%)	0	100	100
1	10	20/305 (7%)	20 (100%)	0	100	100
1	11	20/305 (7%)	20 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	12	20/305 (7%)	20 (100%)	0	100	100
1	13	20/305 (7%)	20 (100%)	0	100	100
1	14	20/305 (7%)	20 (100%)	0	100	100
1	15	20/305 (7%)	20 (100%)	0	100	100
1	16	20/305 (7%)	20 (100%)	0	100	100
1	17	20/305 (7%)	20 (100%)	0	100	100
1	18	20/305 (7%)	20 (100%)	0	100	100
1	19	20/305 (7%)	20 (100%)	0	100	100
1	2	20/305 (7%)	20 (100%)	0	100	100
1	22	18/305 (6%)	18 (100%)	0	100	100
1	23	18/305 (6%)	18 (100%)	0	100	100
1	3	20/305 (7%)	20 (100%)	0	100	100
1	4	20/305 (7%)	20 (100%)	0	100	100
1	5	20/305 (7%)	19 (95%)	1 (5%)	20	48
1	6	20/305 (7%)	20 (100%)	0	100	100
1	7	20/305 (7%)	20 (100%)	0	100	100
1	8	20/305 (7%)	20 (100%)	0	100	100
1	9	20/305 (7%)	20 (100%)	0	100	100
2	A	154/502 (31%)	154 (100%)	0	100	100
2	B	194/502 (39%)	194 (100%)	0	100	100
2	C	38/502 (8%)	38 (100%)	0	100	100
3	A0	359/379 (95%)	359 (100%)	0	100	100
3	A2	359/379 (95%)	359 (100%)	0	100	100
3	A4	359/379 (95%)	359 (100%)	0	100	100
3	A6	359/379 (95%)	359 (100%)	0	100	100
3	A8	359/379 (95%)	359 (100%)	0	100	100
3	B0	359/379 (95%)	359 (100%)	0	100	100
3	B2	359/379 (95%)	359 (100%)	0	100	100
3	B4	359/379 (95%)	359 (100%)	0	100	100
3	B6	359/379 (95%)	359 (100%)	0	100	100
3	B8	359/379 (95%)	359 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C0	359/379 (95%)	358 (100%)	1 (0%)	91	94
3	C2	359/379 (95%)	359 (100%)	0	100	100
3	C4	359/379 (95%)	359 (100%)	0	100	100
3	C6	359/379 (95%)	359 (100%)	0	100	100
3	C8	359/379 (95%)	359 (100%)	0	100	100
3	D0	359/379 (95%)	359 (100%)	0	100	100
3	D2	359/379 (95%)	358 (100%)	1 (0%)	91	94
3	D4	359/379 (95%)	359 (100%)	0	100	100
3	D6	359/379 (95%)	358 (100%)	1 (0%)	91	94
3	D8	359/379 (95%)	359 (100%)	0	100	100
3	E0	359/379 (95%)	359 (100%)	0	100	100
3	E2	359/379 (95%)	359 (100%)	0	100	100
3	E4	359/379 (95%)	359 (100%)	0	100	100
3	E6	359/379 (95%)	359 (100%)	0	100	100
3	E8	358/379 (94%)	358 (100%)	0	100	100
3	F0	359/379 (95%)	359 (100%)	0	100	100
4	A1	364/381 (96%)	364 (100%)	0	100	100
4	A3	364/381 (96%)	364 (100%)	0	100	100
4	A5	364/381 (96%)	364 (100%)	0	100	100
4	A7	364/381 (96%)	364 (100%)	0	100	100
4	A9	364/381 (96%)	363 (100%)	1 (0%)	91	94
4	B1	364/381 (96%)	364 (100%)	0	100	100
4	B3	364/381 (96%)	364 (100%)	0	100	100
4	B5	364/381 (96%)	364 (100%)	0	100	100
4	B7	364/381 (96%)	364 (100%)	0	100	100
4	B9	364/381 (96%)	364 (100%)	0	100	100
4	C1	364/381 (96%)	364 (100%)	0	100	100
4	C3	364/381 (96%)	363 (100%)	1 (0%)	91	94
4	C5	364/381 (96%)	363 (100%)	1 (0%)	91	94
4	C7	364/381 (96%)	364 (100%)	0	100	100
4	C9	364/381 (96%)	363 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D1	364/381 (96%)	364 (100%)	0	100	100
4	D3	364/381 (96%)	363 (100%)	1 (0%)	91	94
4	D5	364/381 (96%)	364 (100%)	0	100	100
4	D7	364/381 (96%)	364 (100%)	0	100	100
4	D9	364/381 (96%)	364 (100%)	0	100	100
4	E1	364/381 (96%)	364 (100%)	0	100	100
4	E3	364/381 (96%)	364 (100%)	0	100	100
4	E5	364/381 (96%)	364 (100%)	0	100	100
4	E7	364/381 (96%)	364 (100%)	0	100	100
4	E9	364/381 (96%)	362 (100%)	2 (0%)	86	91
4	F1	364/381 (96%)	364 (100%)	0	100	100
5	E	76/280 (27%)	76 (100%)	0	100	100
5	F	76/280 (27%)	76 (100%)	0	100	100
5	G	56/280 (20%)	56 (100%)	0	100	100
6	H	185/345 (54%)	185 (100%)	0	100	100
6	I	185/345 (54%)	185 (100%)	0	100	100
6	J	191/345 (55%)	191 (100%)	0	100	100
6	K	183/345 (53%)	183 (100%)	0	100	100
7	a	139/190 (73%)	139 (100%)	0	100	100
7	b	139/190 (73%)	139 (100%)	0	100	100
7	c	174/190 (92%)	174 (100%)	0	100	100
7	d	174/190 (92%)	174 (100%)	0	100	100
7	e	174/190 (92%)	174 (100%)	0	100	100
7	f	174/190 (92%)	174 (100%)	0	100	100
7	g	174/190 (92%)	174 (100%)	0	100	100
7	h	174/190 (92%)	174 (100%)	0	100	100
7	i	174/190 (92%)	174 (100%)	0	100	100
7	j	174/190 (92%)	174 (100%)	0	100	100
7	m	174/190 (92%)	174 (100%)	0	100	100
7	n	174/190 (92%)	174 (100%)	0	100	100
7	o	174/190 (92%)	174 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	p	174/190 (92%)	174 (100%)	0	100	100
7	q	174/190 (92%)	174 (100%)	0	100	100
7	r	174/190 (92%)	174 (100%)	0	100	100
7	s	174/190 (92%)	174 (100%)	0	100	100
7	t	174/190 (92%)	174 (100%)	0	100	100
7	u	174/190 (92%)	174 (100%)	0	100	100
7	v	174/190 (92%)	174 (100%)	0	100	100
7	w	174/190 (92%)	174 (100%)	0	100	100
7	x	174/190 (92%)	174 (100%)	0	100	100
8	k	122/164 (74%)	122 (100%)	0	100	100
8	l	122/164 (74%)	122 (100%)	0	100	100
All	All	24573/34704 (71%)	24562 (100%)	11 (0%)	100	100

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D3	247	ASN
3	D6	256	GLN
4	E9	329	GLN
4	E9	256	ASN
4	C5	195	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 312 such sidechains are listed below:

Mol	Chain	Res	Type
4	E7	99	ASN
8	l	147	GLN
4	E9	245	GLN
7	a	59	ASN
7	s	25	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 78 ligands modelled in this entry, 26 are monoatomic - leaving 52 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	C3	501	-	25,30,30	1.02	1 (4%)	30,47,47	1.17	2 (6%)
9	GDP	A1	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.25	4 (13%)
10	GTP	C4	501	11	29,34,34	1.25	1 (3%)	35,54,54	1.25	4 (11%)
9	GDP	D1	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	3 (10%)
10	GTP	A4	501	11	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
10	GTP	D8	501	11	29,34,34	1.23	2 (6%)	35,54,54	1.31	6 (17%)
9	GDP	A3	502	-	25,30,30	0.97	1 (4%)	30,47,47	1.17	1 (3%)
10	GTP	D0	501	11	29,34,34	1.21	2 (6%)	35,54,54	1.36	5 (14%)
10	GTP	E0	501	11	29,34,34	1.20	2 (6%)	35,54,54	1.39	5 (14%)
9	GDP	A	601	-	25,30,30	0.99	1 (4%)	30,47,47	1.19	3 (10%)
9	GDP	C1	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.30	5 (16%)
9	GDP	D7	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.05	2 (6%)
9	GDP	C5	501	-	25,30,30	0.93	1 (4%)	30,47,47	0.99	2 (6%)
9	GDP	B3	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.13	1 (3%)
10	GTP	B2	501	11	29,34,34	1.23	2 (6%)	35,54,54	1.36	5 (14%)
10	GTP	D2	501	11	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
10	GTP	B0	501	11	29,34,34	1.23	2 (6%)	35,54,54	1.34	4 (11%)
10	GTP	E4	501	11	29,34,34	1.18	2 (6%)	35,54,54	1.33	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GTP	A2	501	11	29,34,34	1.21	2 (6%)	35,54,54	1.37	5 (14%)
10	GTP	E8	501	11	29,34,34	1.19	2 (6%)	35,54,54	1.32	3 (8%)
9	GDP	D3	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.10	2 (6%)
9	GDP	A7	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.12	2 (6%)
9	GDP	D9	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.07	1 (3%)
9	GDP	E5	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.02	1 (3%)
9	GDP	F1	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.14	3 (10%)
10	GTP	D4	501	11	29,34,34	1.23	1 (3%)	35,54,54	1.33	5 (14%)
9	GDP	E1	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.05	2 (6%)
10	GTP	B6	501	11	29,34,34	1.22	2 (6%)	35,54,54	1.30	4 (11%)
10	GTP	D6	501	11	29,34,34	1.22	2 (6%)	35,54,54	1.32	4 (11%)
10	GTP	B4	501	11	29,34,34	1.23	2 (6%)	35,54,54	1.34	6 (17%)
9	GDP	B9	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	1 (3%)
10	GTP	A0	501	11	29,34,34	1.32	2 (6%)	35,54,54	1.38	5 (14%)
10	GTP	A8	501	11	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
9	GDP	E7	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.06	1 (3%)
10	GTP	C6	501	11	29,34,34	1.25	2 (6%)	35,54,54	1.35	4 (11%)
10	GTP	F0	501	11	29,34,34	1.23	1 (3%)	35,54,54	1.33	3 (8%)
9	GDP	B	601	-	25,30,30	1.03	1 (4%)	30,47,47	1.23	4 (13%)
9	GDP	B5	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.03	1 (3%)
10	GTP	B8	501	11	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)
9	GDP	E9	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.14	3 (10%)
9	GDP	B7	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	1 (3%)
9	GDP	C9	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
10	GTP	C8	501	11	29,34,34	1.20	2 (6%)	35,54,54	1.30	5 (14%)
10	GTP	E2	501	11	29,34,34	1.21	2 (6%)	35,54,54	1.33	5 (14%)
9	GDP	D5	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.12	2 (6%)
10	GTP	E6	501	11	29,34,34	1.20	2 (6%)	35,54,54	1.31	4 (11%)
9	GDP	C7	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.22	3 (10%)
10	GTP	A6	501	11	29,34,34	1.23	2 (6%)	35,54,54	1.40	6 (17%)
9	GDP	A5	501	-	25,30,30	0.93	1 (4%)	30,47,47	1.06	1 (3%)
9	GDP	E3	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.02	2 (6%)
10	GTP	C2	501	11	29,34,34	1.27	2 (6%)	35,54,54	1.52	8 (22%)
10	GTP	C0	501	11	29,34,34	1.29	3 (10%)	35,54,54	1.41	7 (20%)

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	C3	501	-	-	3/12/32/32	0/3/3/3
9	GDP	A1	501	-	-	5/12/32/32	0/3/3/3
10	GTP	C4	501	11	-	7/18/38/38	0/3/3/3
9	GDP	D1	501	-	-	2/12/32/32	0/3/3/3
10	GTP	A4	501	11	-	3/18/38/38	0/3/3/3
10	GTP	D8	501	11	-	6/18/38/38	0/3/3/3
9	GDP	A3	502	-	-	4/12/32/32	0/3/3/3
10	GTP	D0	501	11	-	6/18/38/38	0/3/3/3
10	GTP	E0	501	11	-	2/18/38/38	0/3/3/3
9	GDP	A	601	-	-	5/12/32/32	0/3/3/3
9	GDP	C1	501	-	-	2/12/32/32	0/3/3/3
9	GDP	D7	501	-	-	4/12/32/32	0/3/3/3
9	GDP	C5	501	-	-	4/12/32/32	0/3/3/3
9	GDP	B3	501	-	-	3/12/32/32	0/3/3/3
10	GTP	B2	501	11	-	6/18/38/38	0/3/3/3
10	GTP	D2	501	11	-	9/18/38/38	0/3/3/3
10	GTP	B0	501	11	-	8/18/38/38	0/3/3/3
10	GTP	E4	501	11	-	8/18/38/38	0/3/3/3
10	GTP	A2	501	11	-	9/18/38/38	0/3/3/3
10	GTP	E8	501	11	-	5/18/38/38	0/3/3/3
9	GDP	D3	501	-	-	3/12/32/32	0/3/3/3
9	GDP	A7	501	-	-	3/12/32/32	0/3/3/3
9	GDP	D9	501	-	-	4/12/32/32	0/3/3/3
9	GDP	E5	501	-	-	1/12/32/32	0/3/3/3
9	GDP	F1	501	-	-	4/12/32/32	0/3/3/3
10	GTP	D4	501	11	-	5/18/38/38	0/3/3/3
9	GDP	E1	501	-	-	4/12/32/32	0/3/3/3
10	GTP	B6	501	11	-	7/18/38/38	0/3/3/3
10	GTP	D6	501	11	-	7/18/38/38	0/3/3/3
10	GTP	B4	501	11	-	8/18/38/38	0/3/3/3
9	GDP	B9	501	-	-	3/12/32/32	0/3/3/3
10	GTP	A0	501	11	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GTP	A8	501	11	-	7/18/38/38	0/3/3/3
9	GDP	E7	501	-	-	6/12/32/32	0/3/3/3
10	GTP	C6	501	11	-	9/18/38/38	0/3/3/3
10	GTP	F0	501	11	-	7/18/38/38	0/3/3/3
9	GDP	B	601	-	-	4/12/32/32	0/3/3/3
9	GDP	B5	501	-	-	5/12/32/32	0/3/3/3
10	GTP	B8	501	11	-	8/18/38/38	0/3/3/3
9	GDP	E9	501	-	-	5/12/32/32	0/3/3/3
9	GDP	B7	501	-	-	3/12/32/32	0/3/3/3
9	GDP	C9	501	-	-	3/12/32/32	0/3/3/3
10	GTP	C8	501	11	-	4/18/38/38	0/3/3/3
10	GTP	E2	501	11	-	1/18/38/38	0/3/3/3
9	GDP	D5	501	-	-	9/12/32/32	0/3/3/3
10	GTP	E6	501	11	-	7/18/38/38	0/3/3/3
9	GDP	C7	501	-	-	2/12/32/32	0/3/3/3
10	GTP	A6	501	11	-	6/18/38/38	0/3/3/3
9	GDP	A5	501	-	-	2/12/32/32	0/3/3/3
9	GDP	E3	501	-	-	5/12/32/32	0/3/3/3
10	GTP	C2	501	11	-	6/18/38/38	0/3/3/3
10	GTP	C0	501	11	-	7/18/38/38	0/3/3/3

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A0	501	GTP	C5-C6	-4.71	1.38	1.47
10	C4	501	GTP	C5-C6	-4.63	1.38	1.47
10	C6	501	GTP	C5-C6	-4.55	1.38	1.47
10	D6	501	GTP	C5-C6	-4.51	1.38	1.47
10	C2	501	GTP	C5-C6	-4.51	1.38	1.47

The worst 5 of 178 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E8	501	GTP	C8-N7-C5	3.77	108.97	102.55
10	F0	501	GTP	C8-N7-C5	3.73	108.90	102.55
10	C0	501	GTP	C8-N7-C5	3.72	108.88	102.55
10	A8	501	GTP	C8-N7-C5	3.68	108.82	102.55
10	A6	501	GTP	C8-N7-C5	3.68	108.82	102.55

There are no chirality outliers.

5 of 259 torsion outliers are listed below:

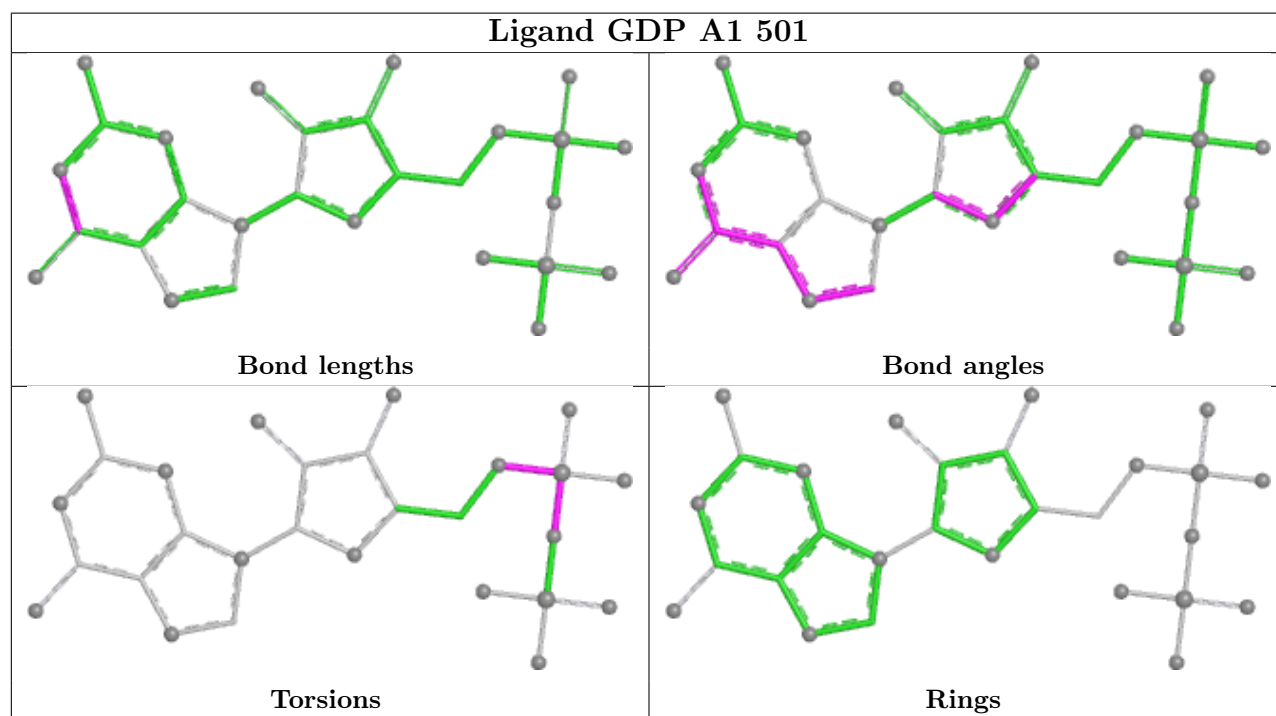
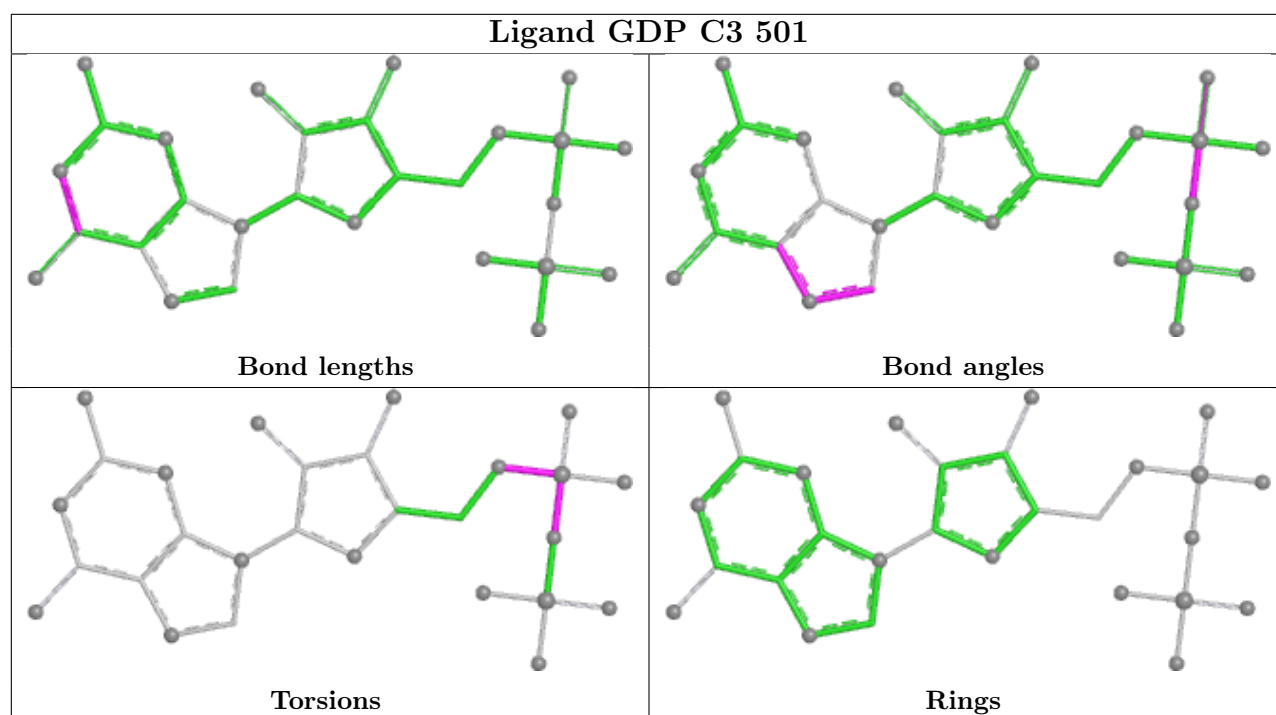
Mol	Chain	Res	Type	Atoms
9	A	601	GDP	C5'-O5'-PA-O3A
9	A	601	GDP	C5'-O5'-PA-O1A
9	A	601	GDP	C5'-O5'-PA-O2A
9	A1	501	GDP	C5'-O5'-PA-O3A
9	A1	501	GDP	C5'-O5'-PA-O1A

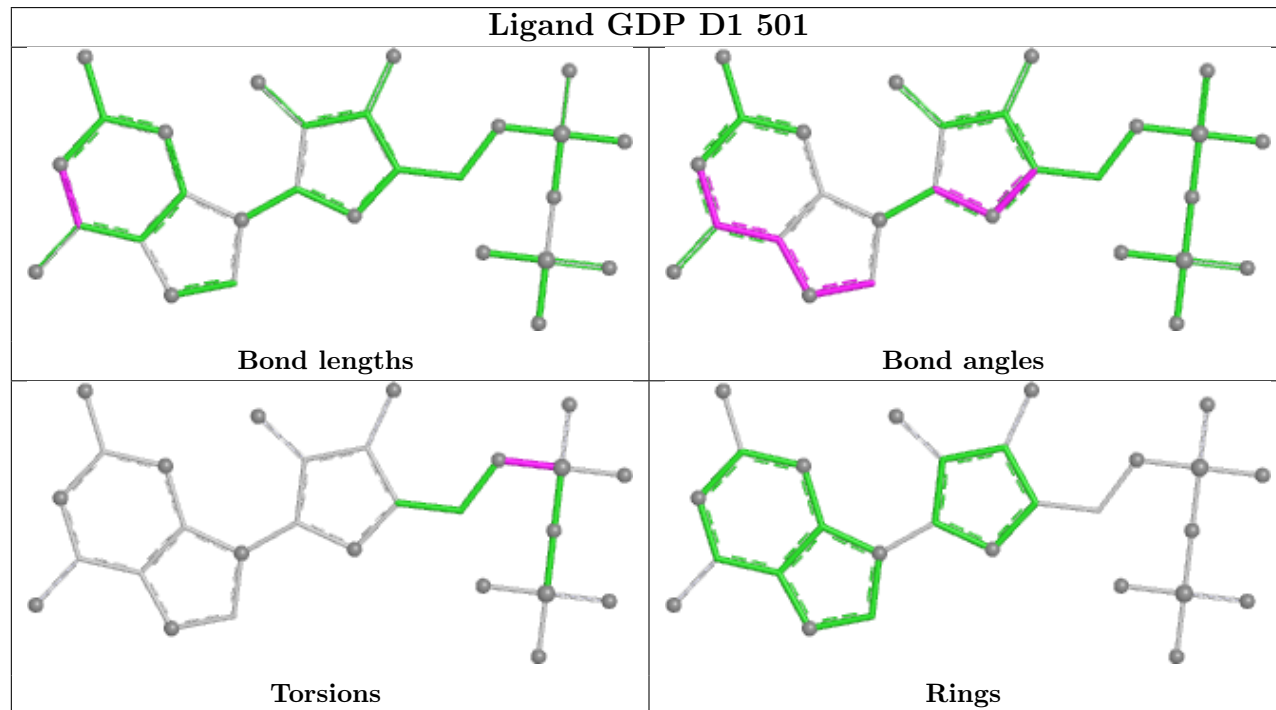
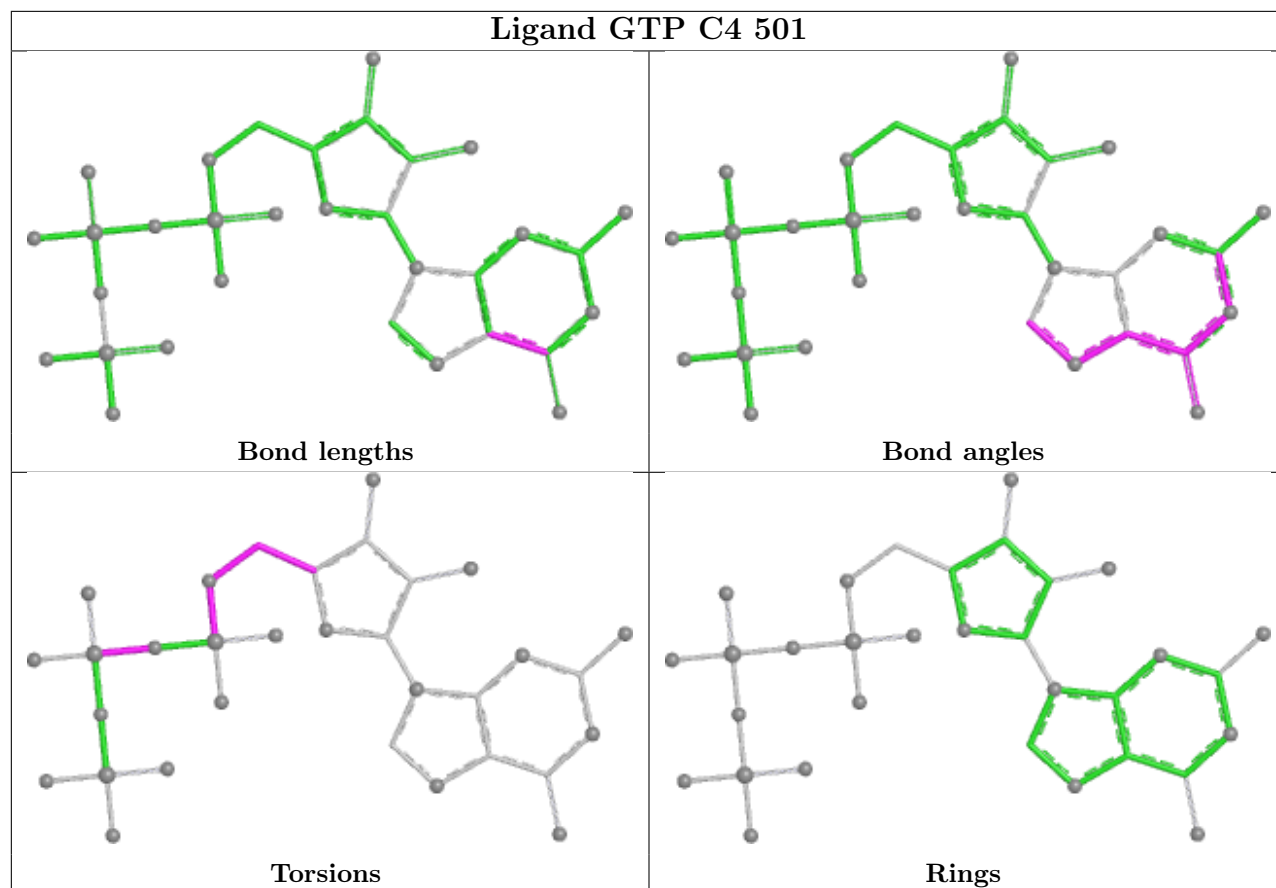
There are no ring outliers.

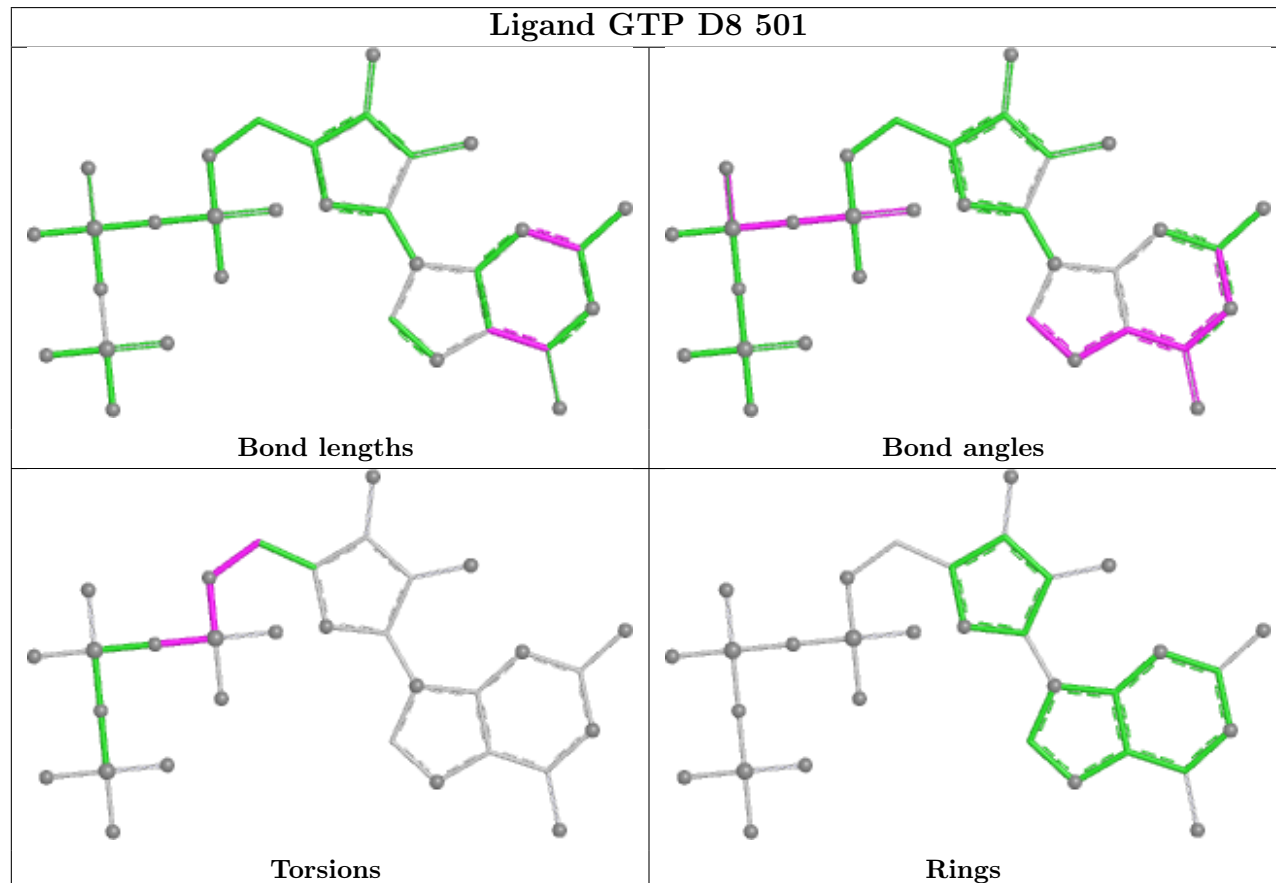
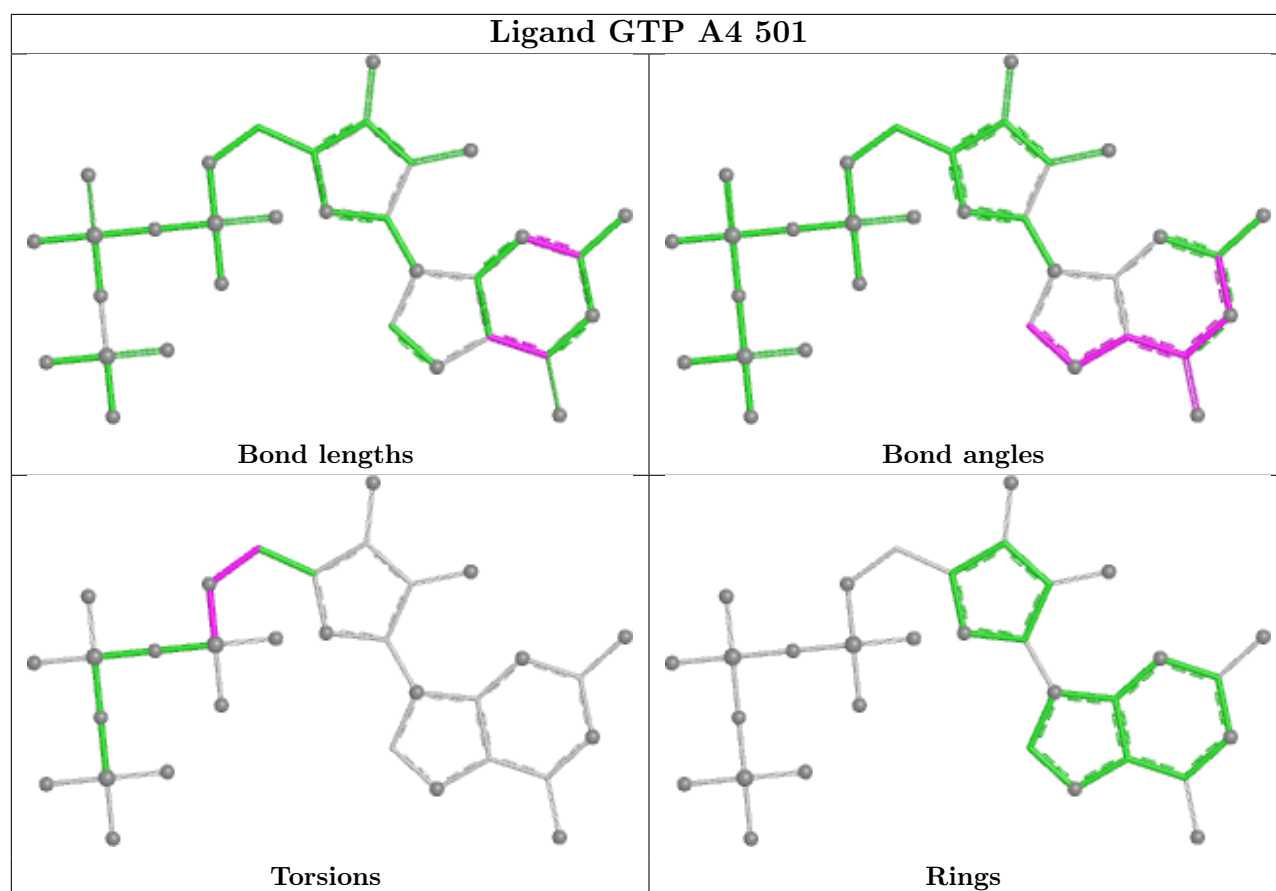
2 monomers are involved in 4 short contacts:

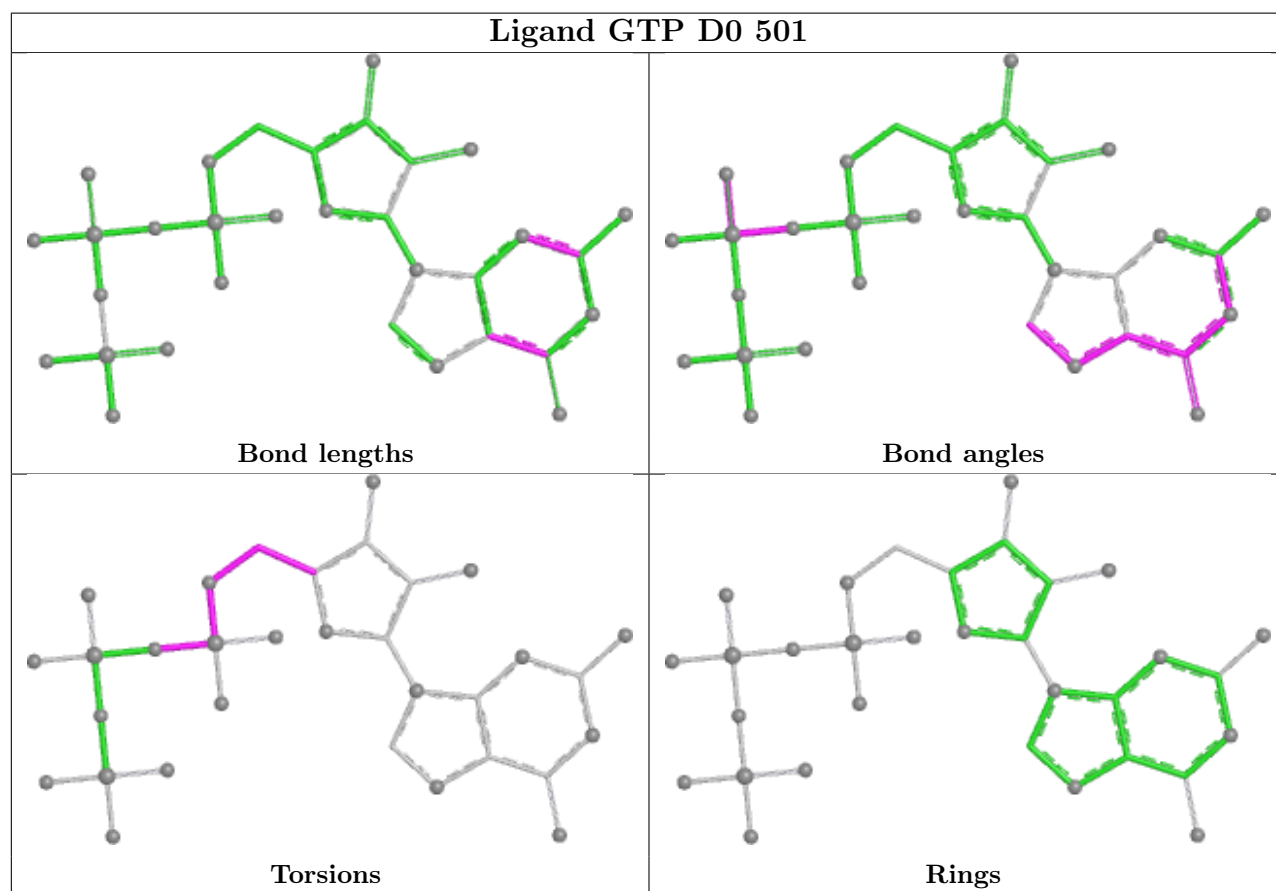
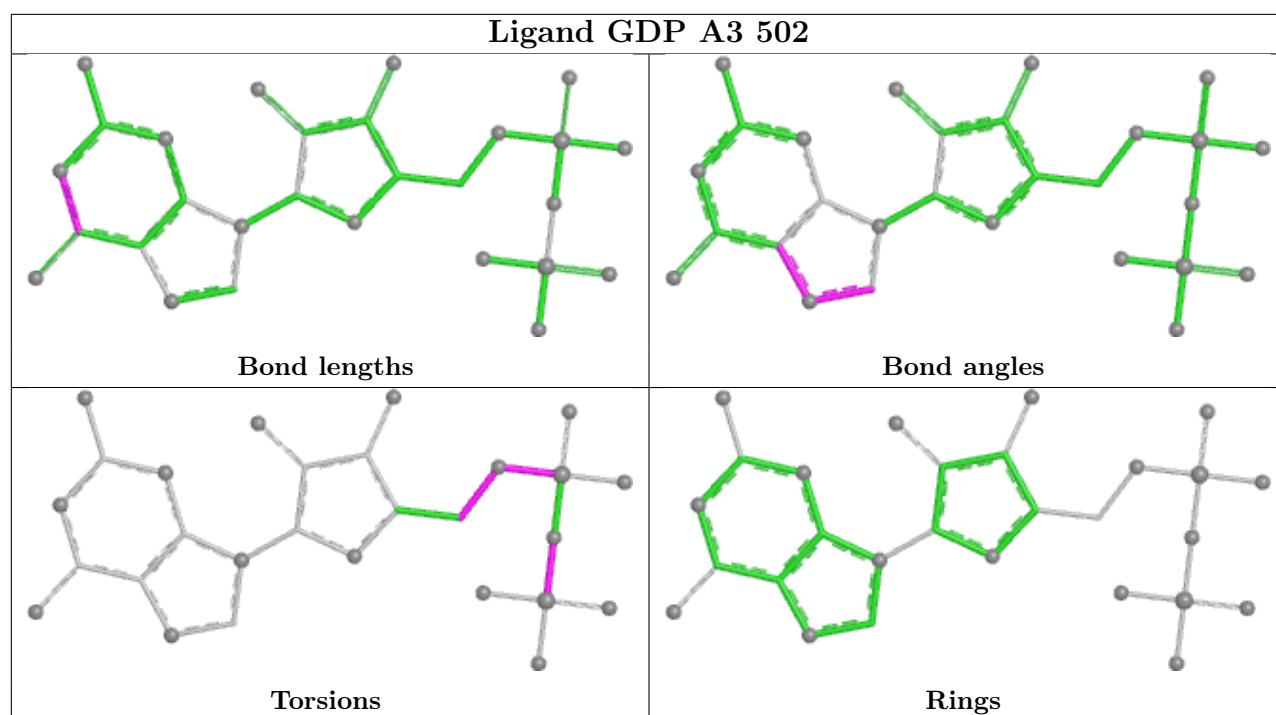
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E9	501	GDP	3	0
10	C0	501	GTP	1	0

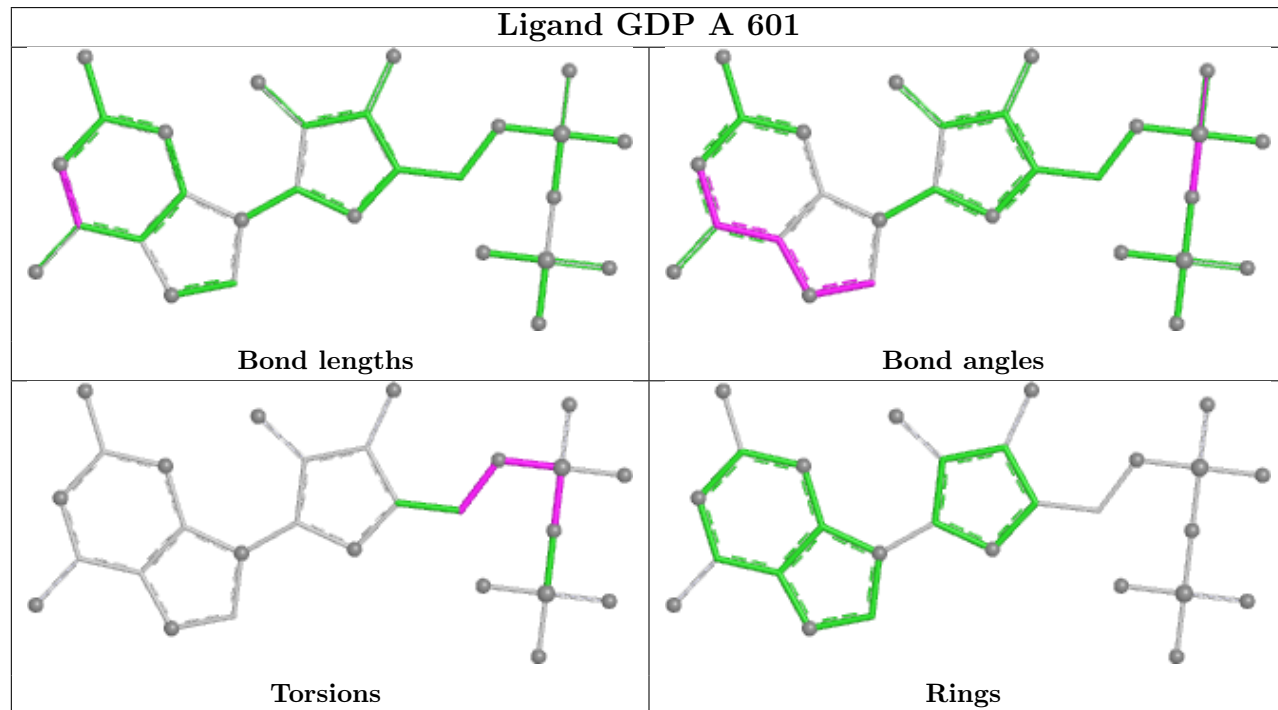
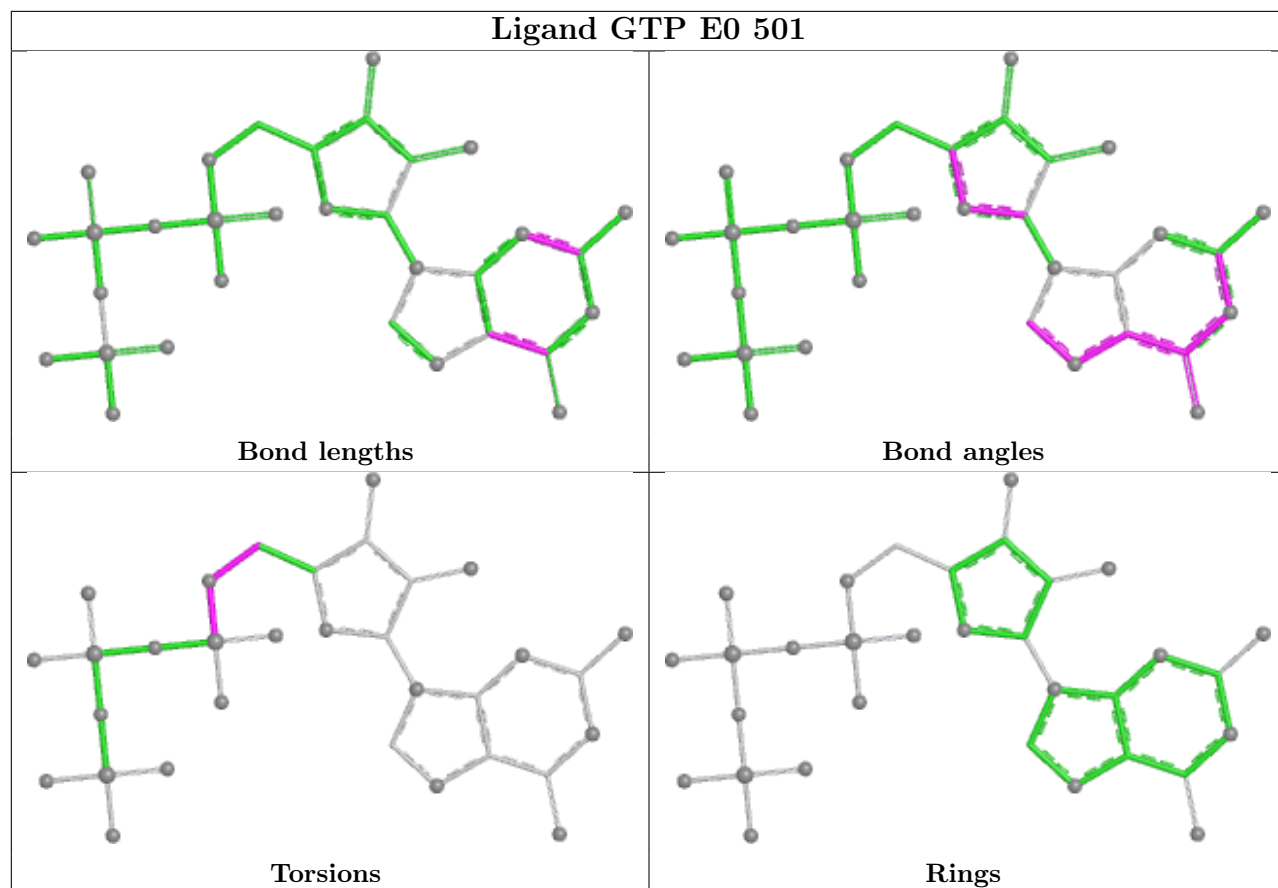
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

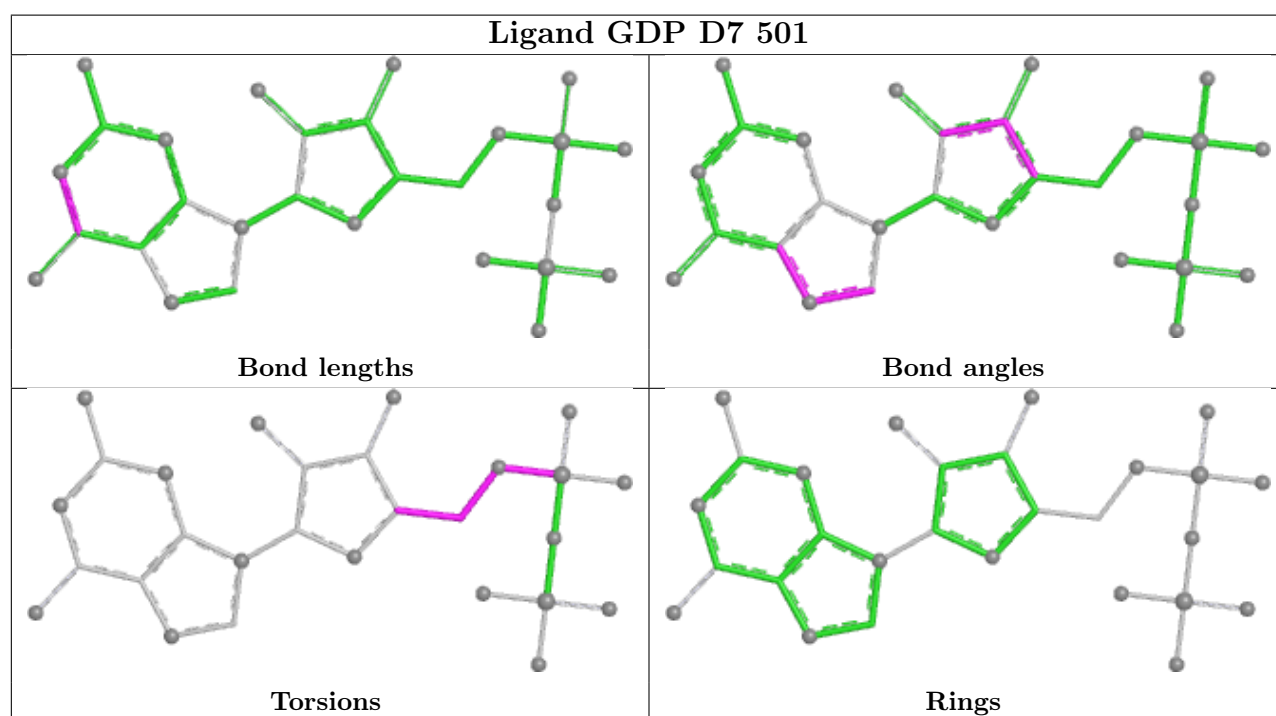
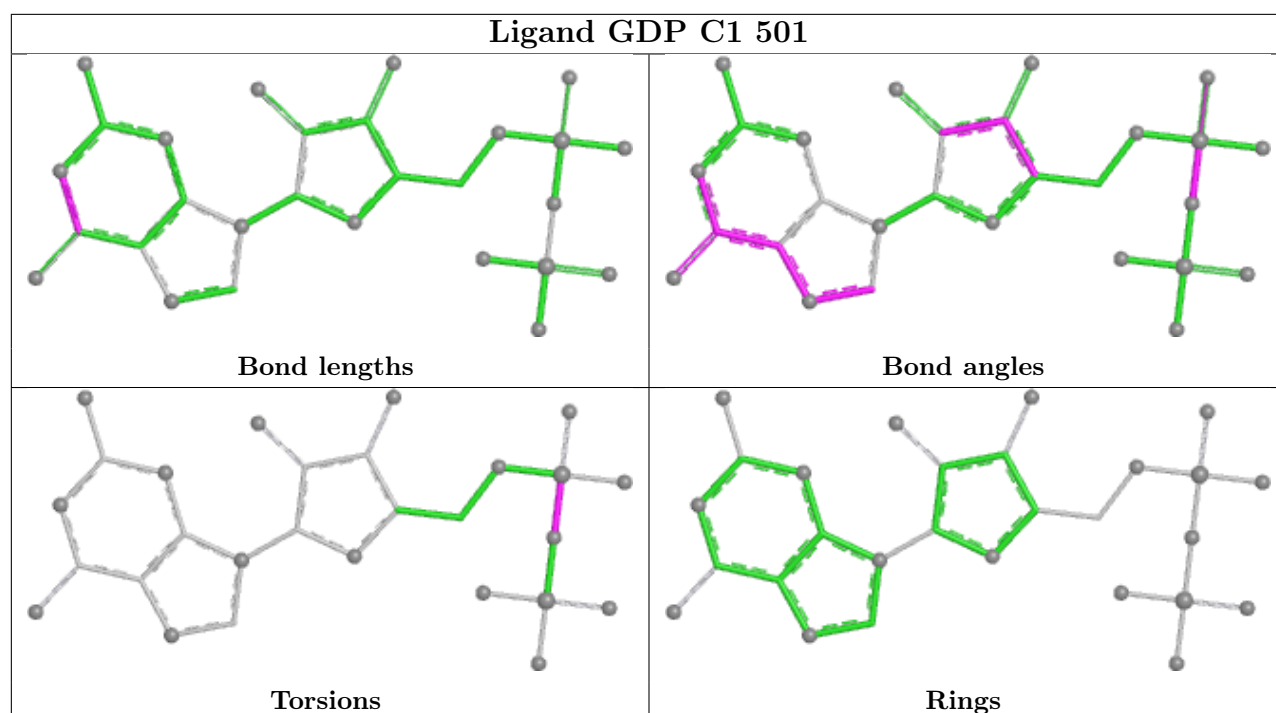


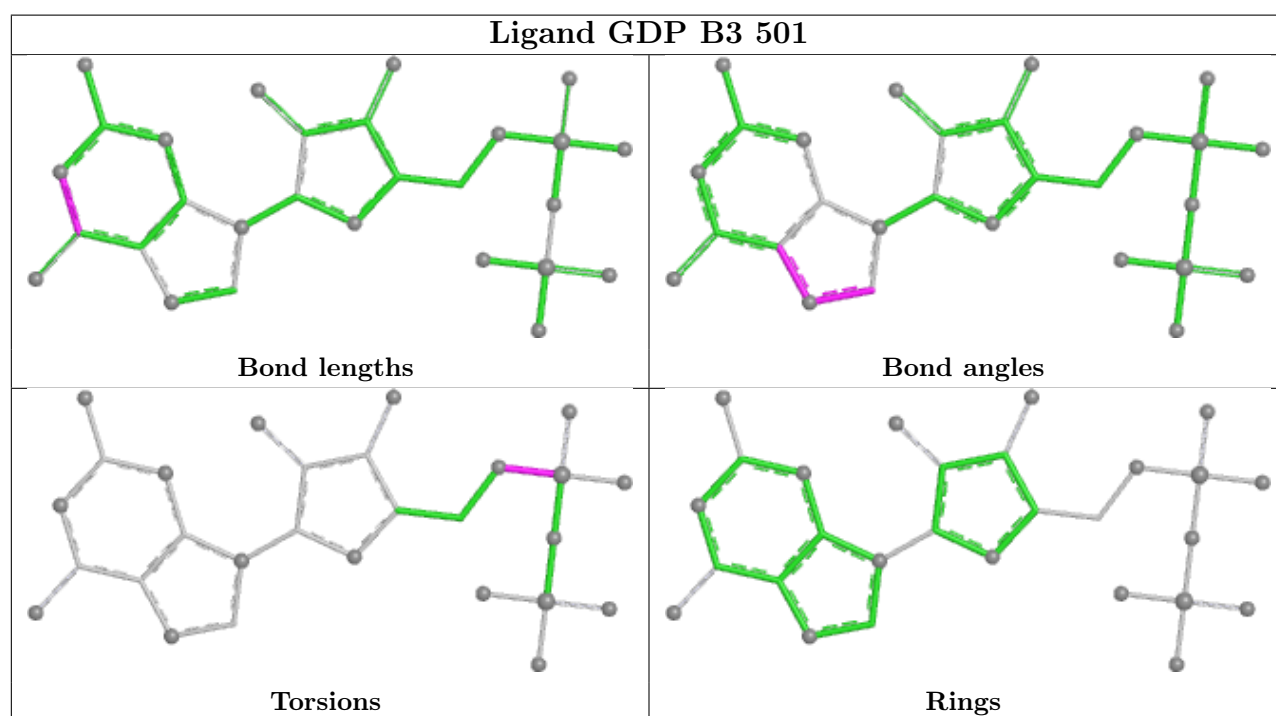
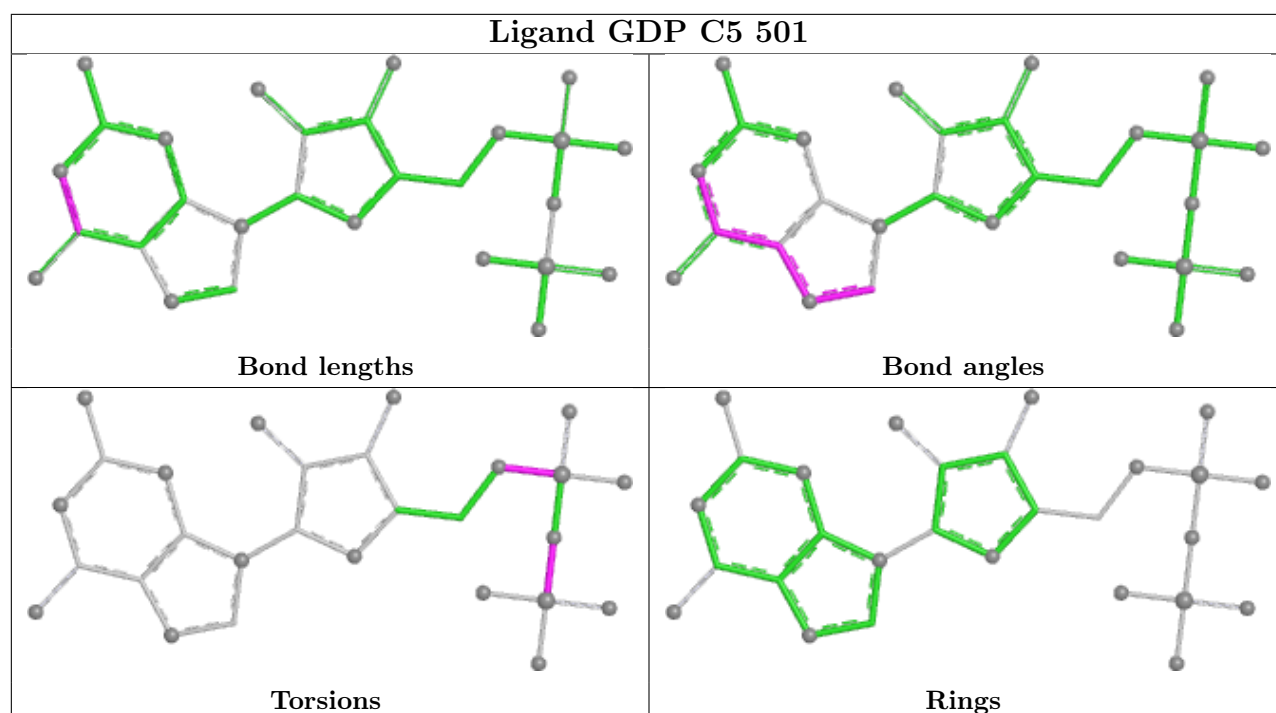


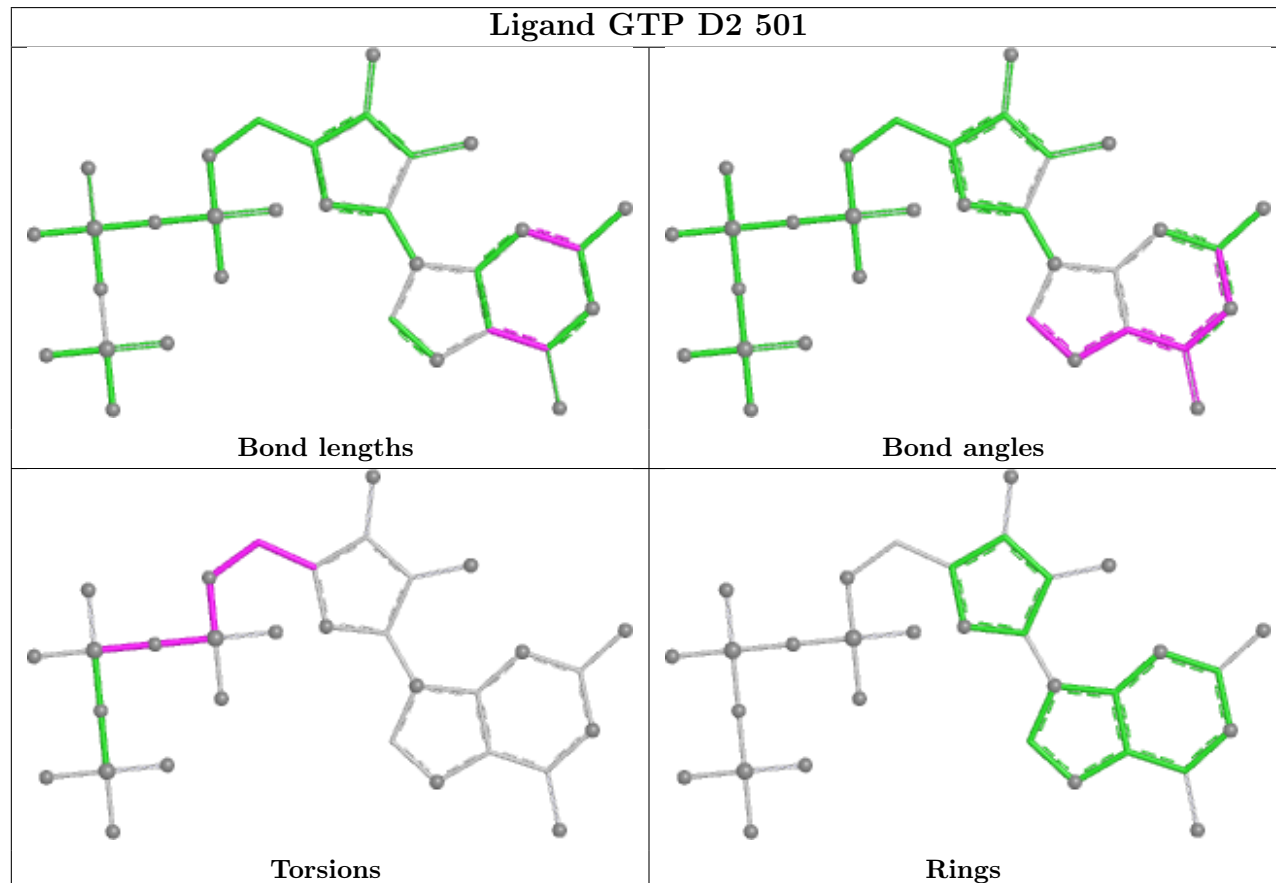
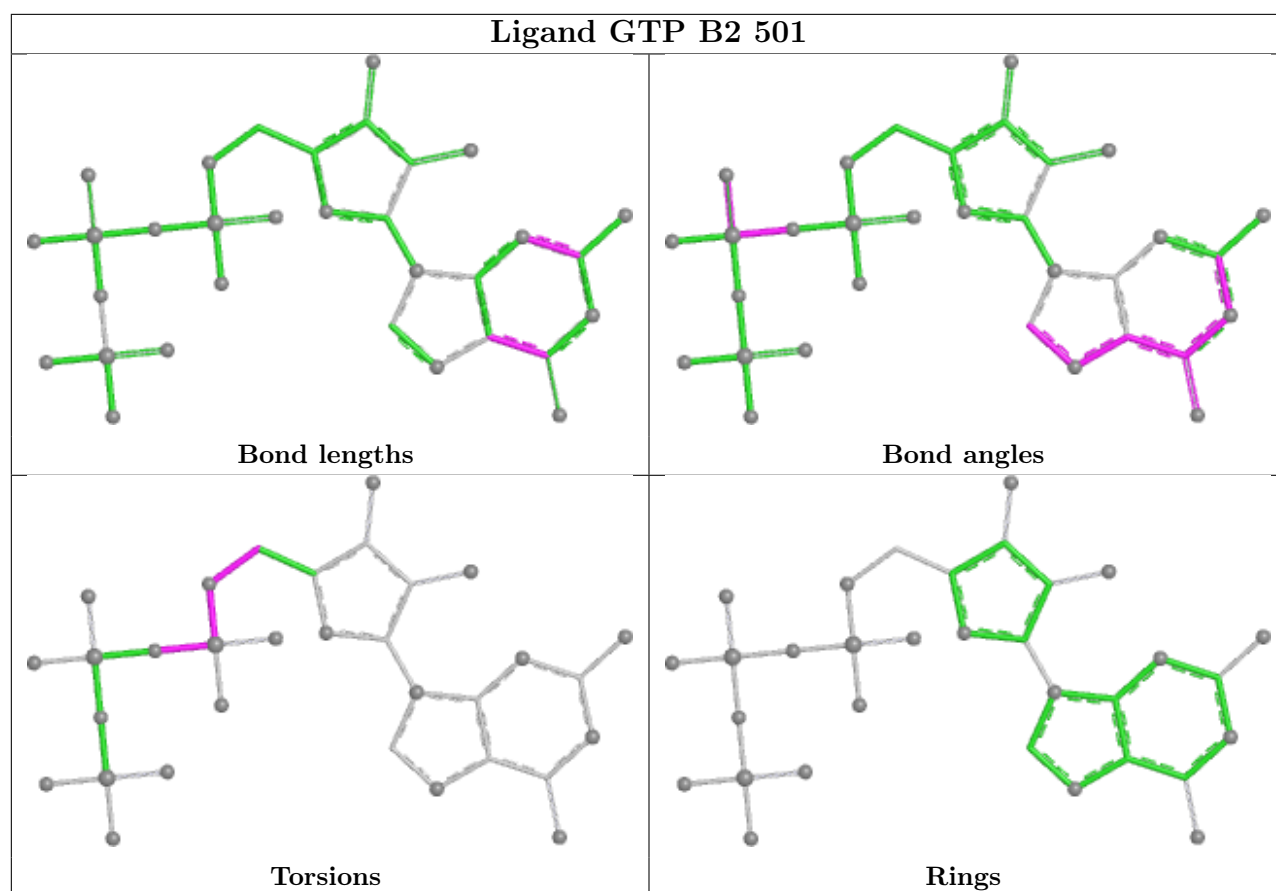




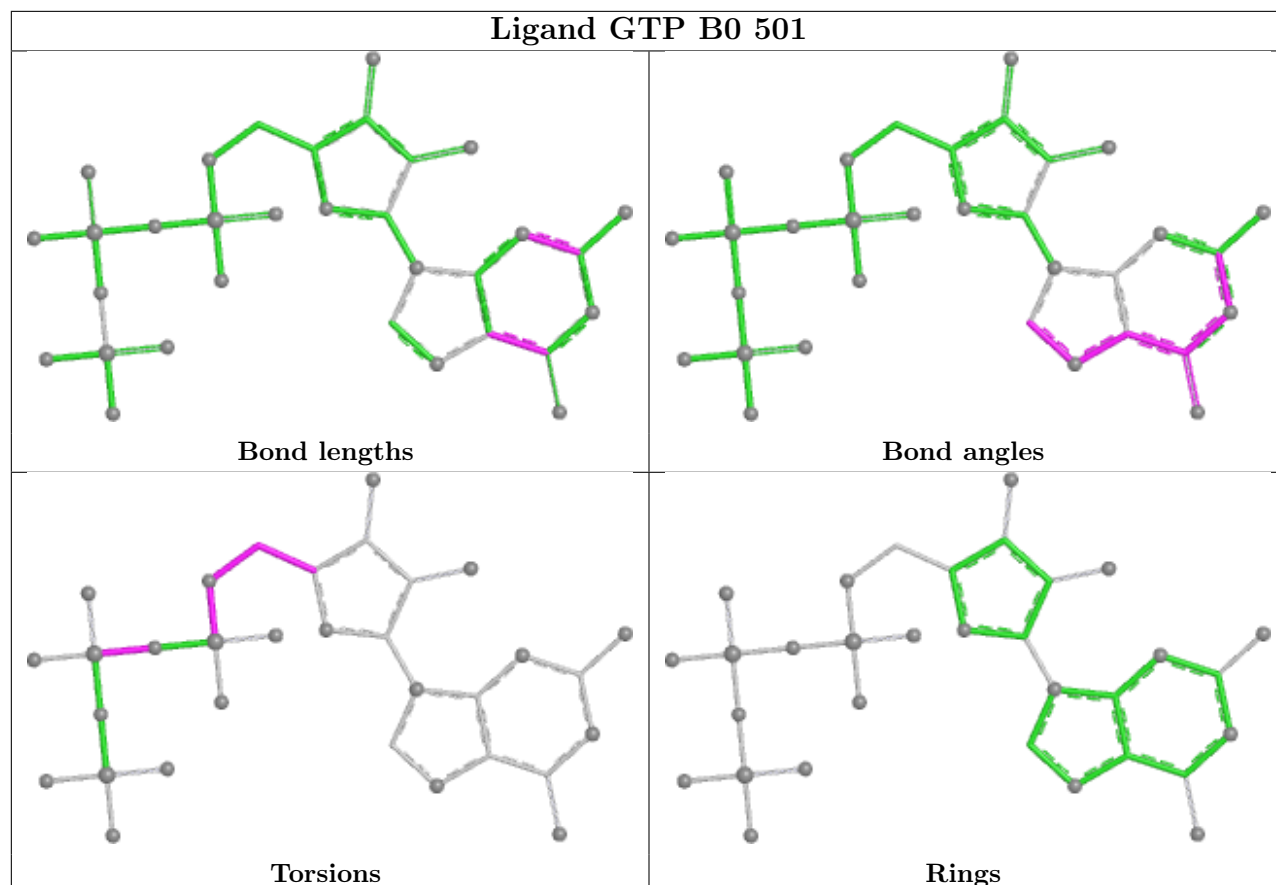




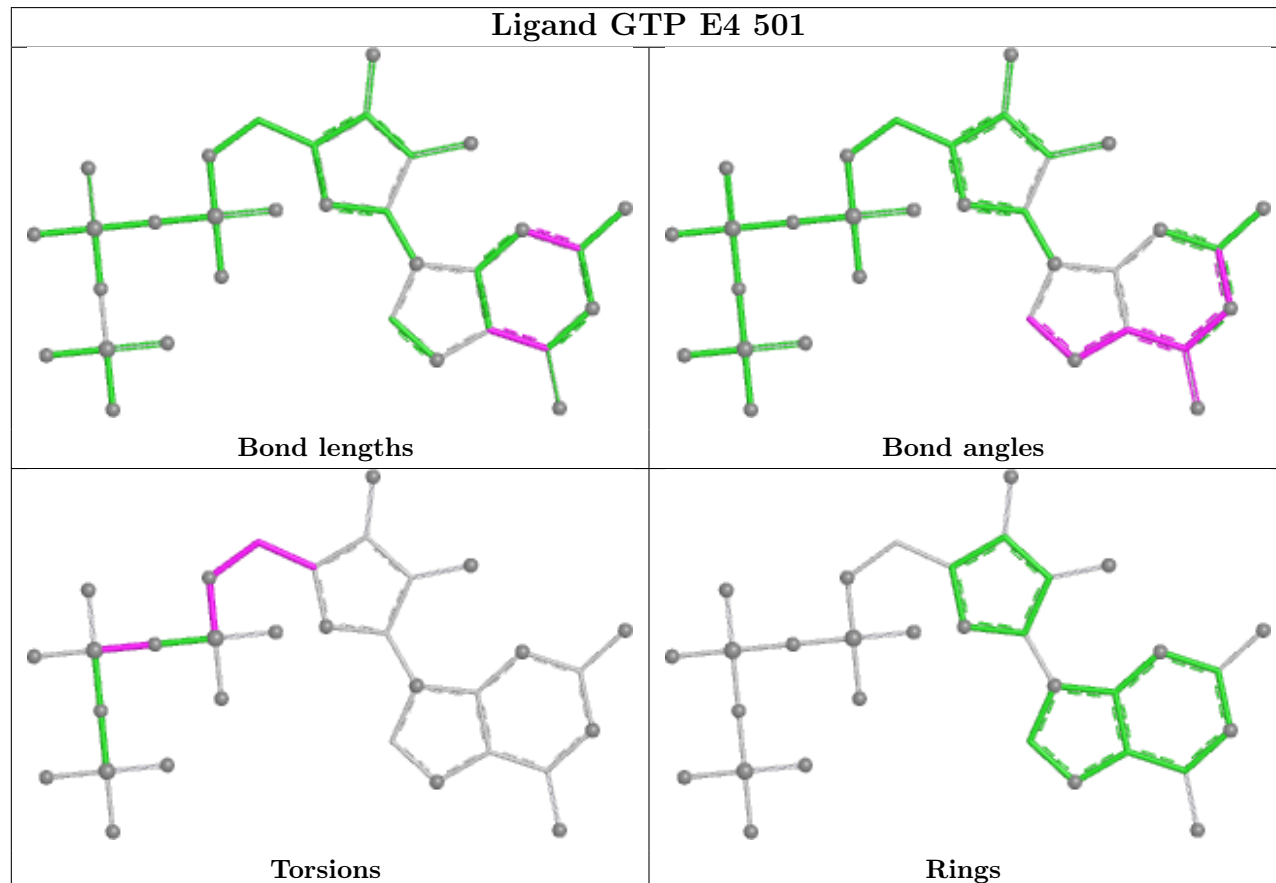




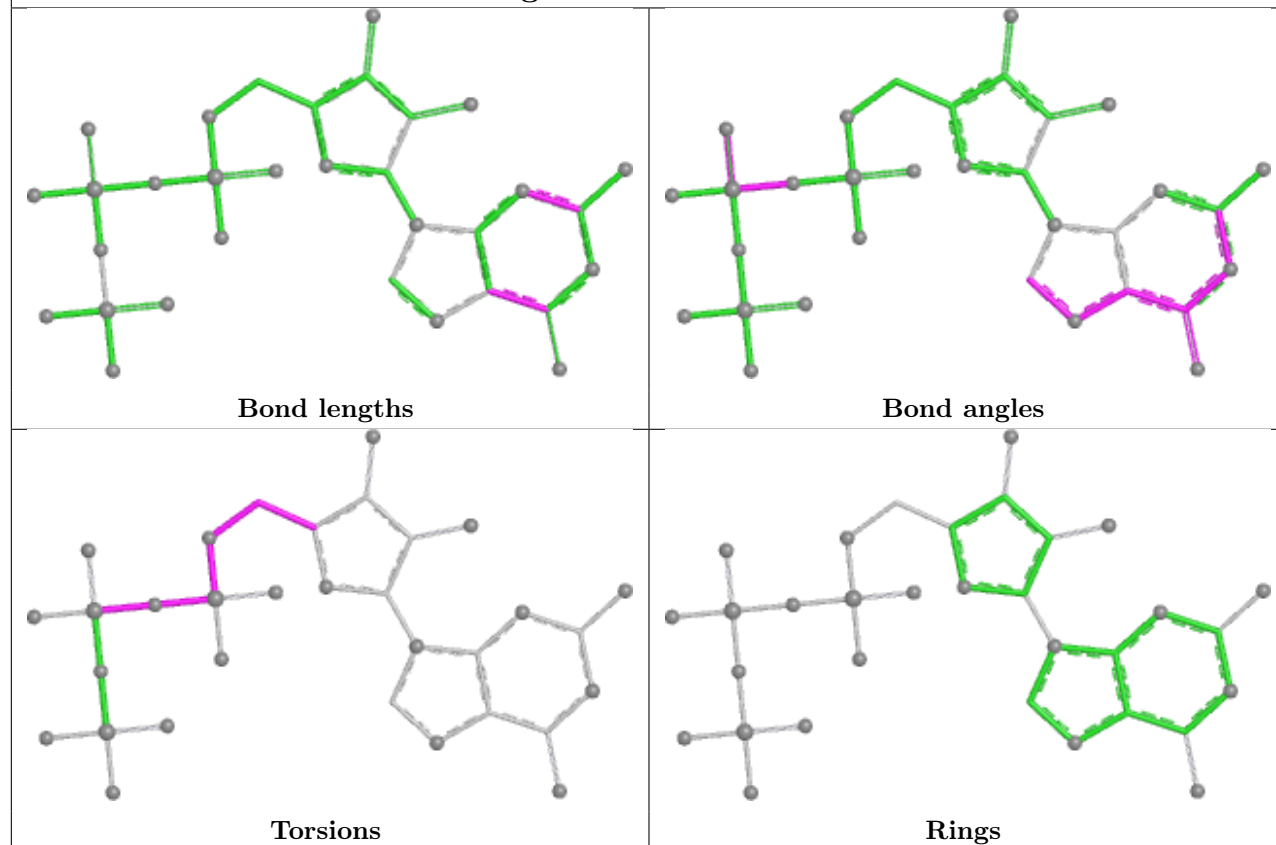
Ligand GTP B0 501



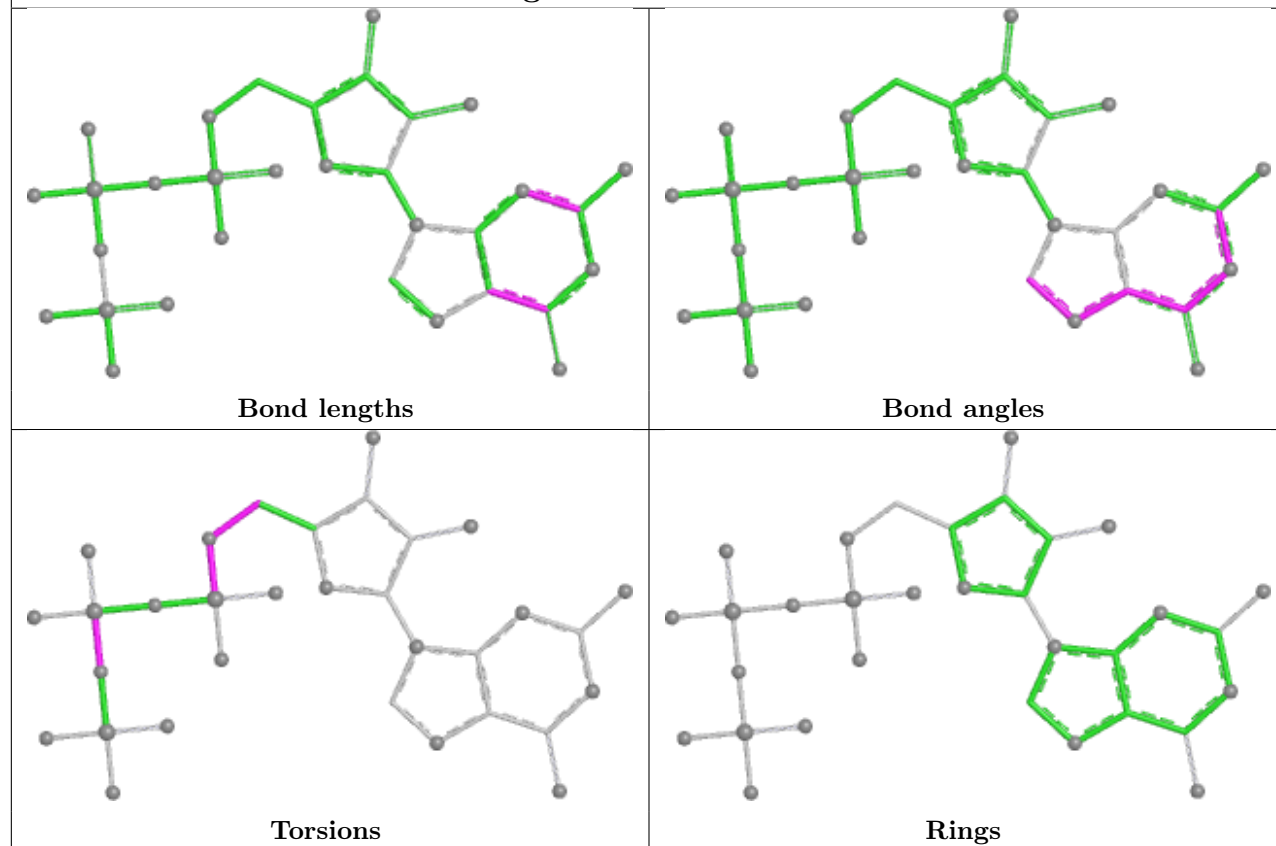
Ligand GTP E4 501

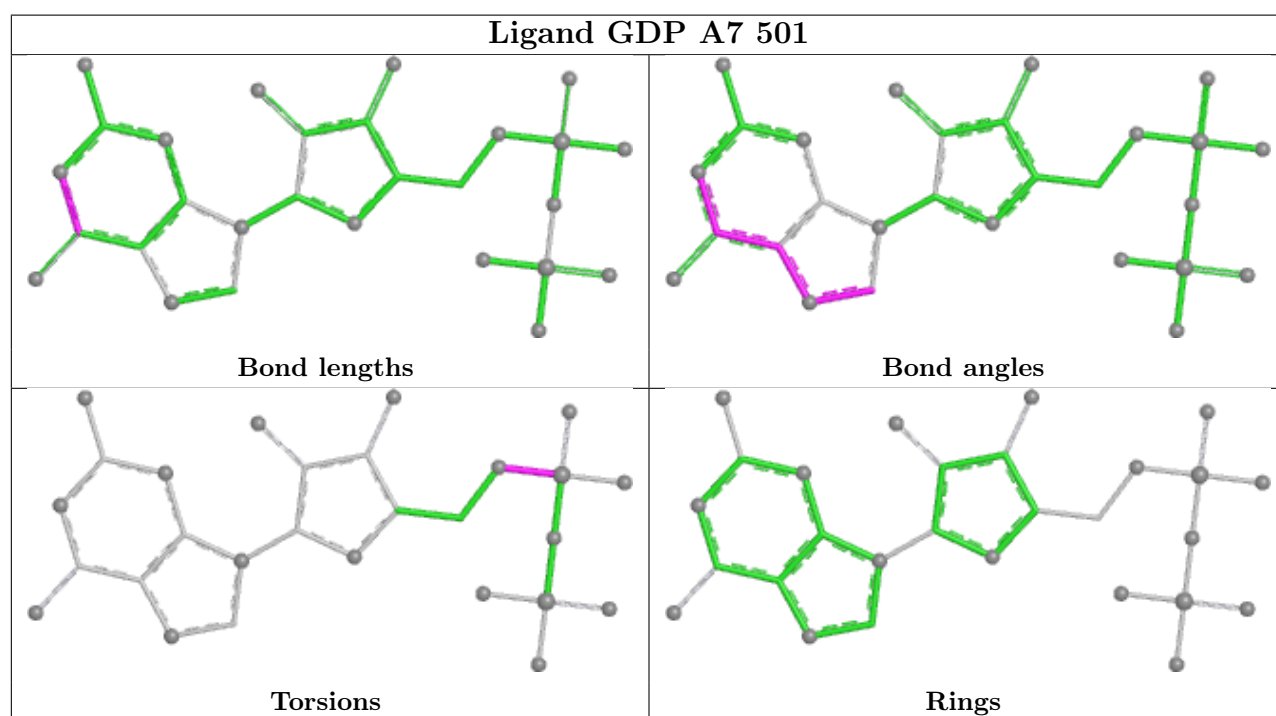
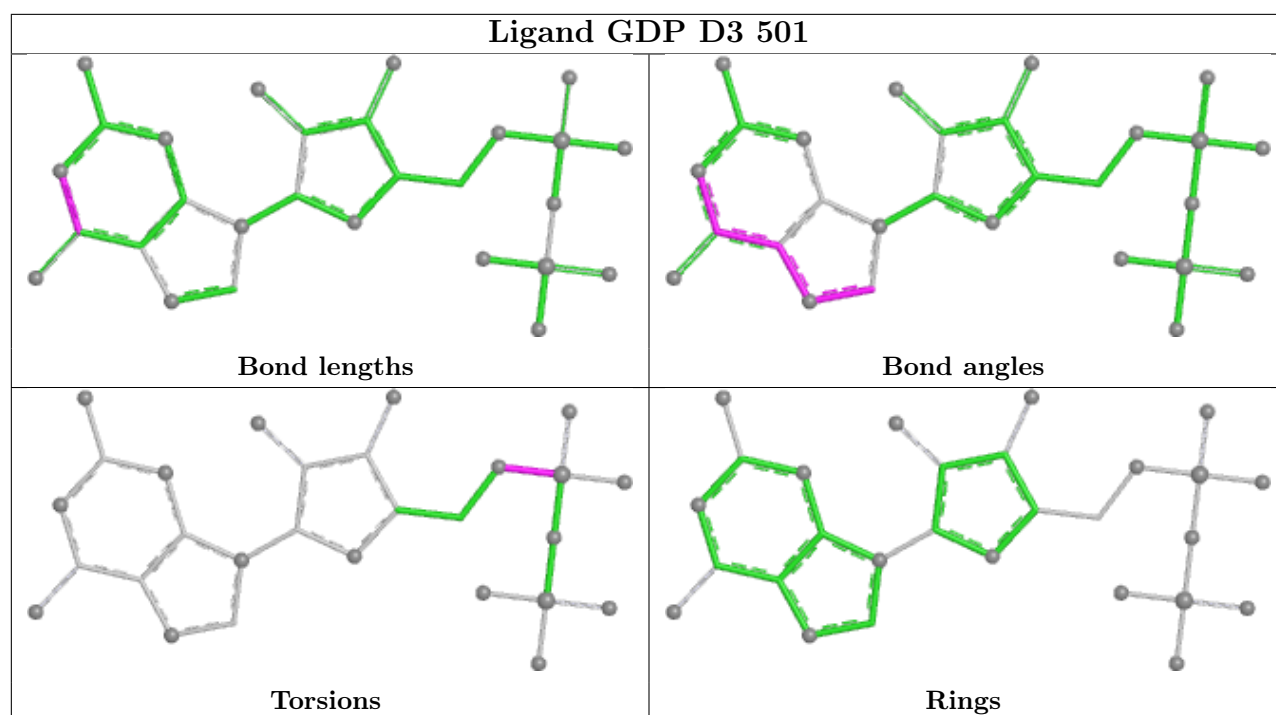


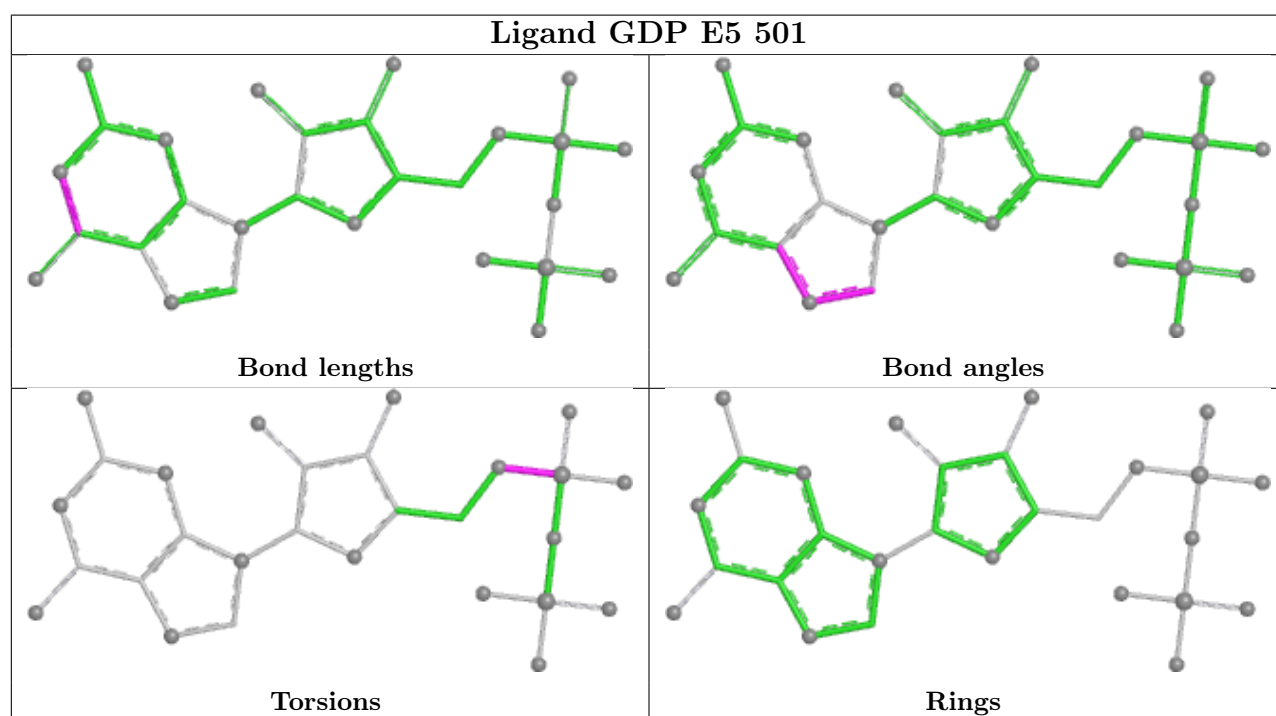
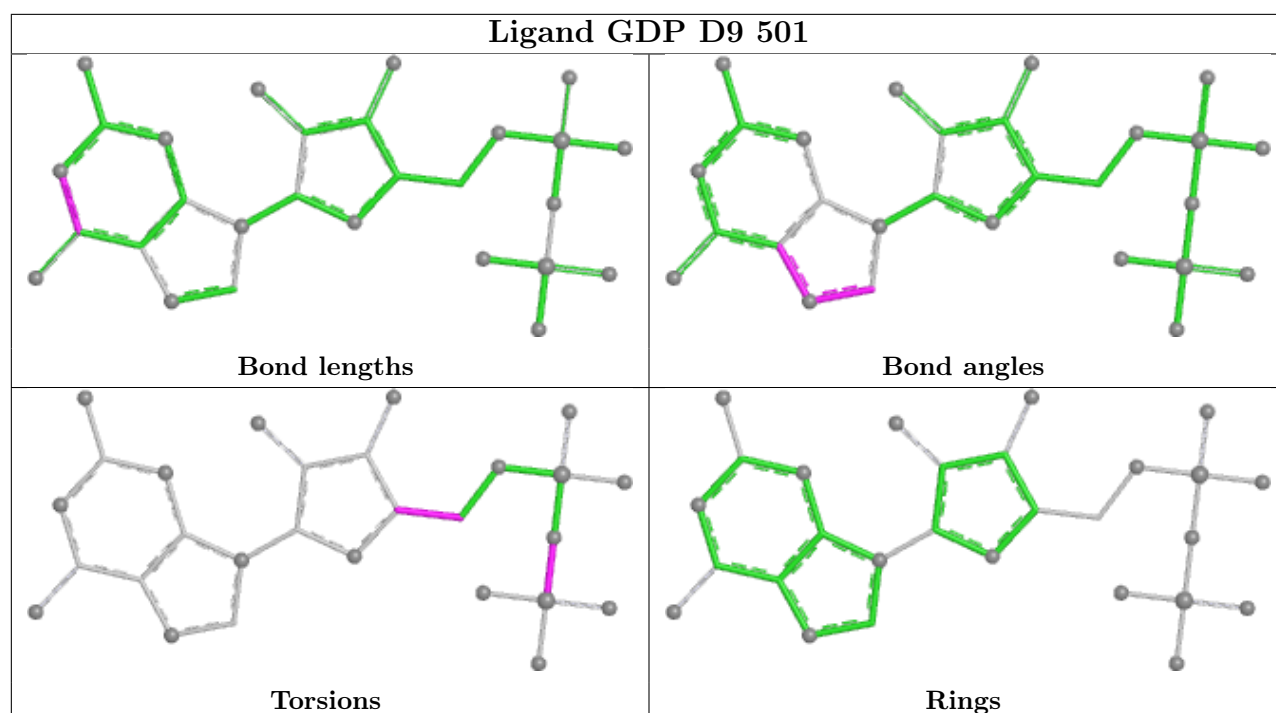
Ligand GTP A2 501

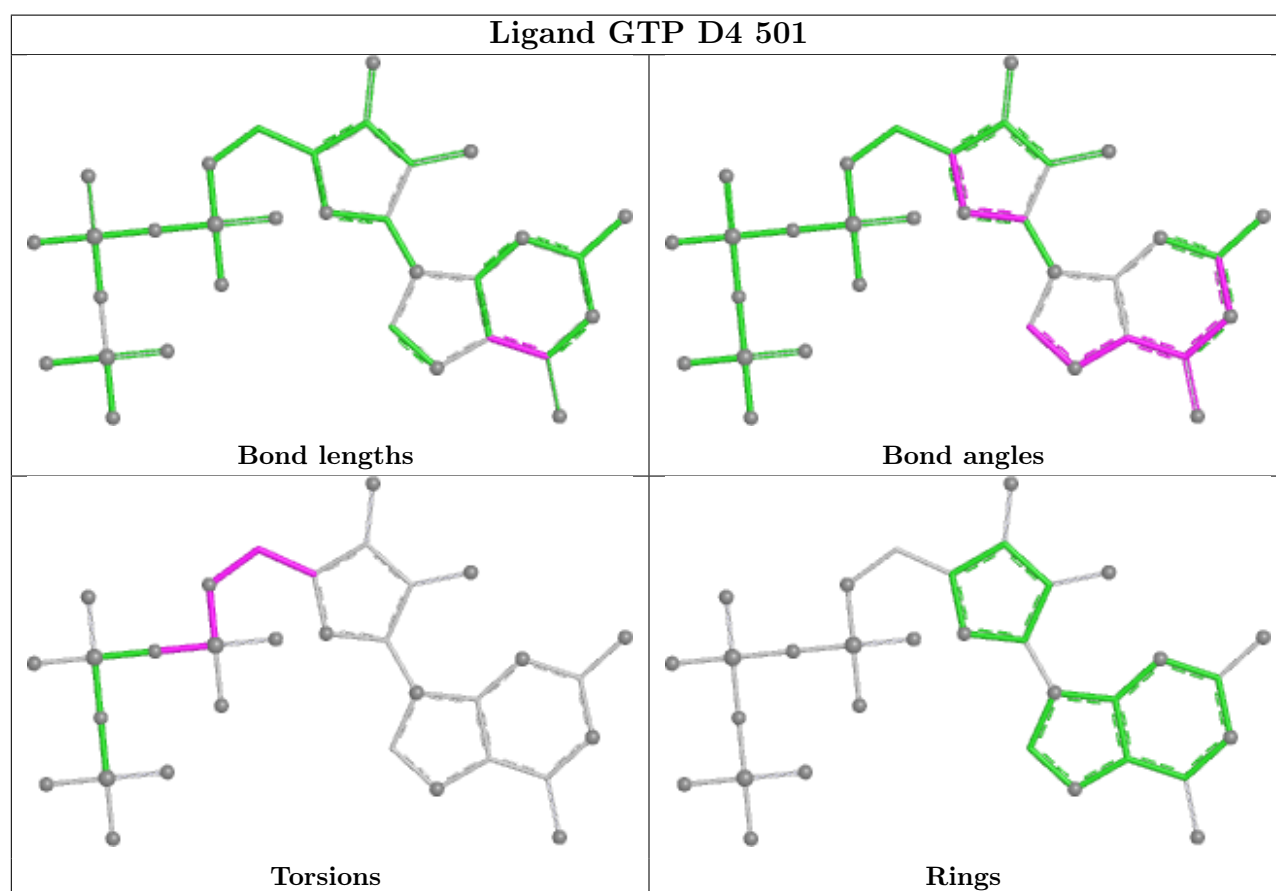
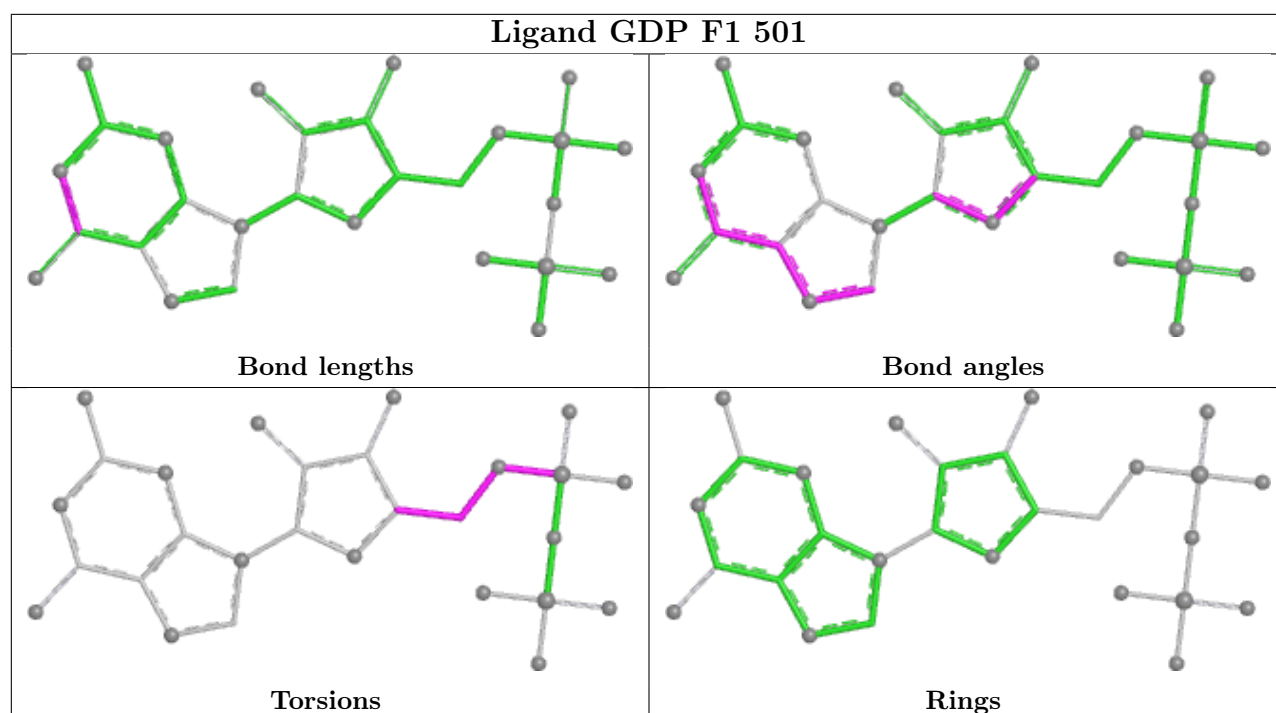


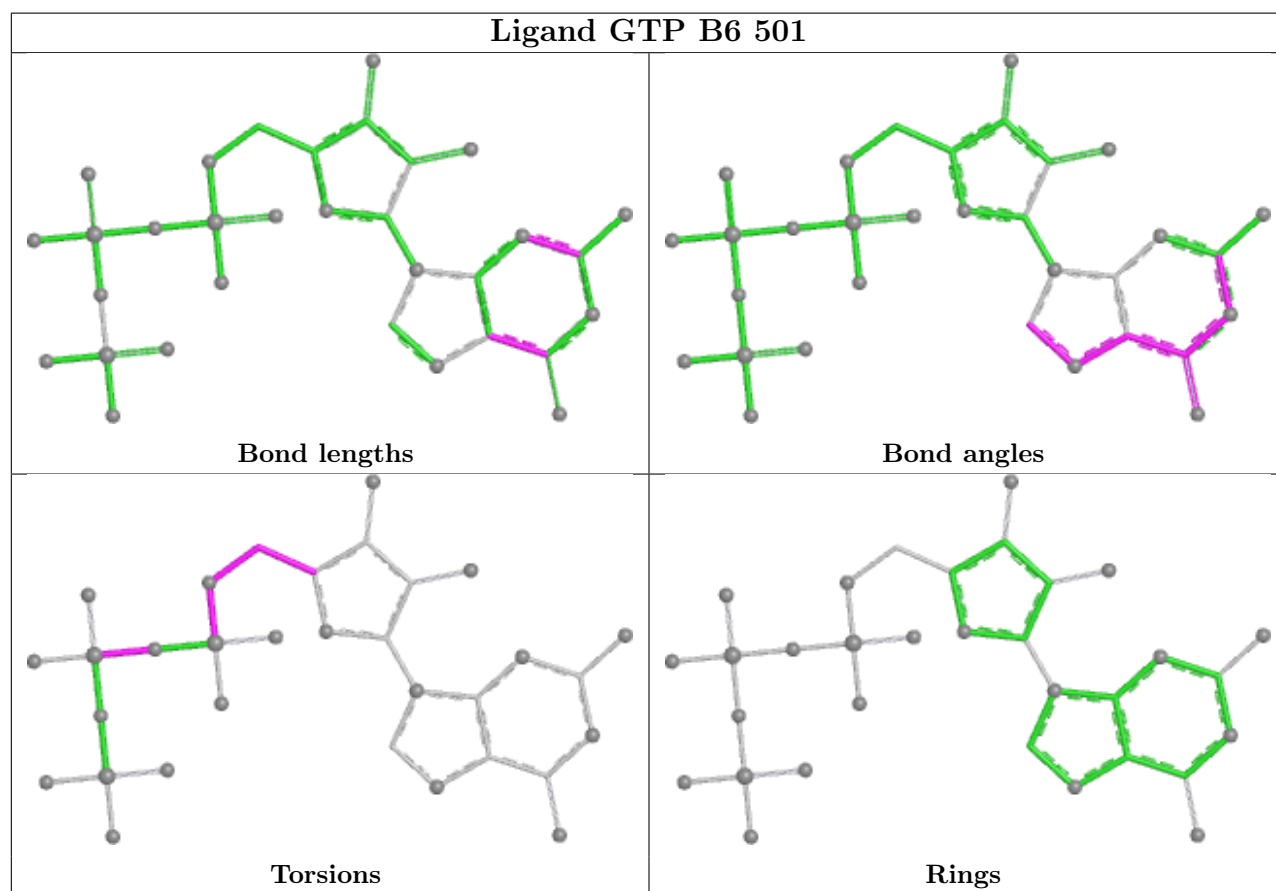
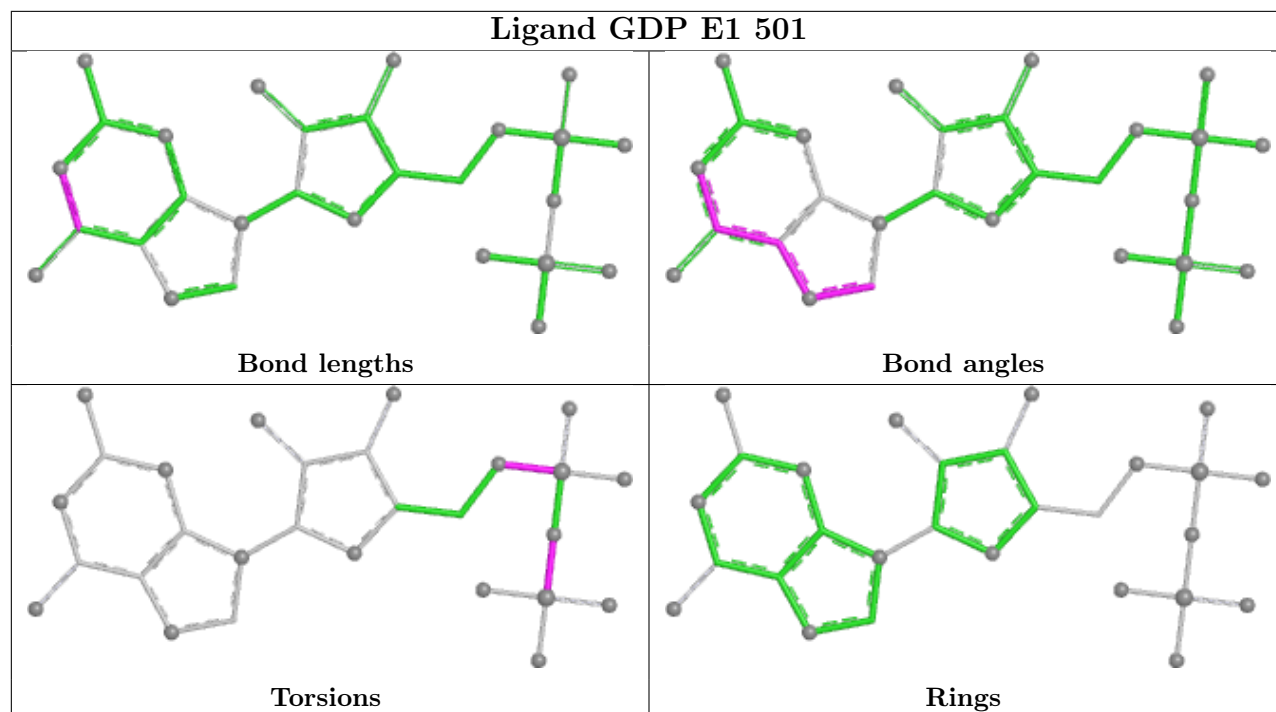
Ligand GTP E8 501



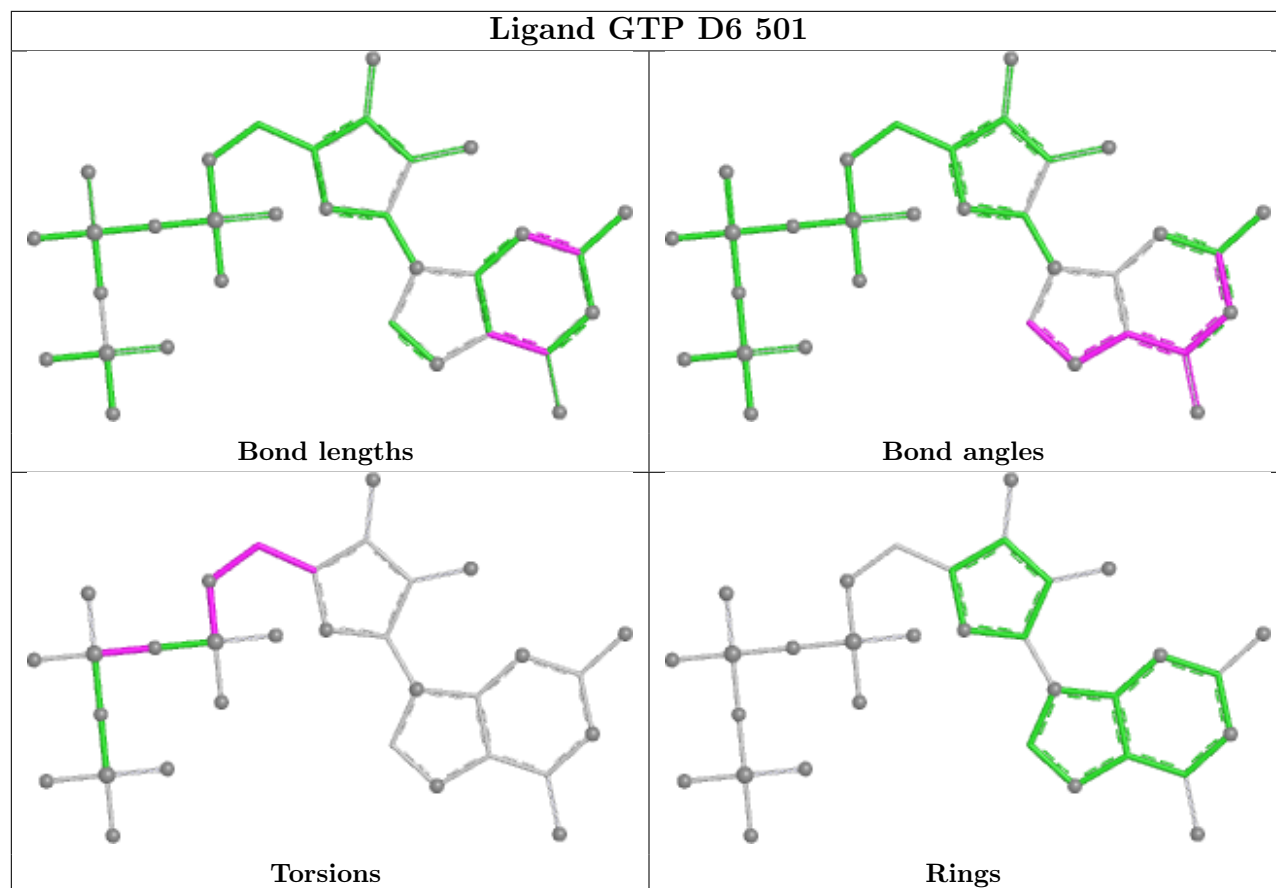




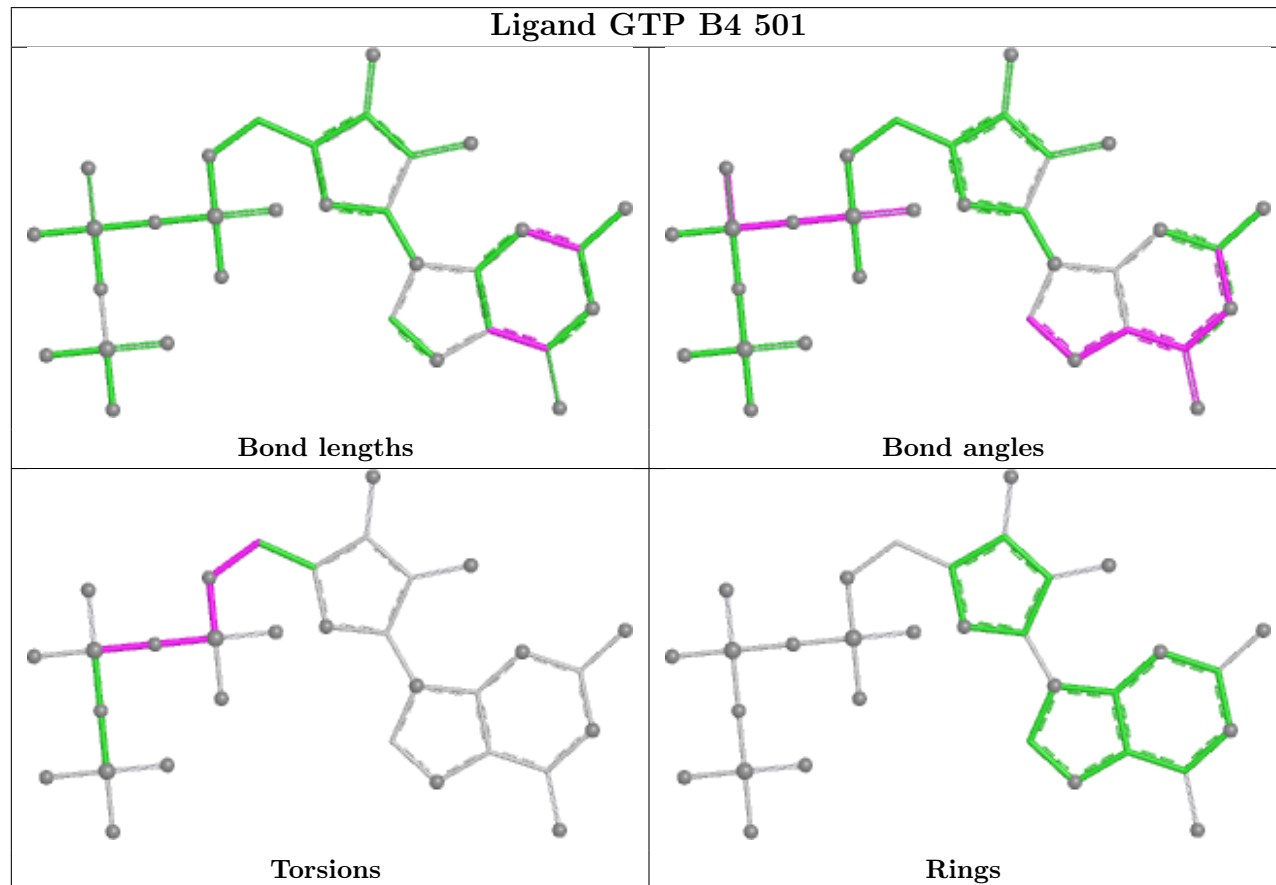


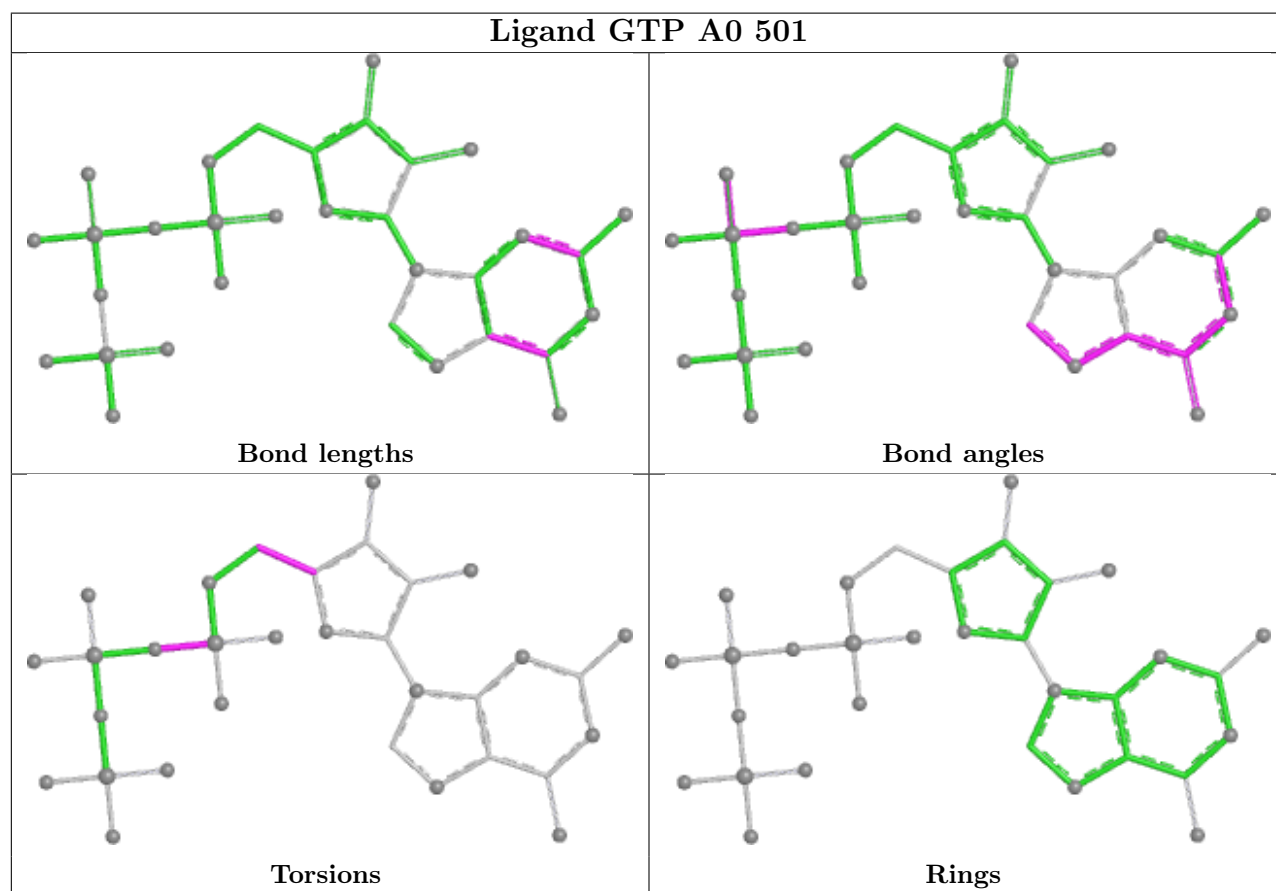
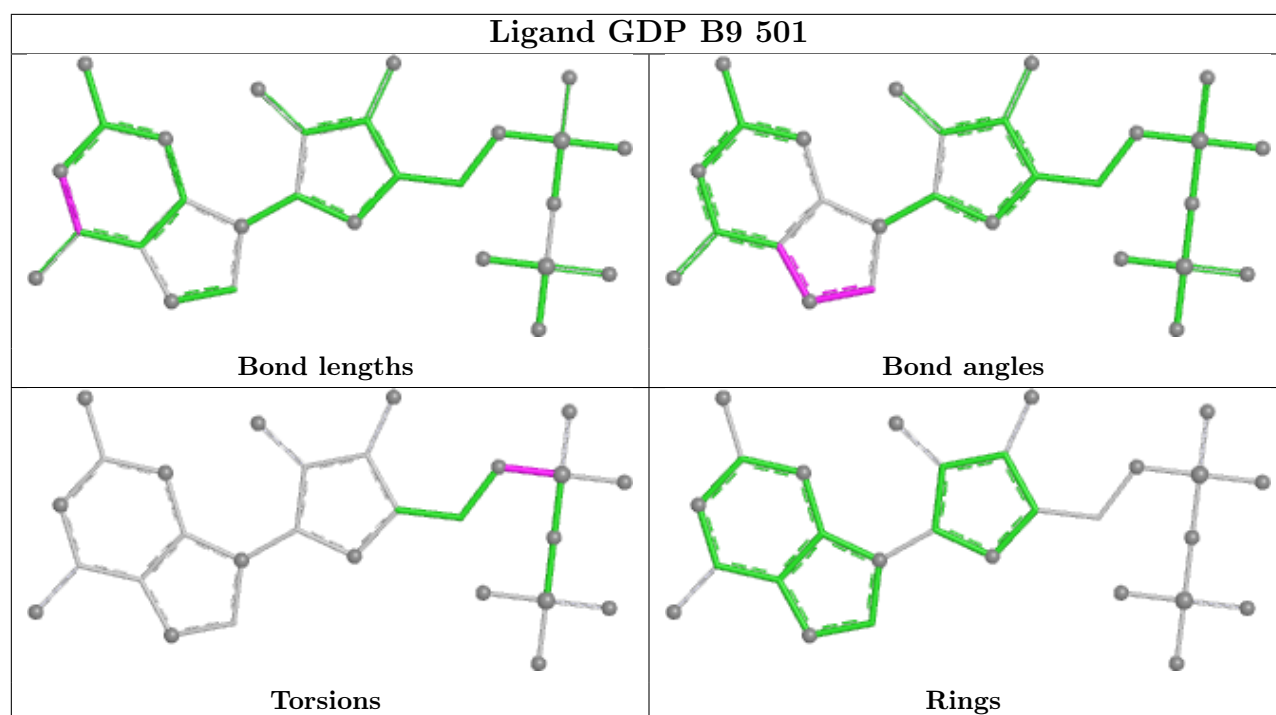


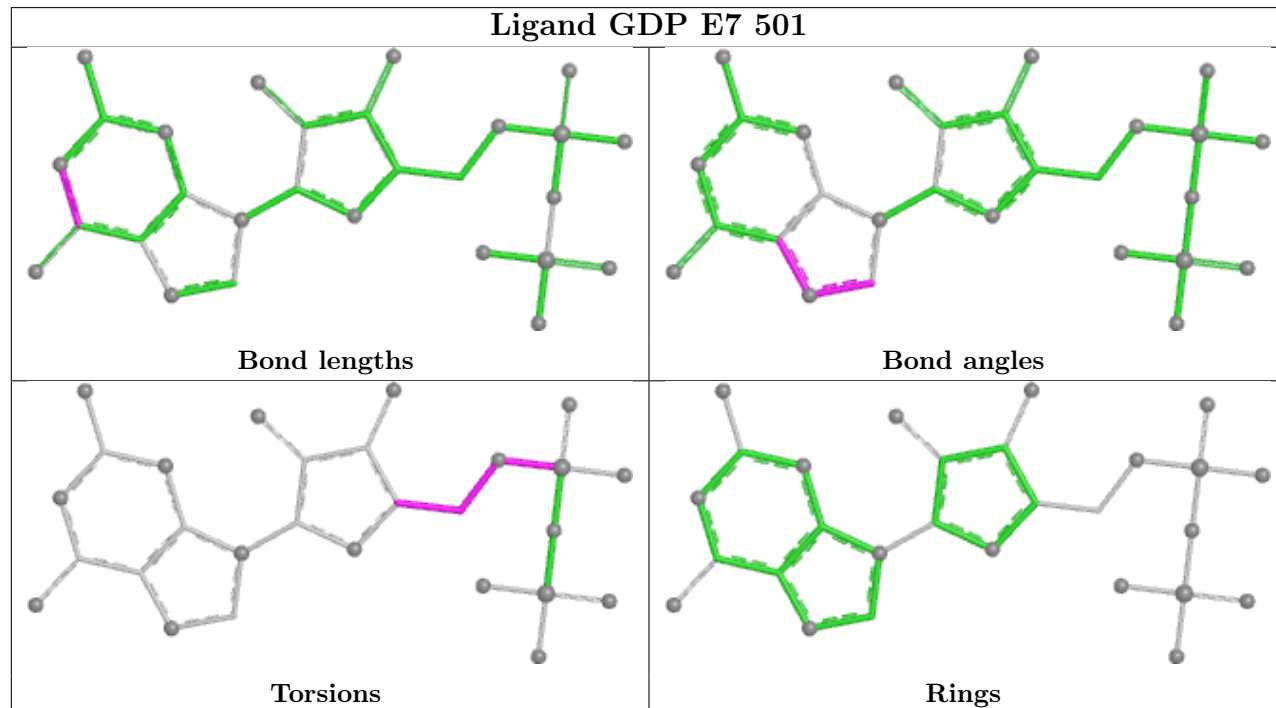
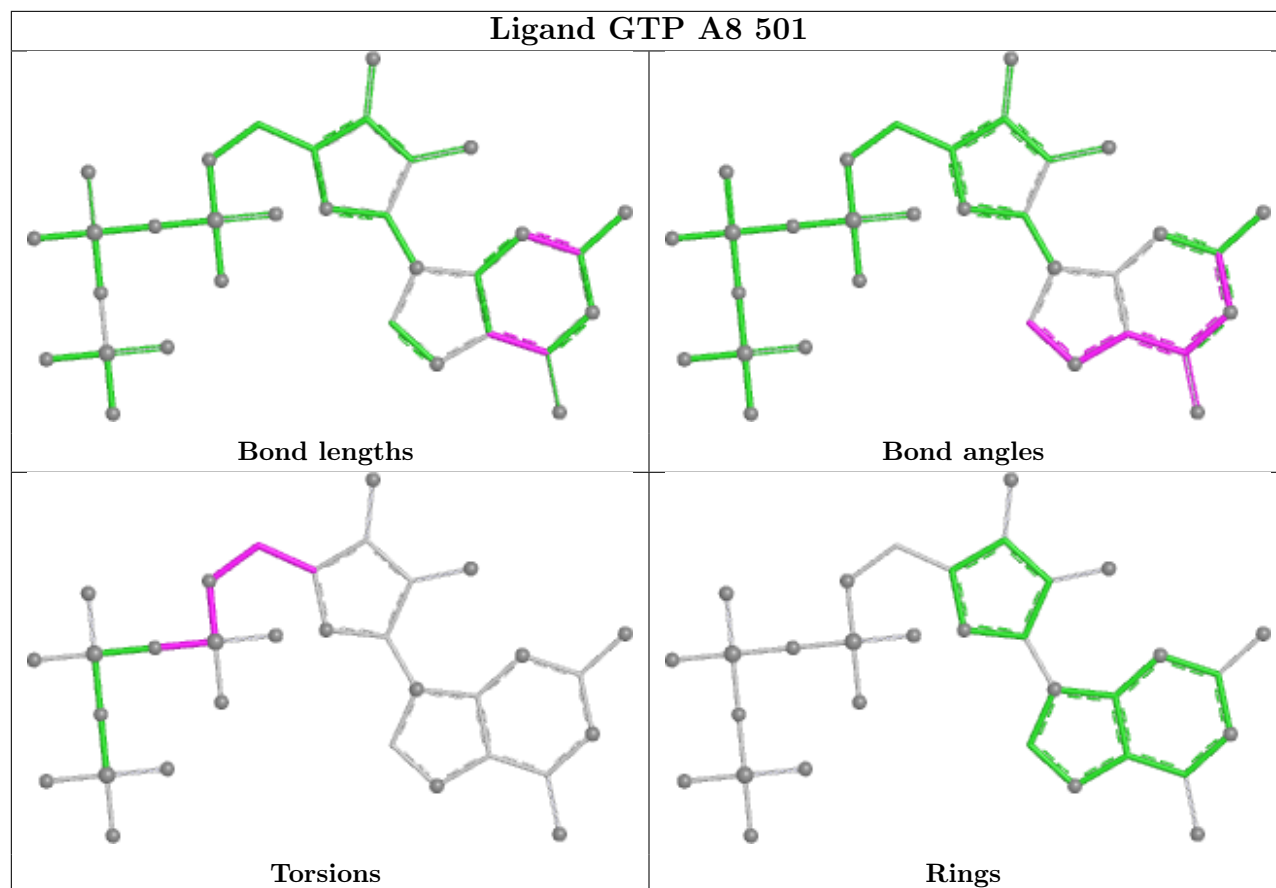
Ligand GTP D6 501



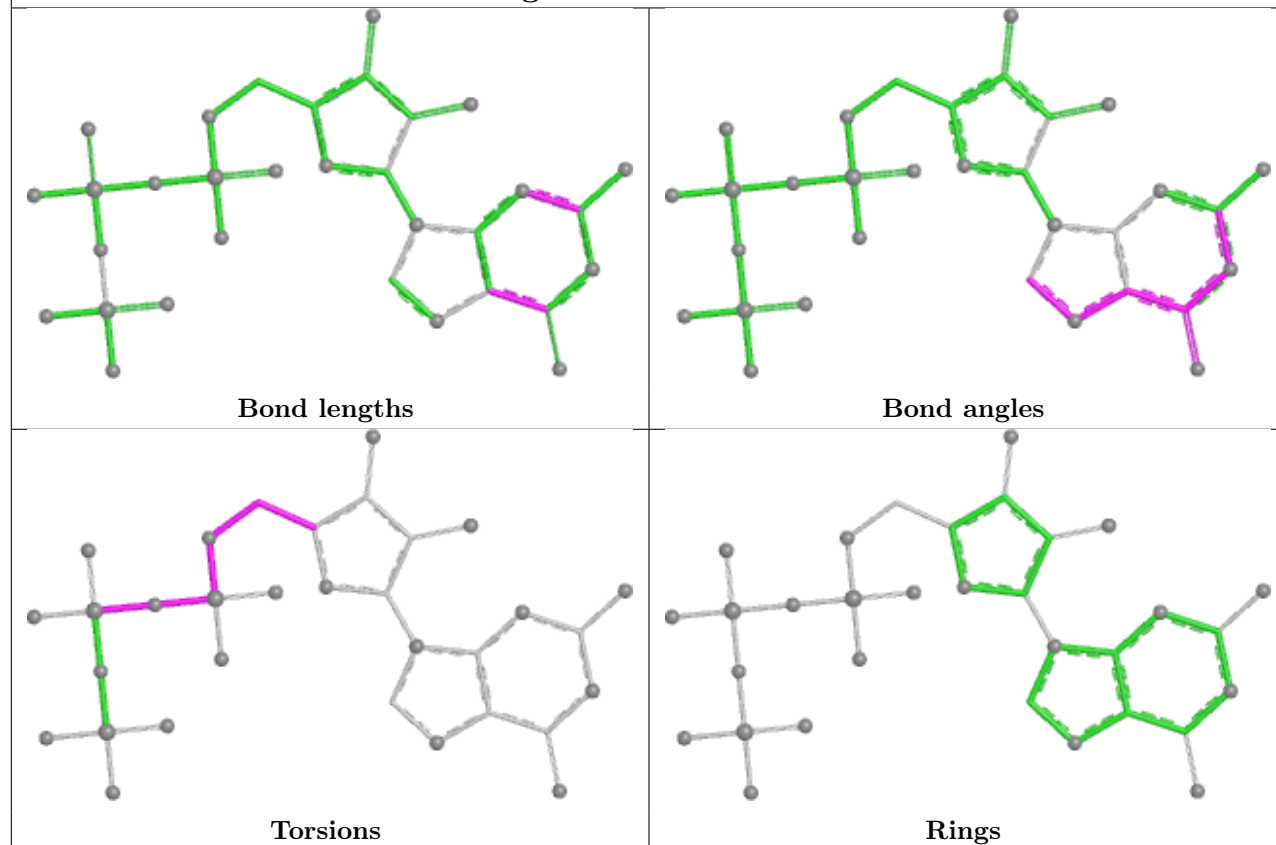
Ligand GTP B4 501



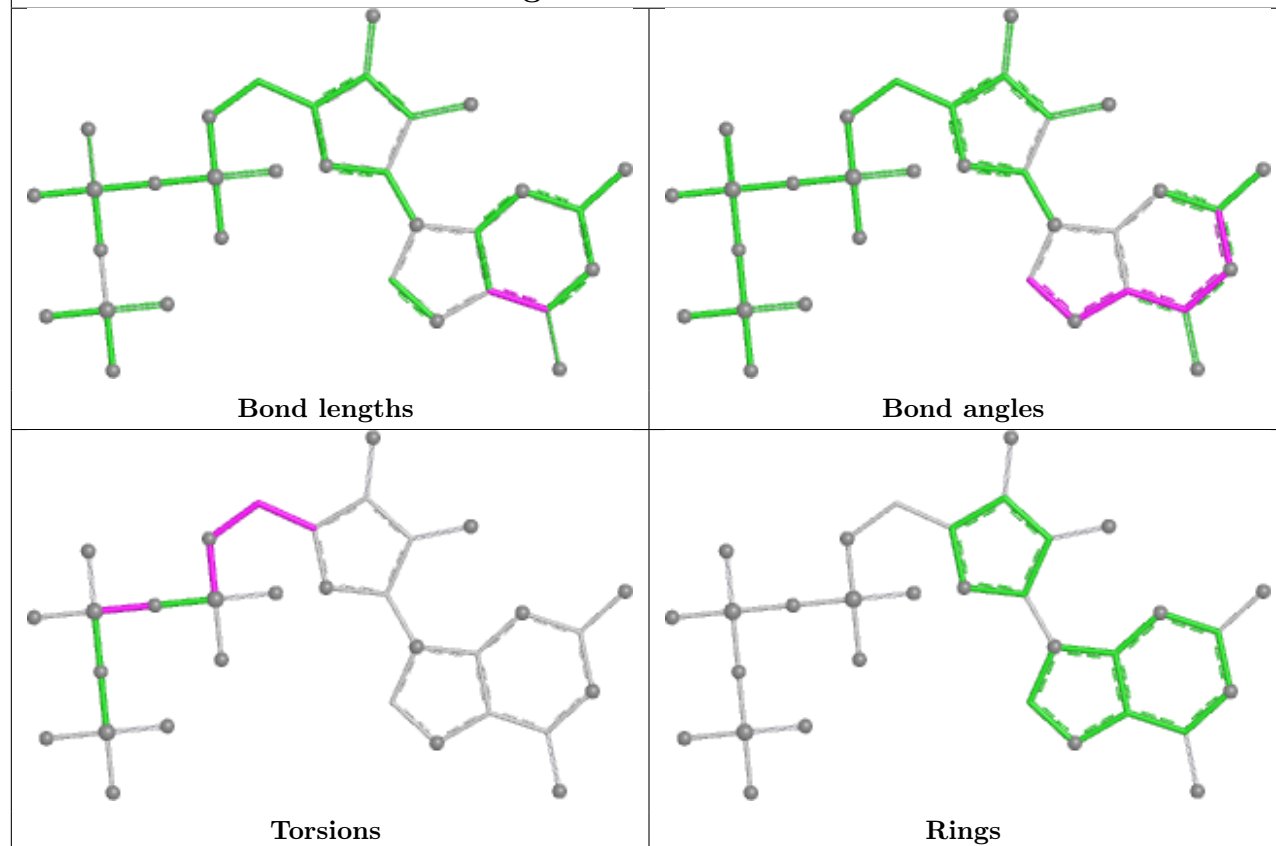


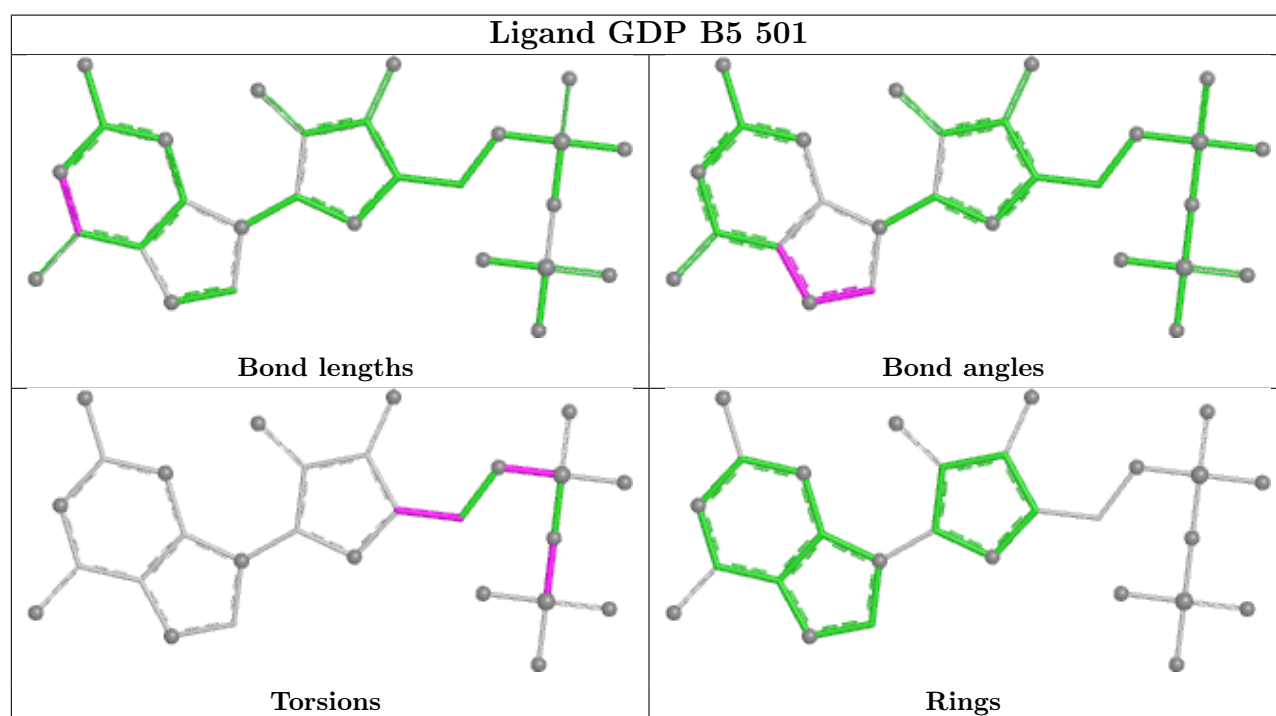
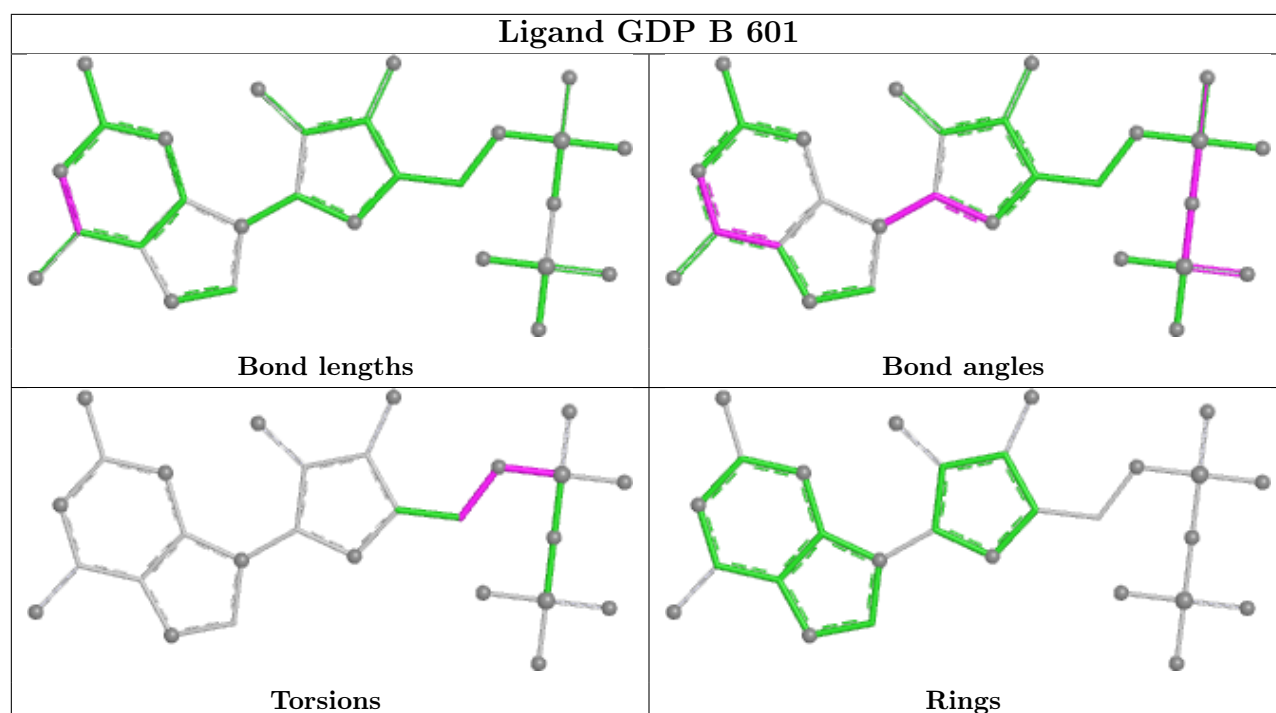


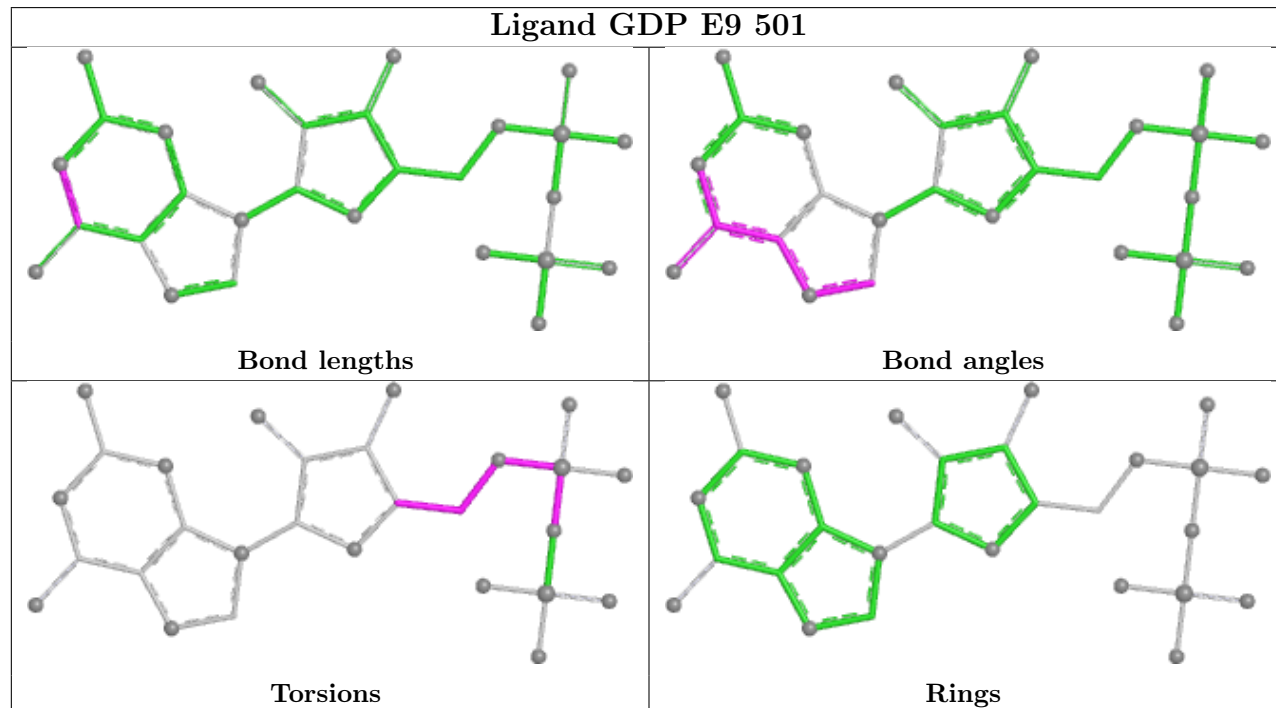
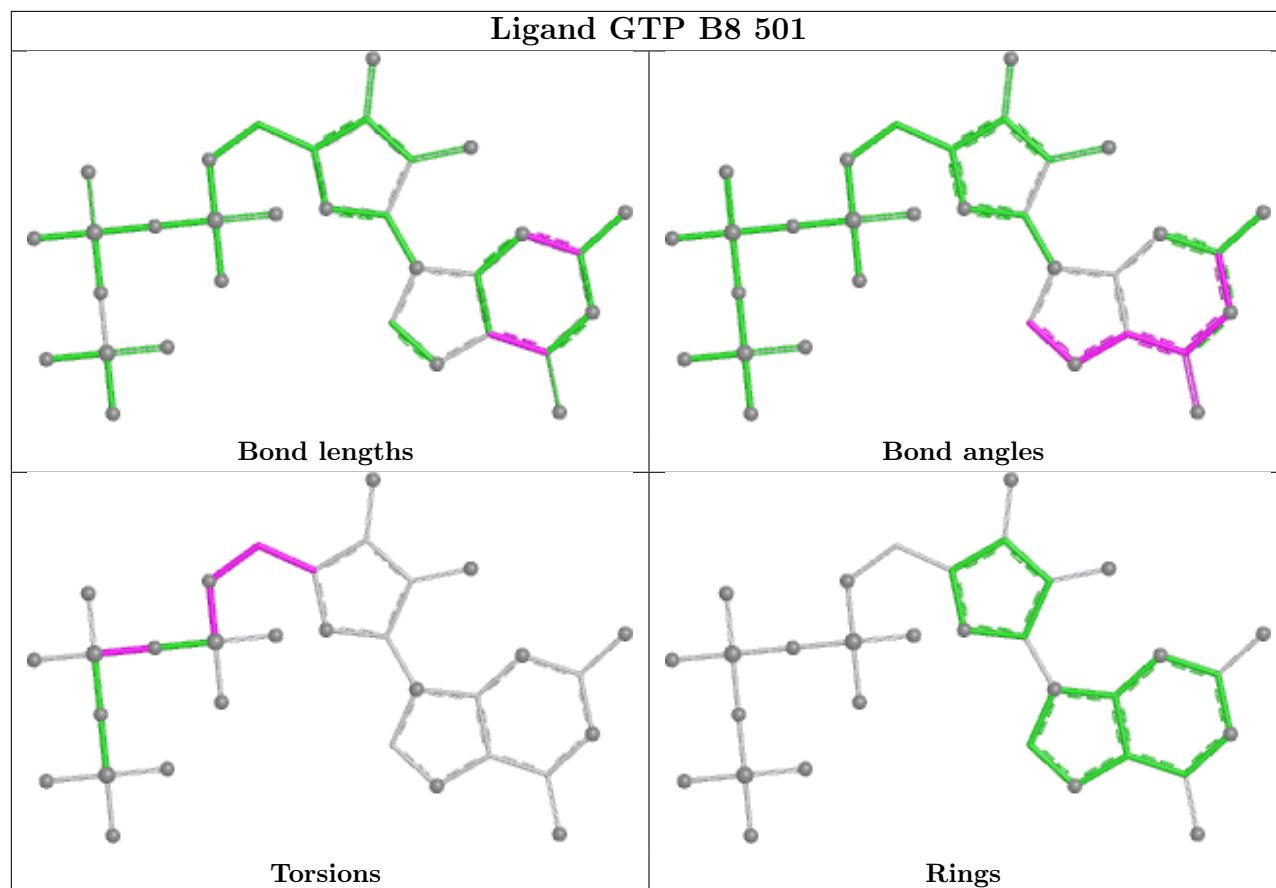
Ligand GTP C6 501

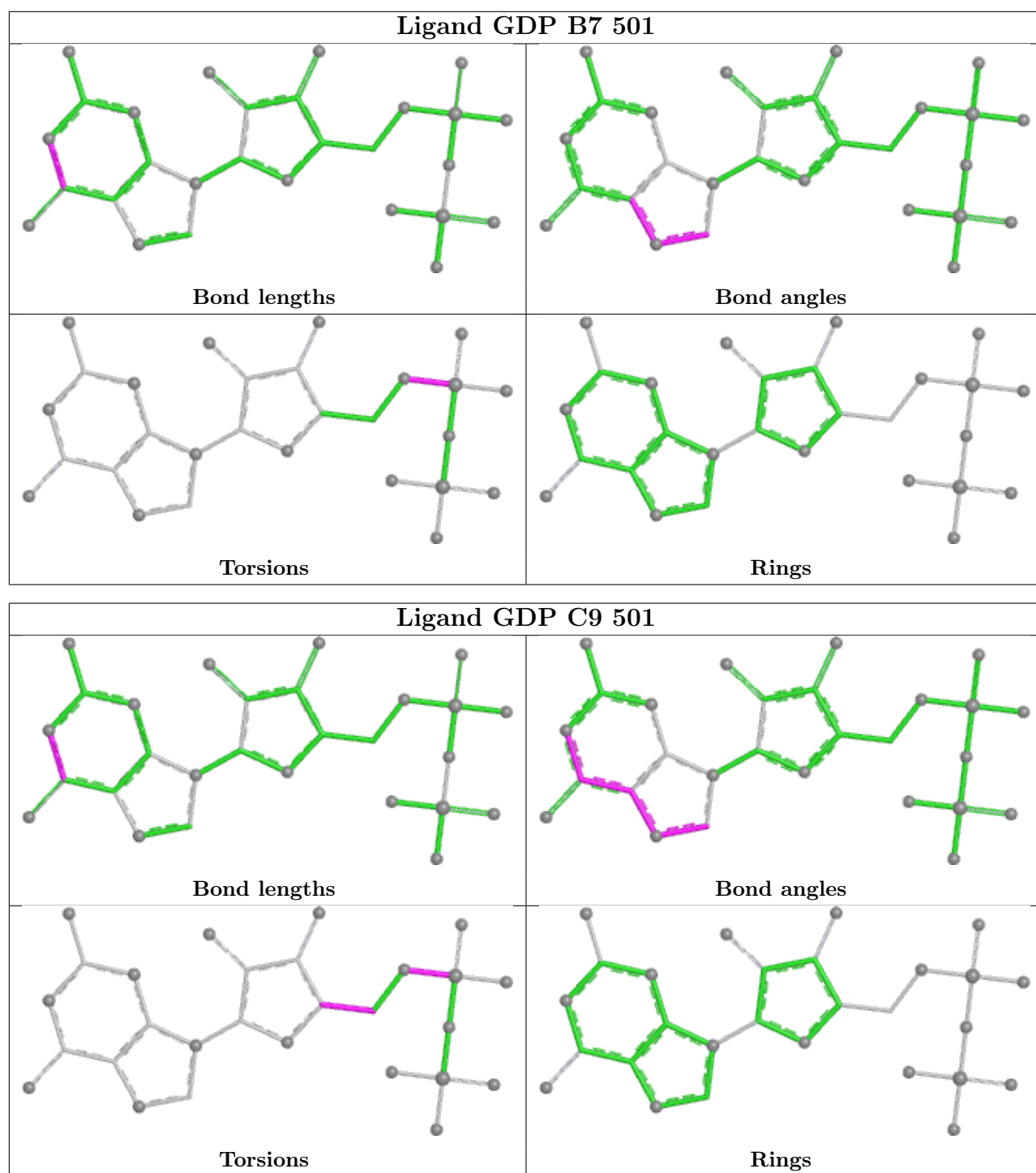


Ligand GTP F0 501

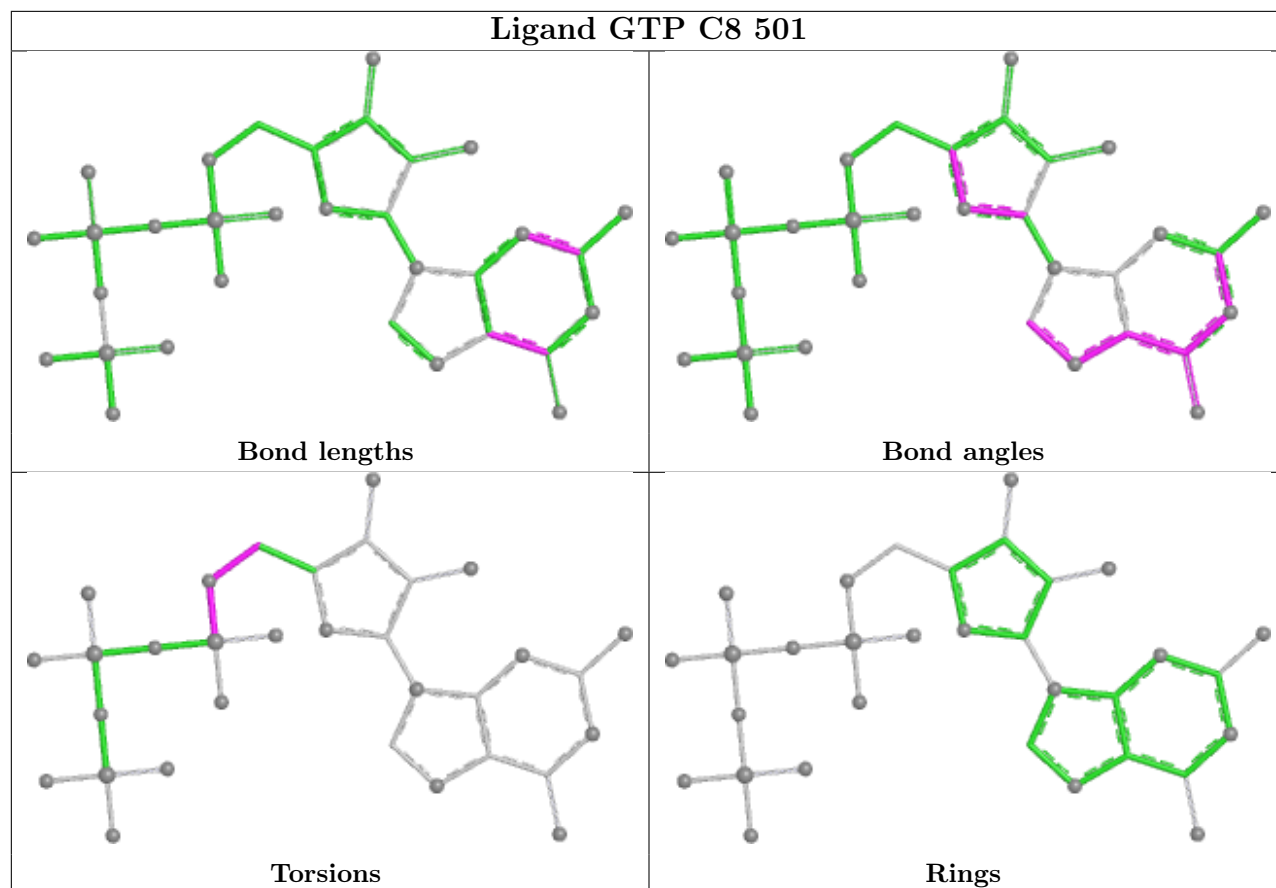




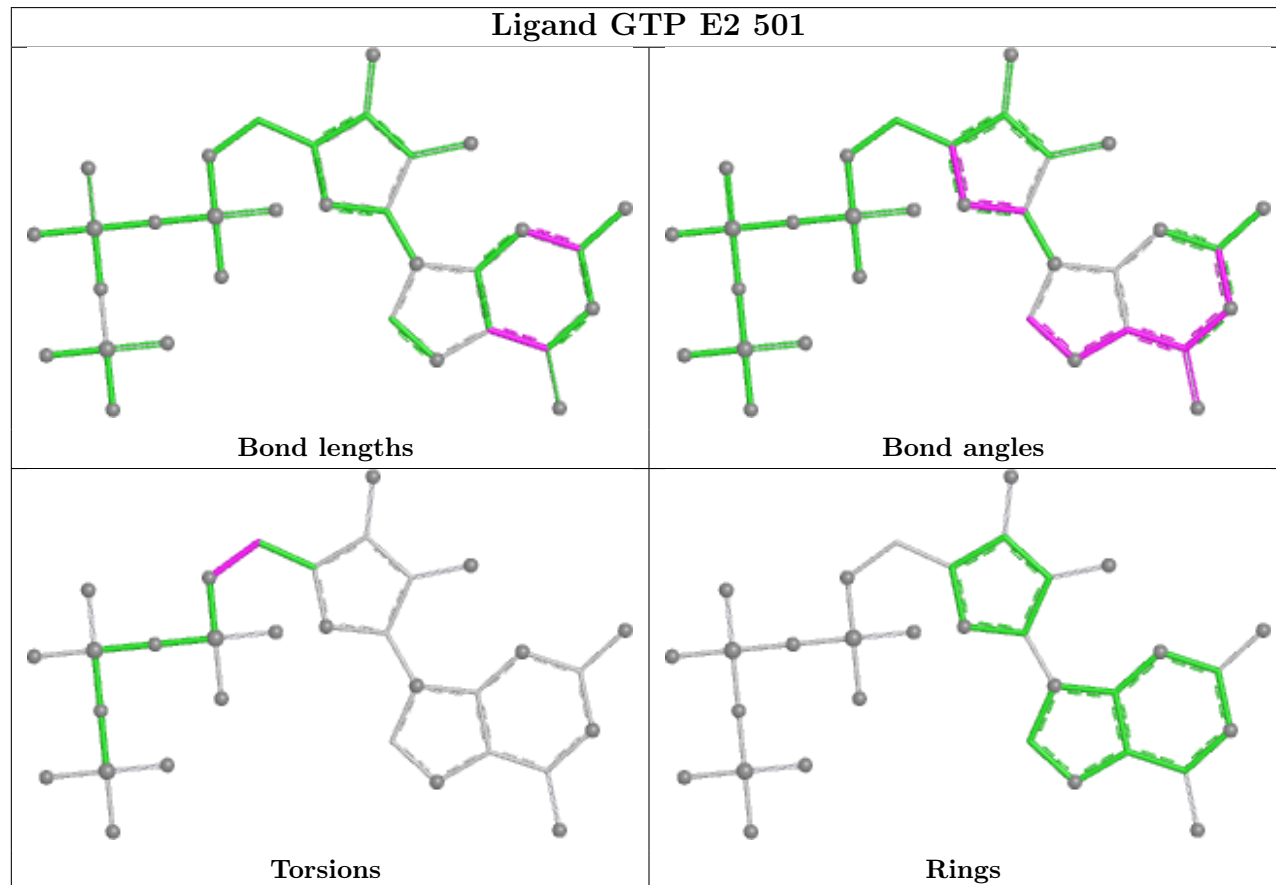


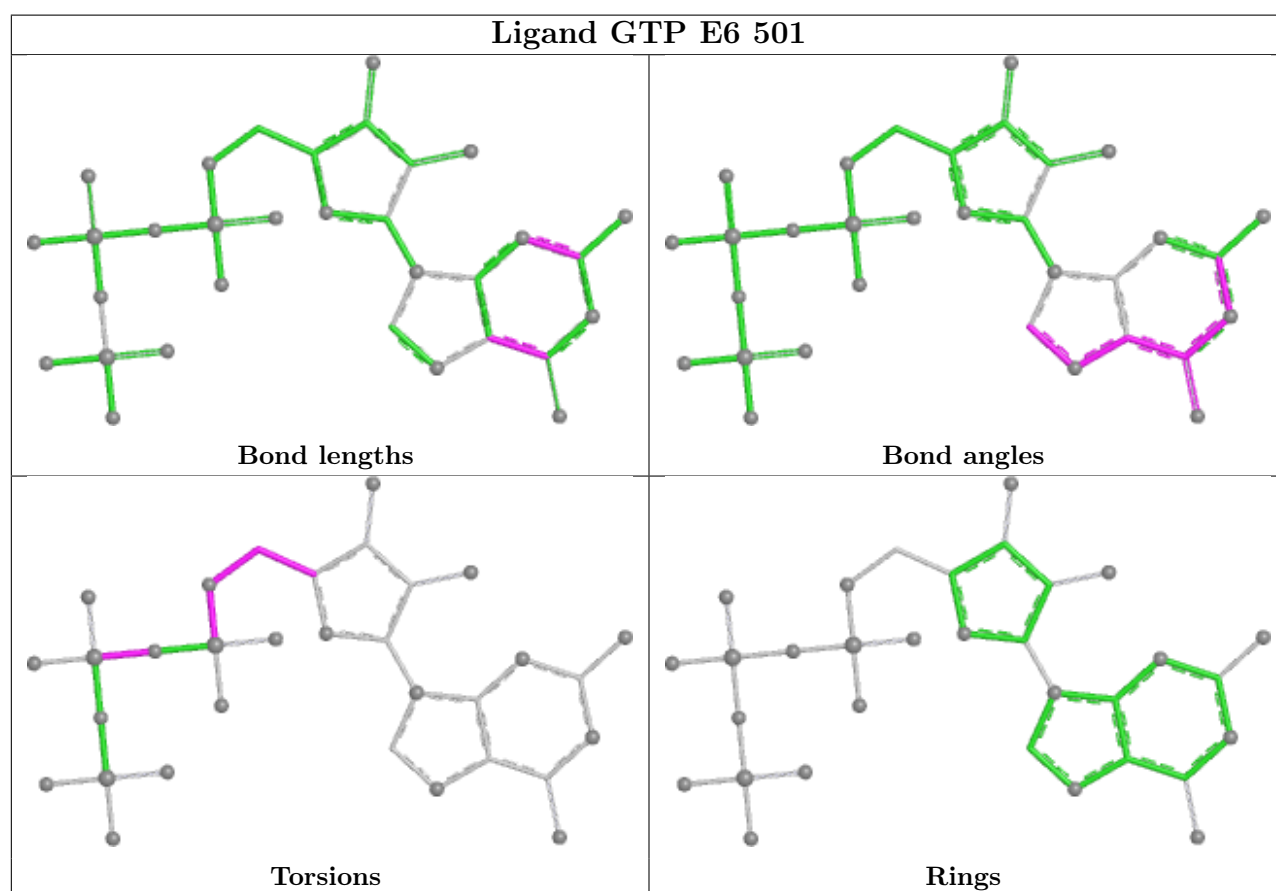
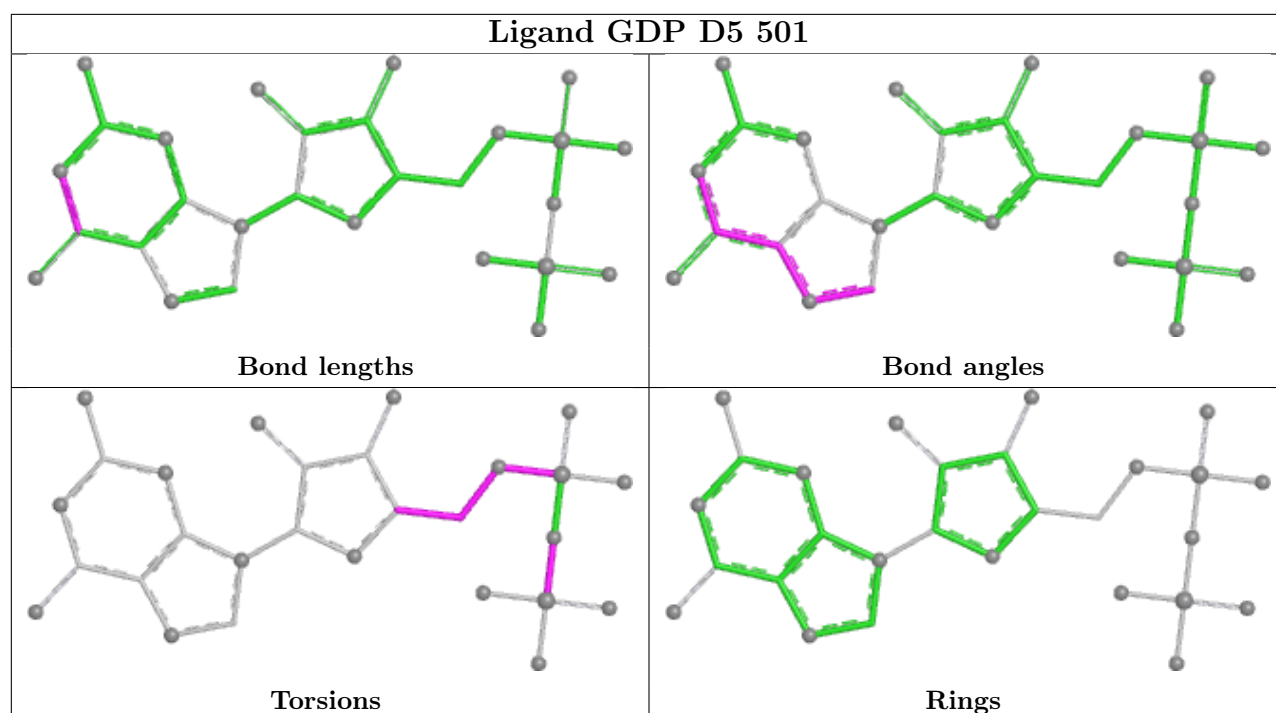


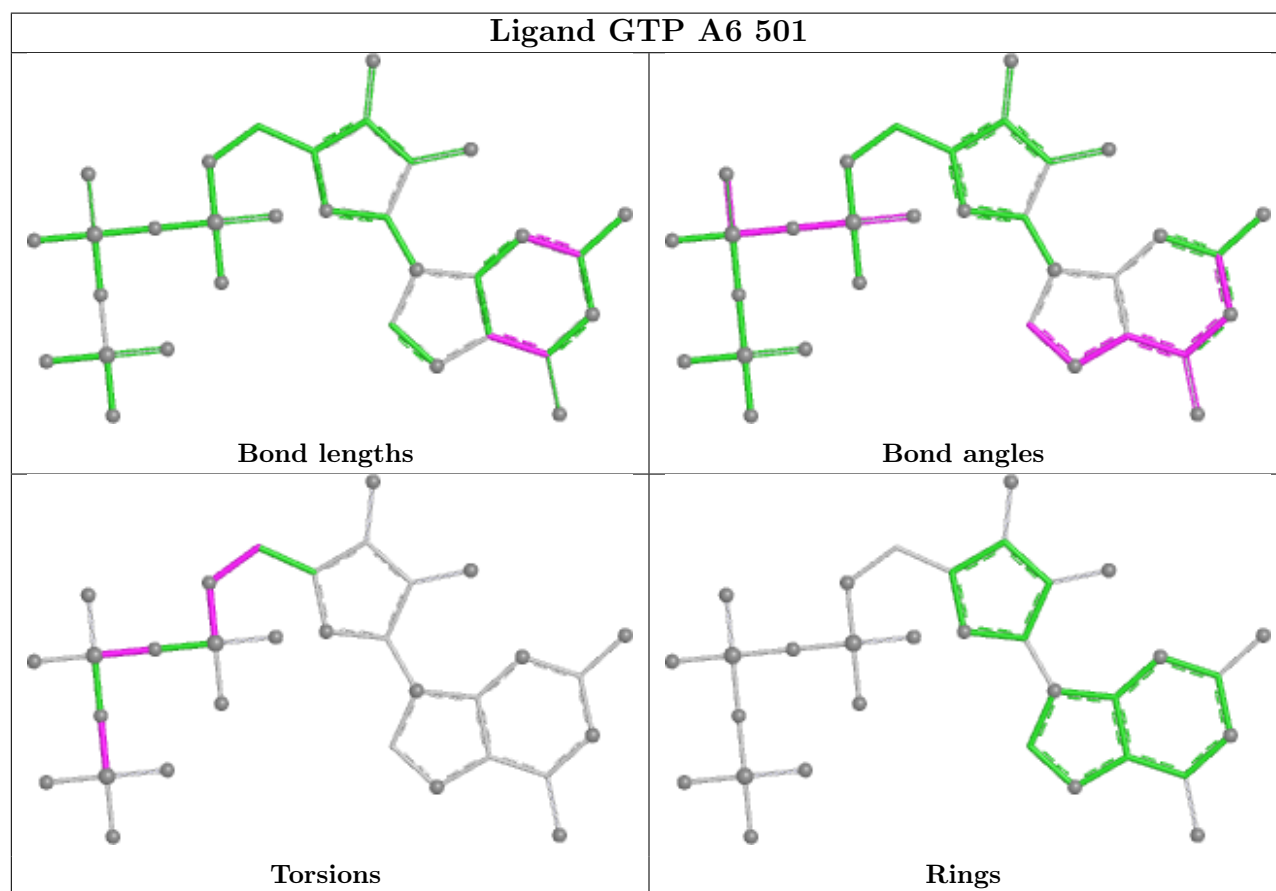
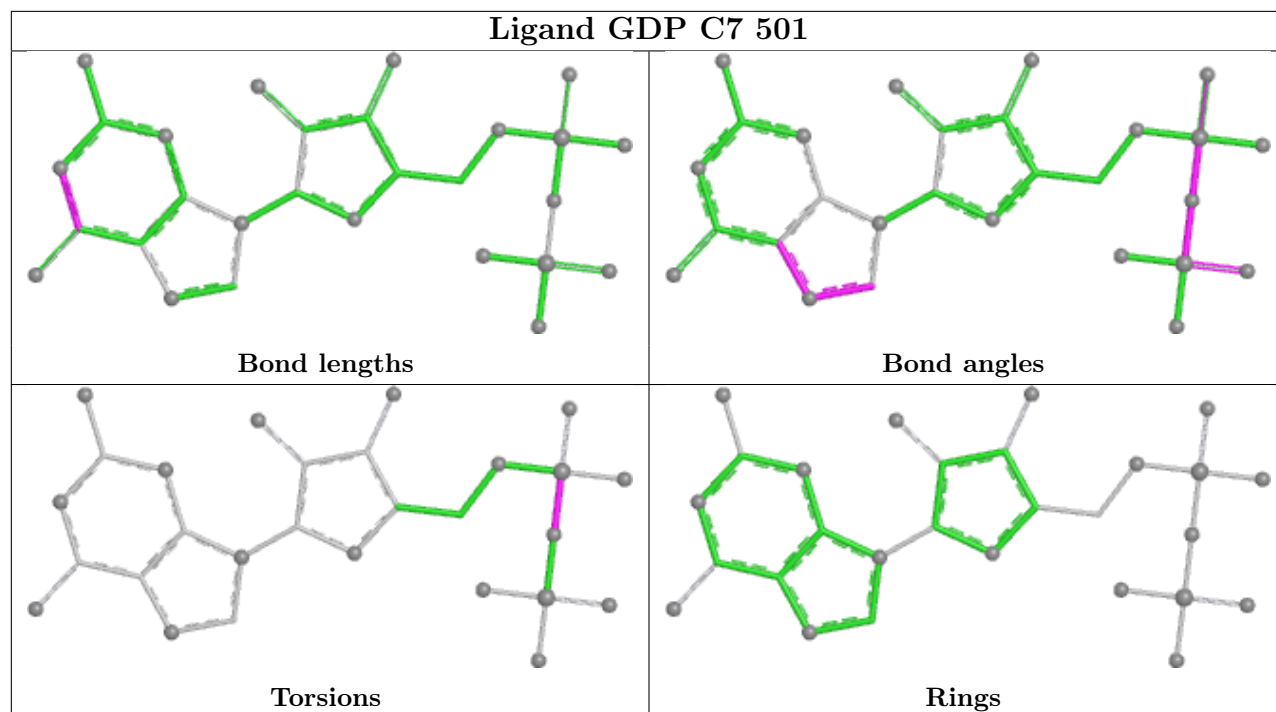
Ligand GTP C8 501

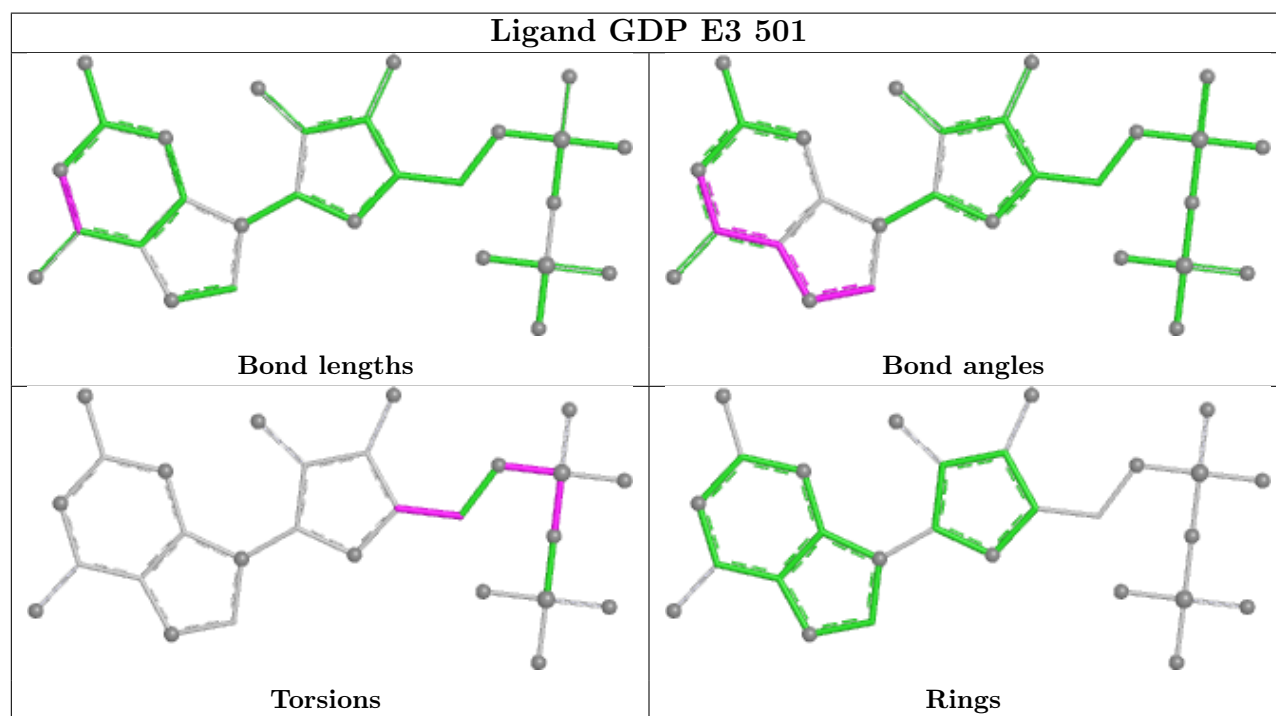
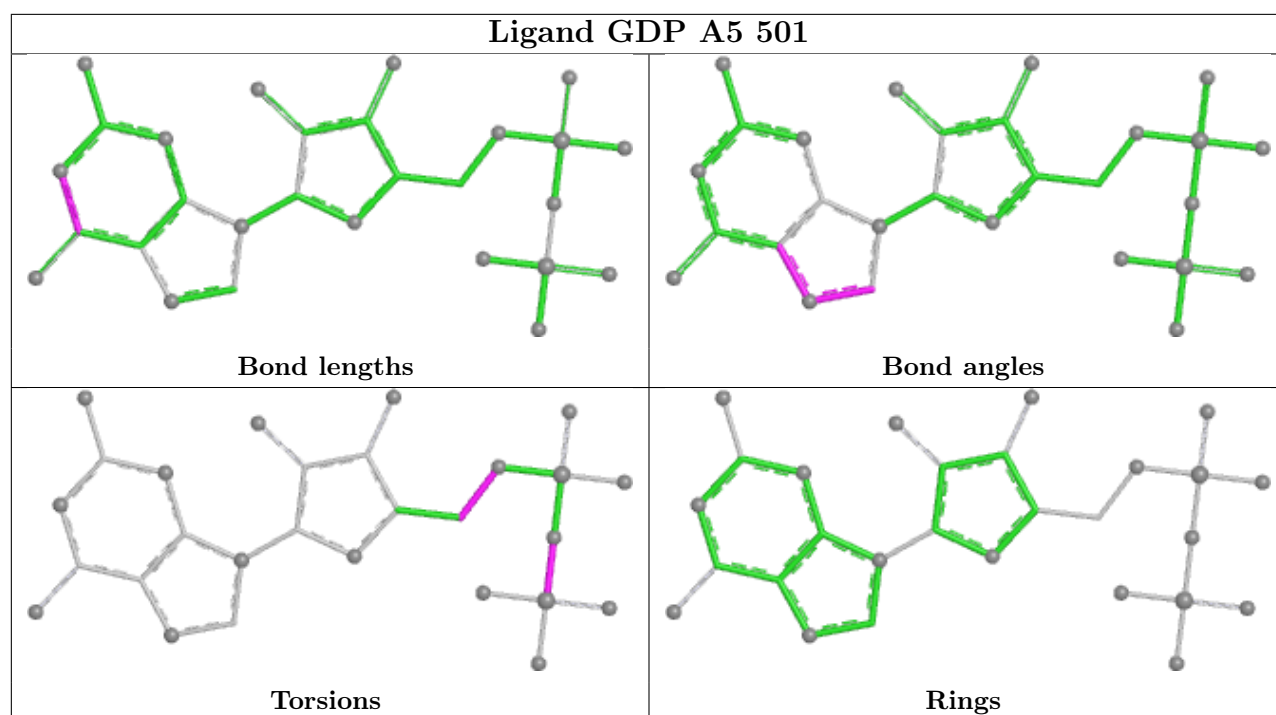


Ligand GTP E2 501

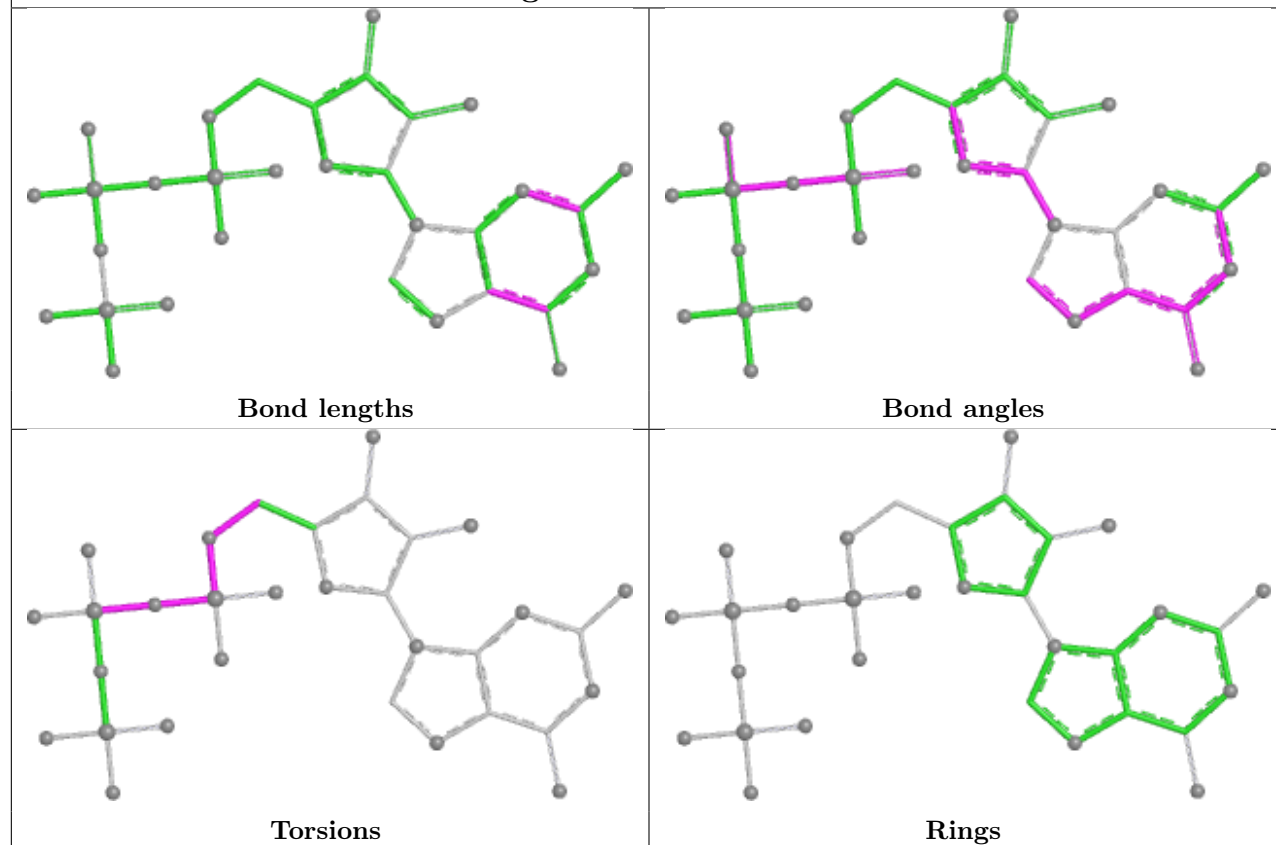




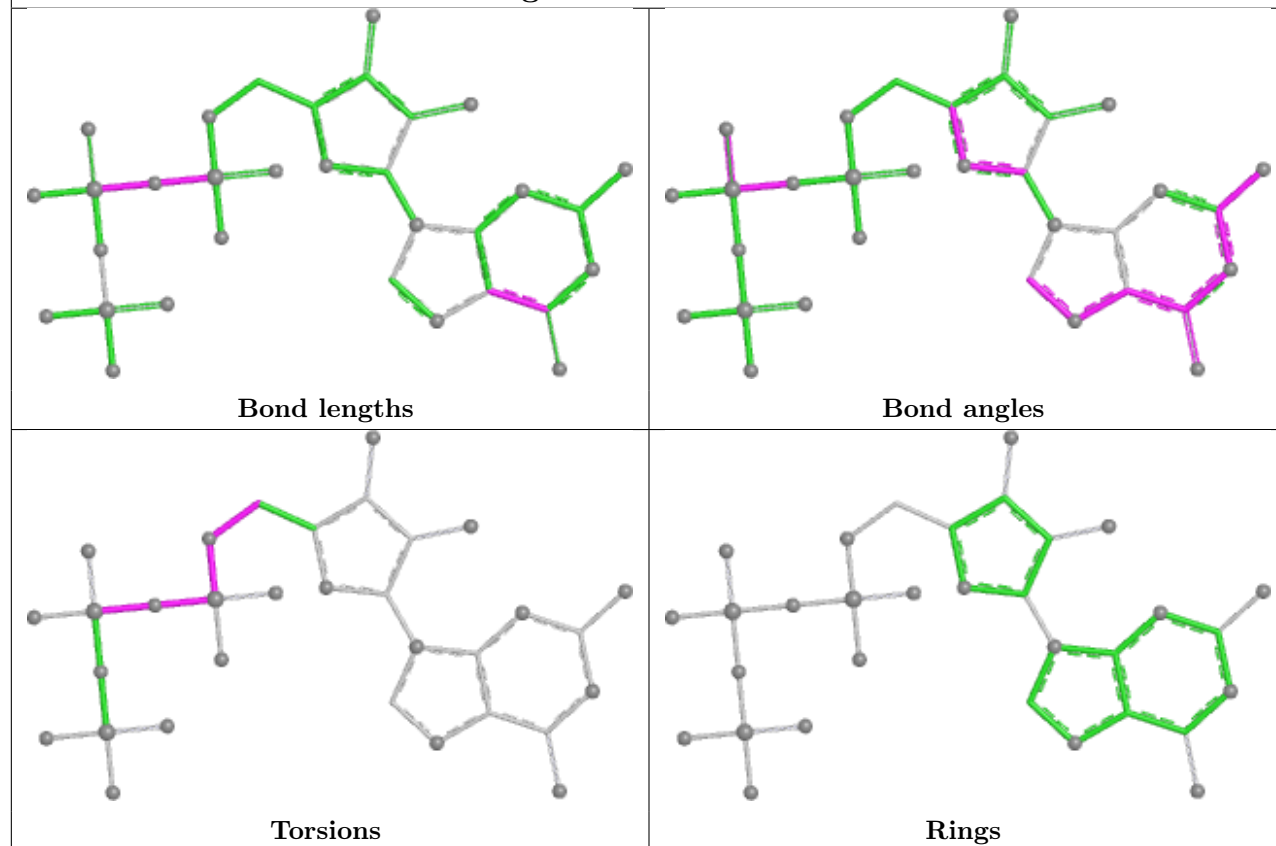




Ligand GTP C2 501



Ligand GTP C0 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.

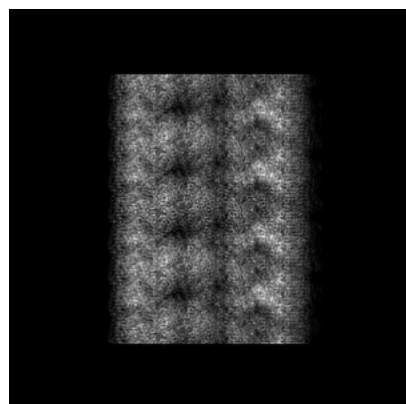
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72719. These allow visual inspection of the internal detail of the map and identification of artifacts.

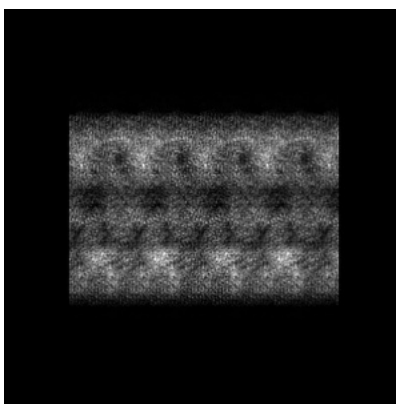
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

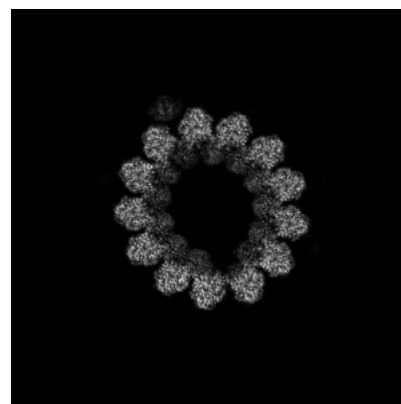
6.1.1 Primary map



X

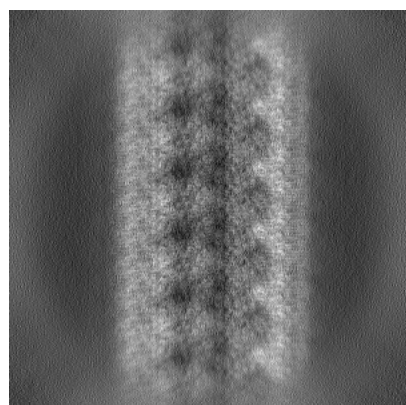


Y

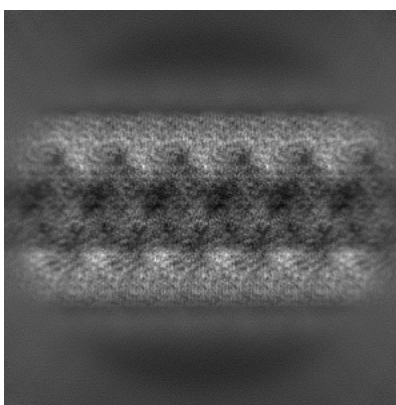


Z

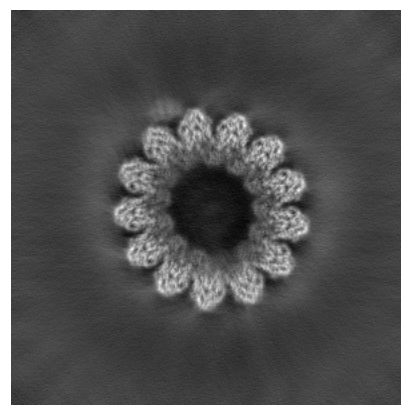
6.1.2 Raw map



X



Y

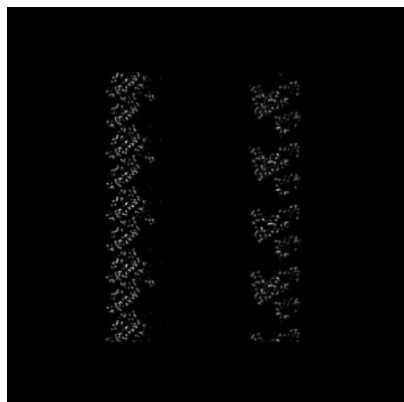


Z

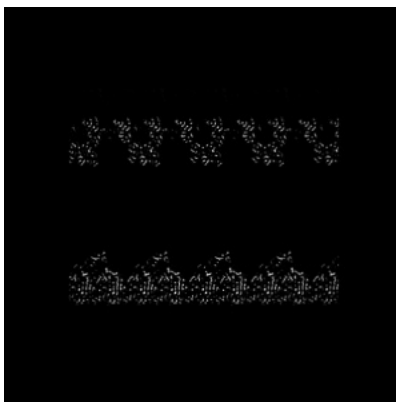
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

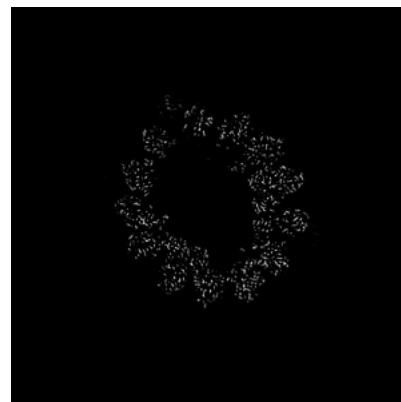
6.2.1 Primary map



X Index: 200

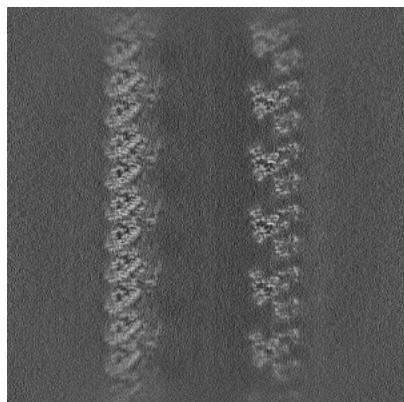


Y Index: 200

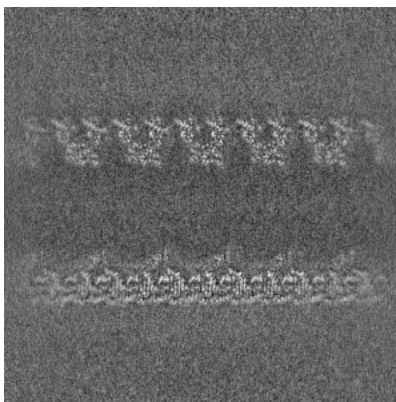


Z Index: 200

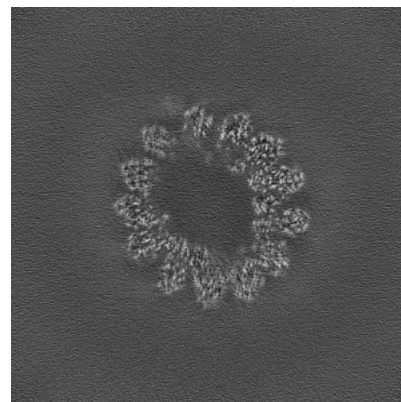
6.2.2 Raw map



X Index: 200



Y Index: 200

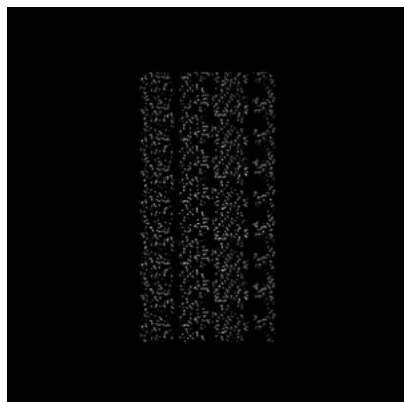


Z Index: 200

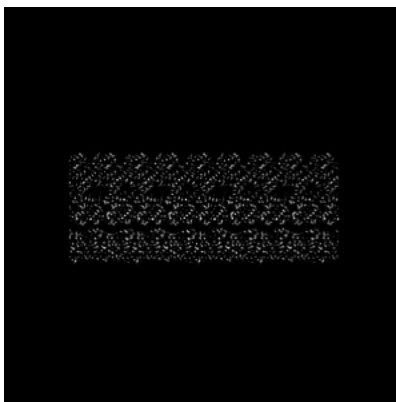
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

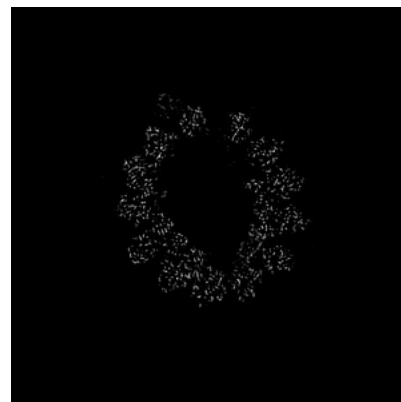
6.3.1 Primary map



X Index: 270

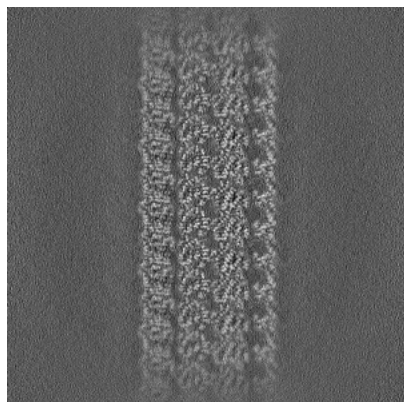


Y Index: 126

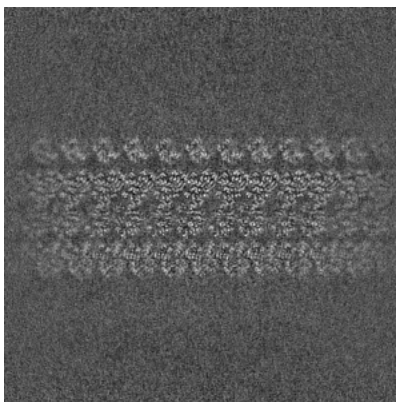


Z Index: 206

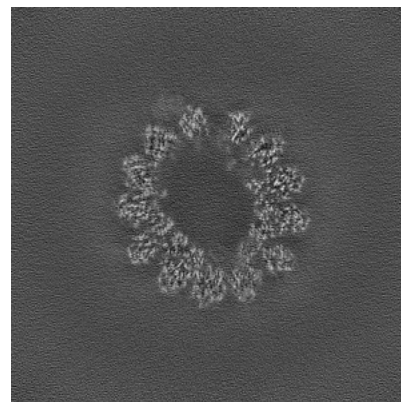
6.3.2 Raw map



X Index: 270



Y Index: 270

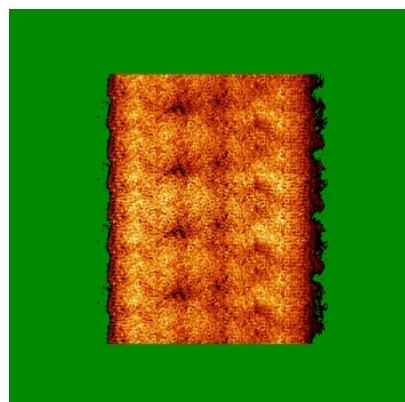


Z Index: 206

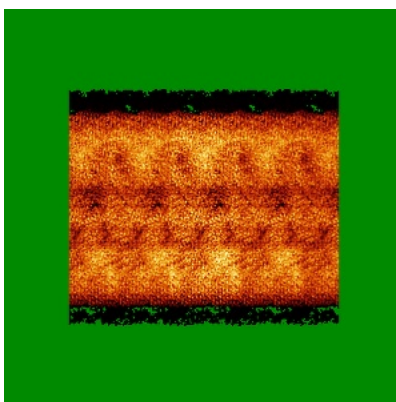
The images above show the largest variance slices of the map in three orthogonal directions.

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

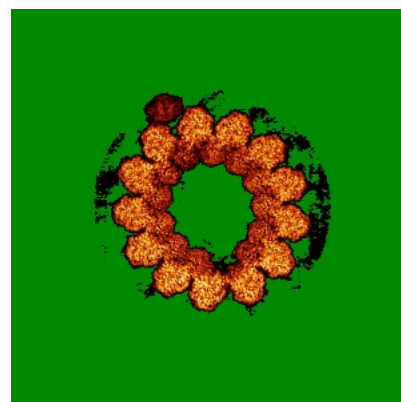
6.4.1 Primary map



X

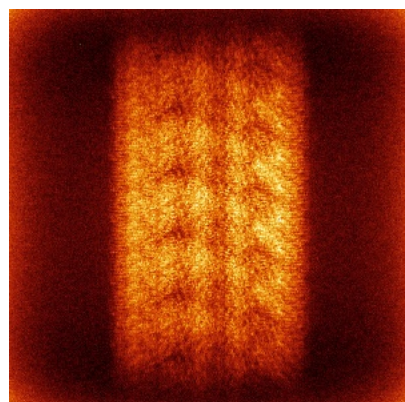


Y

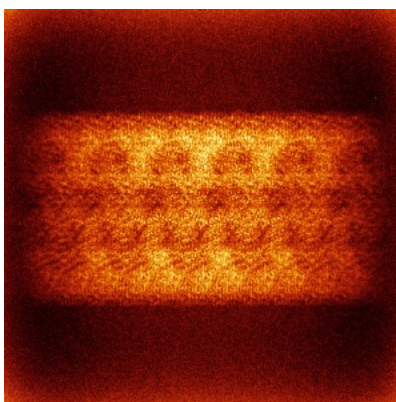


Z

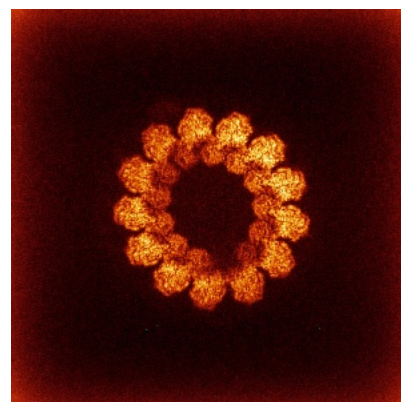
6.4.2 Raw map



X



Y

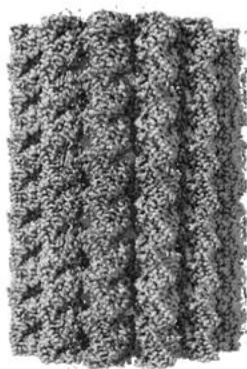


Z

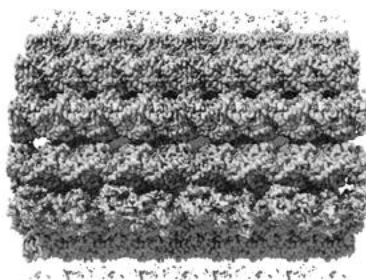
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

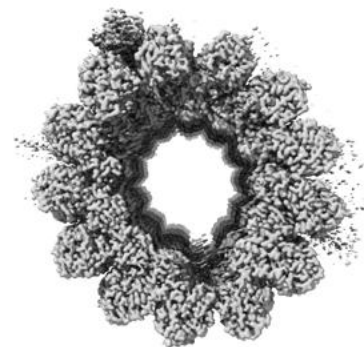
6.5.1 Primary map



X



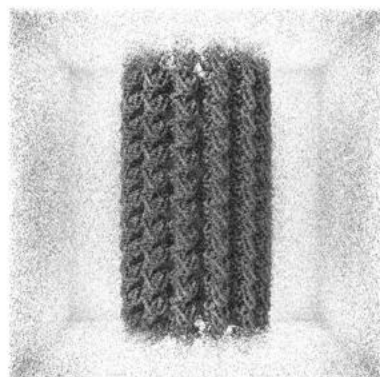
Y



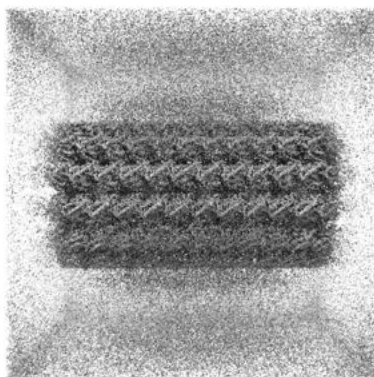
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

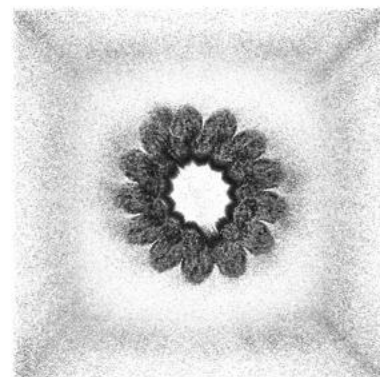
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

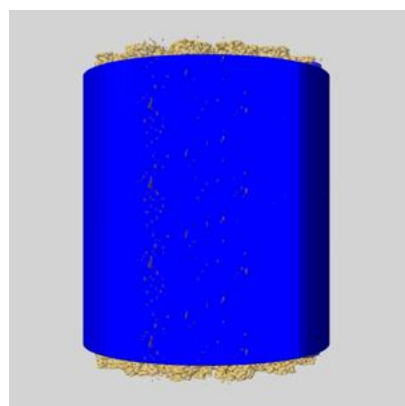
6.6 Mask visualisation [i](#)

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

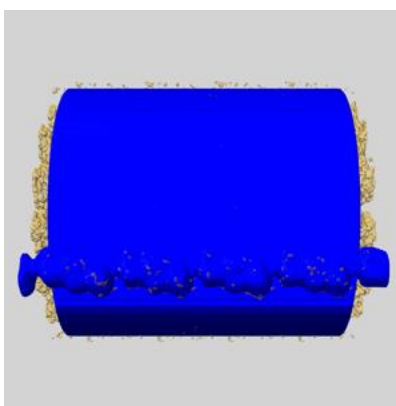
A mask typically either:

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

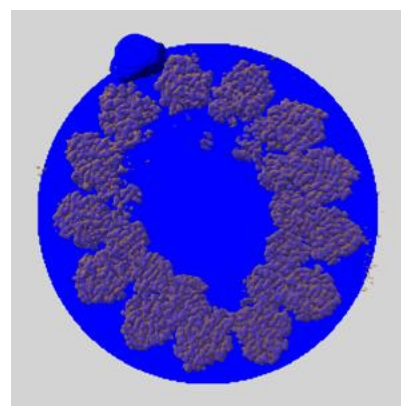
6.6.1 emd_72719_msk_1.map [i](#)



X



Y

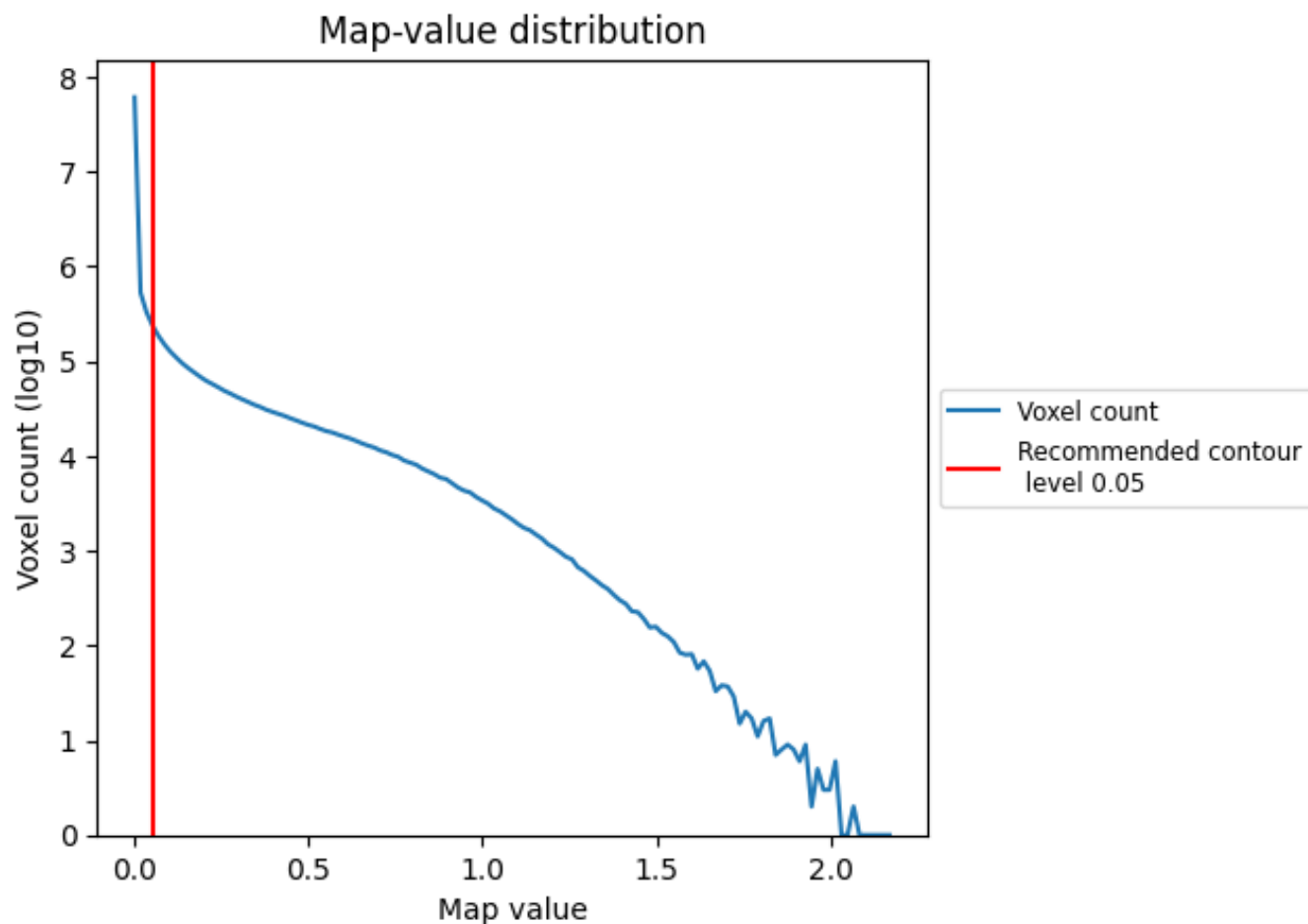


Z

7 Map analysis [i](#)

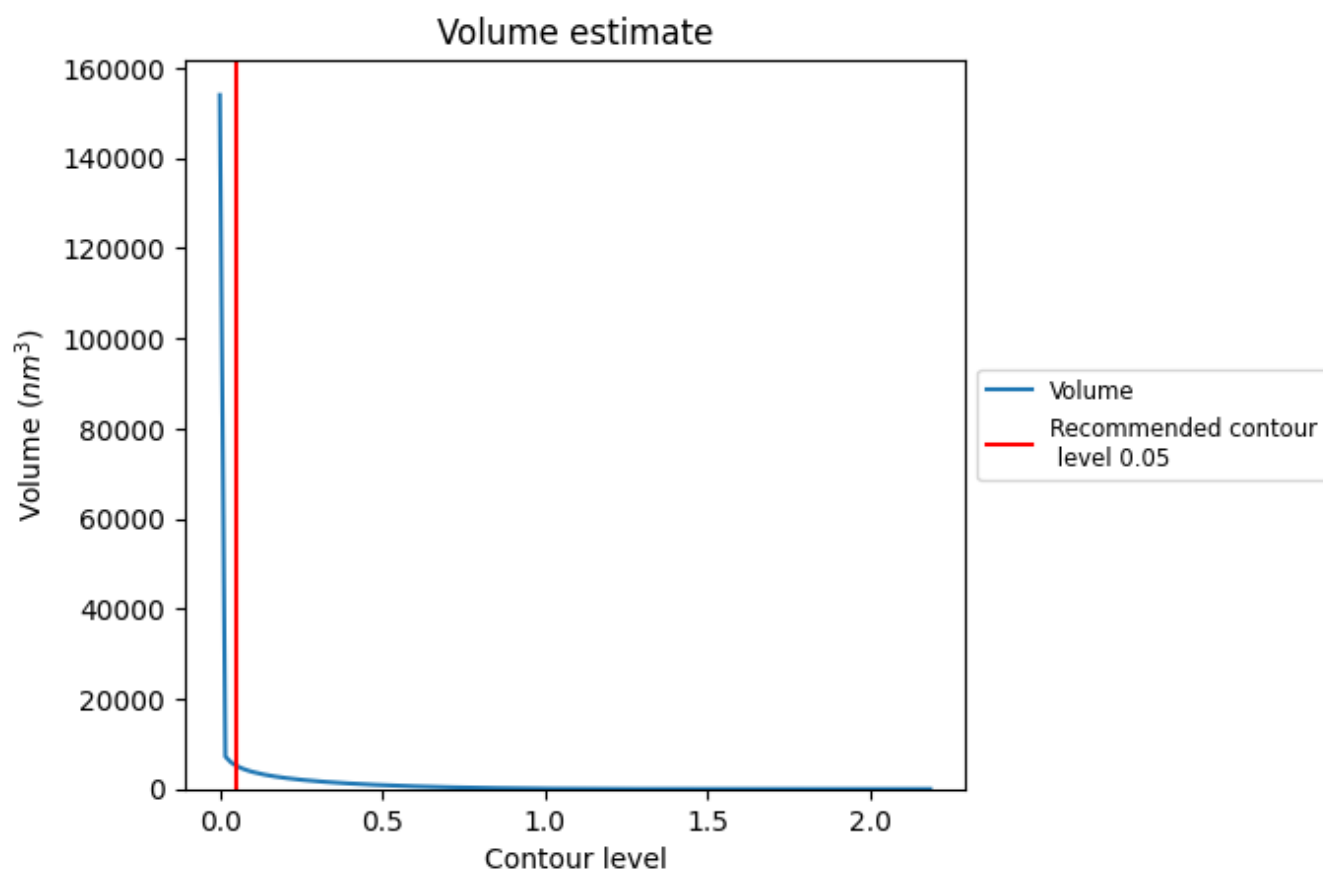
This section contains the results of statistical analysis of the map.

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.

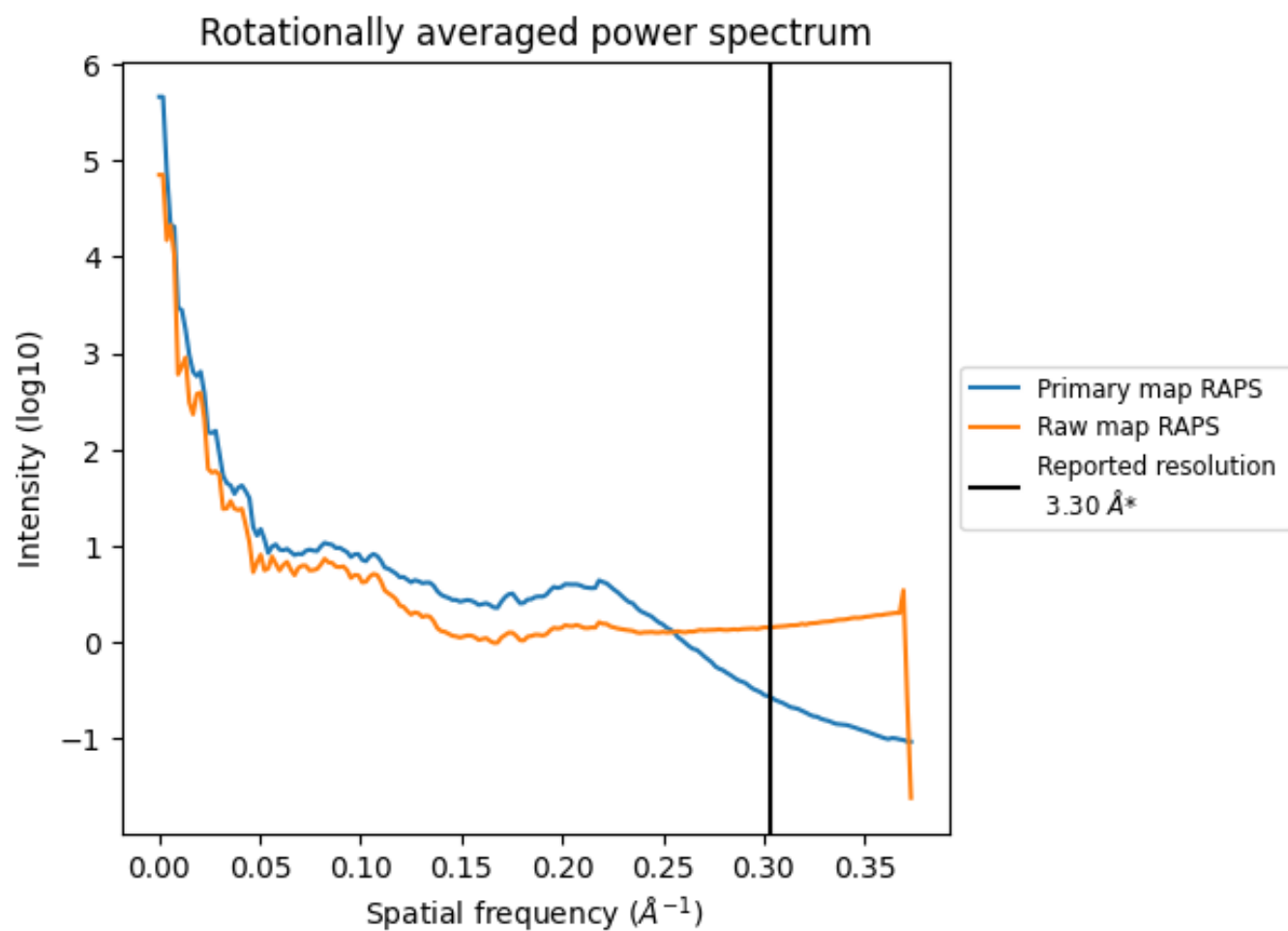
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5187 nm³; this corresponds to an approximate mass of 4686 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 ⓘ

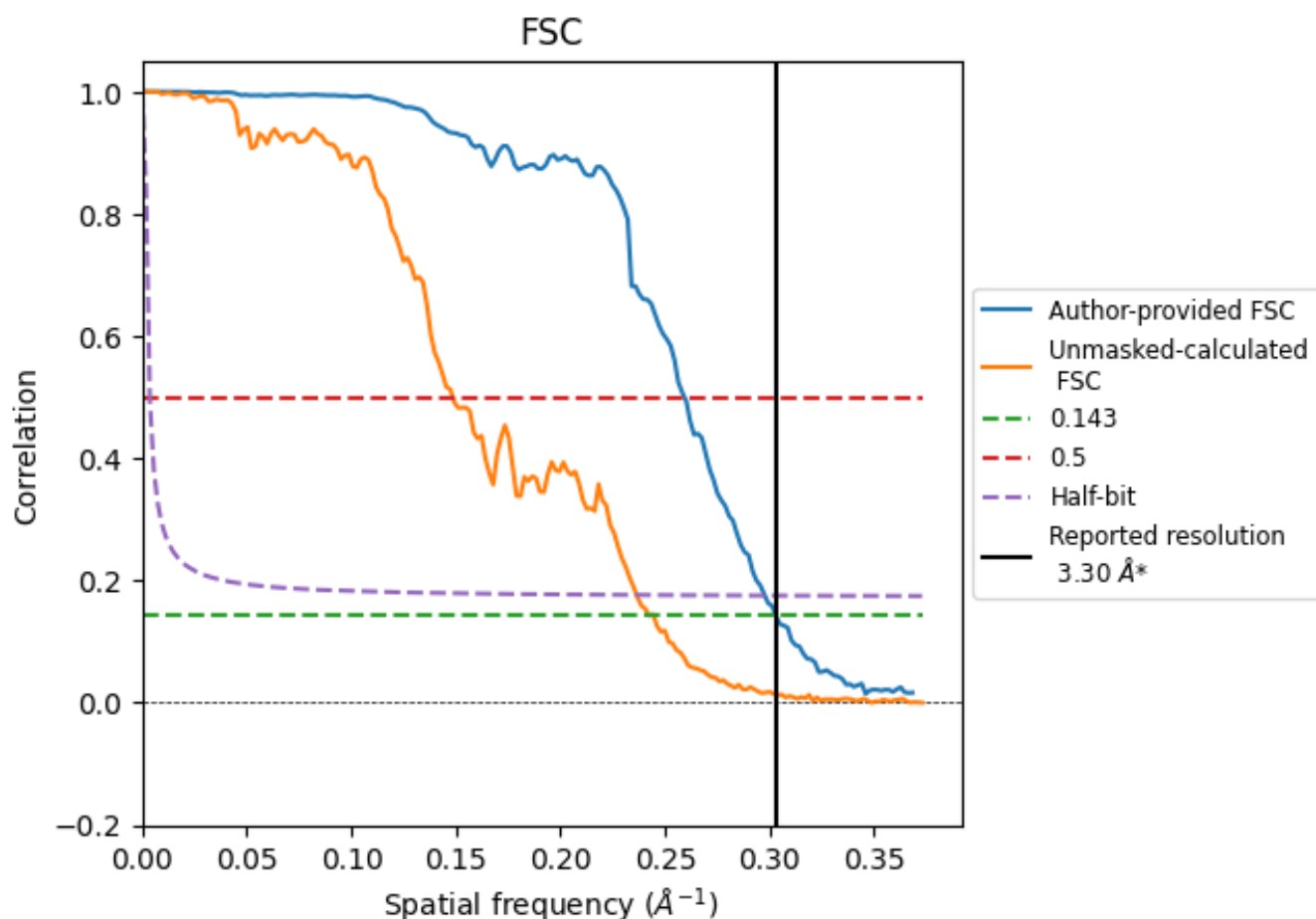


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8.2 Resolution estimates [i](#)

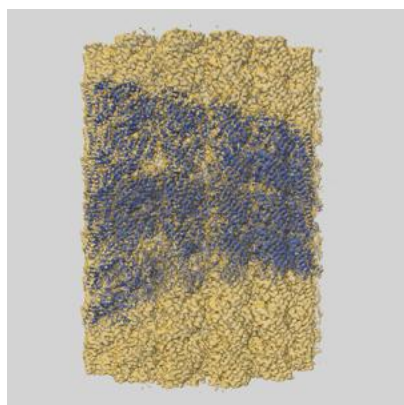
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.30	3.86	3.36
Unmasked-calculated*	4.13	6.73	4.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.13 differs from the reported value 3.3 by more than 10 %

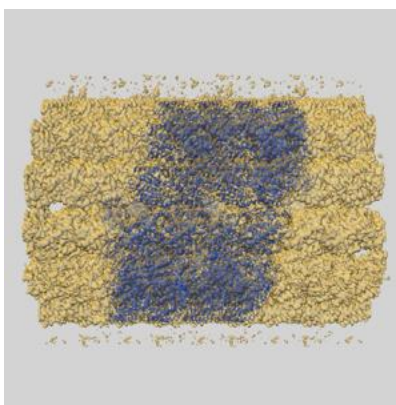
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72719 and PDB model 9YA3. Per-residue inclusion information can be found in section [3](#) on page [21](#).

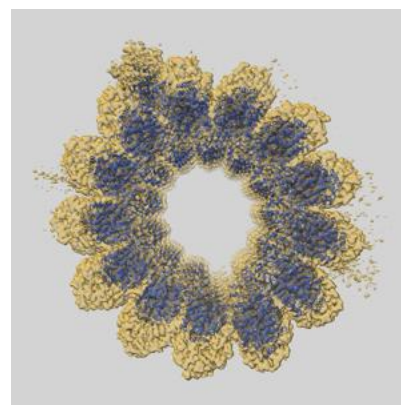
9.1 Map-model overlay [i](#)



X



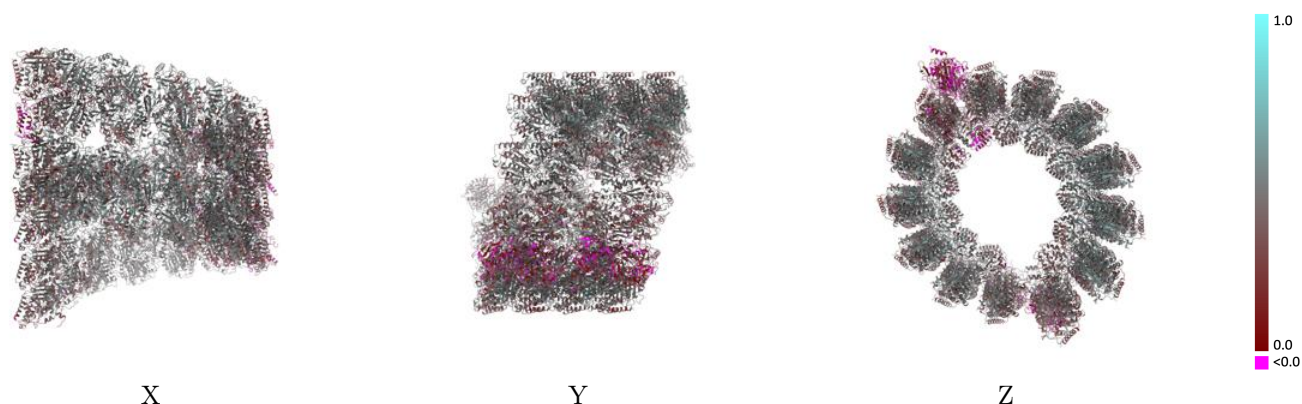
Y



Z

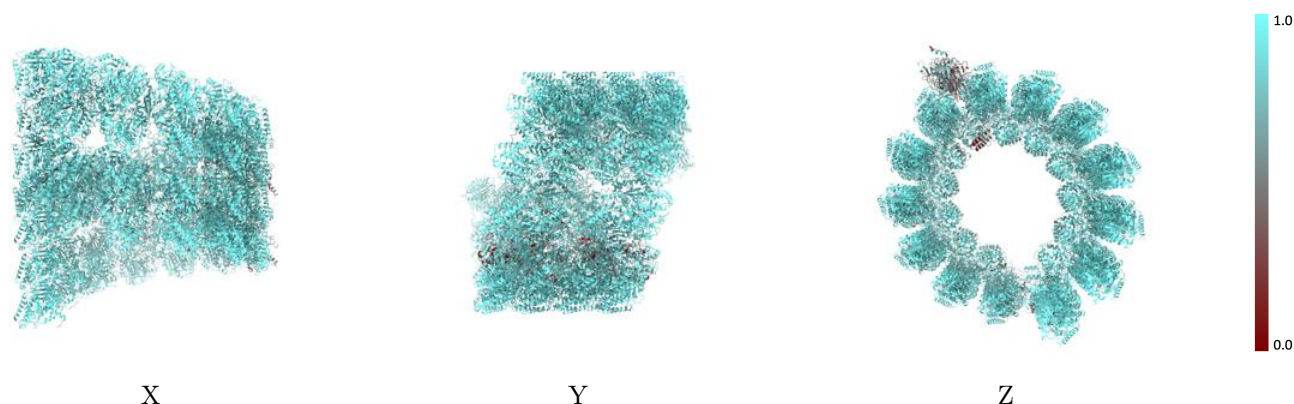
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



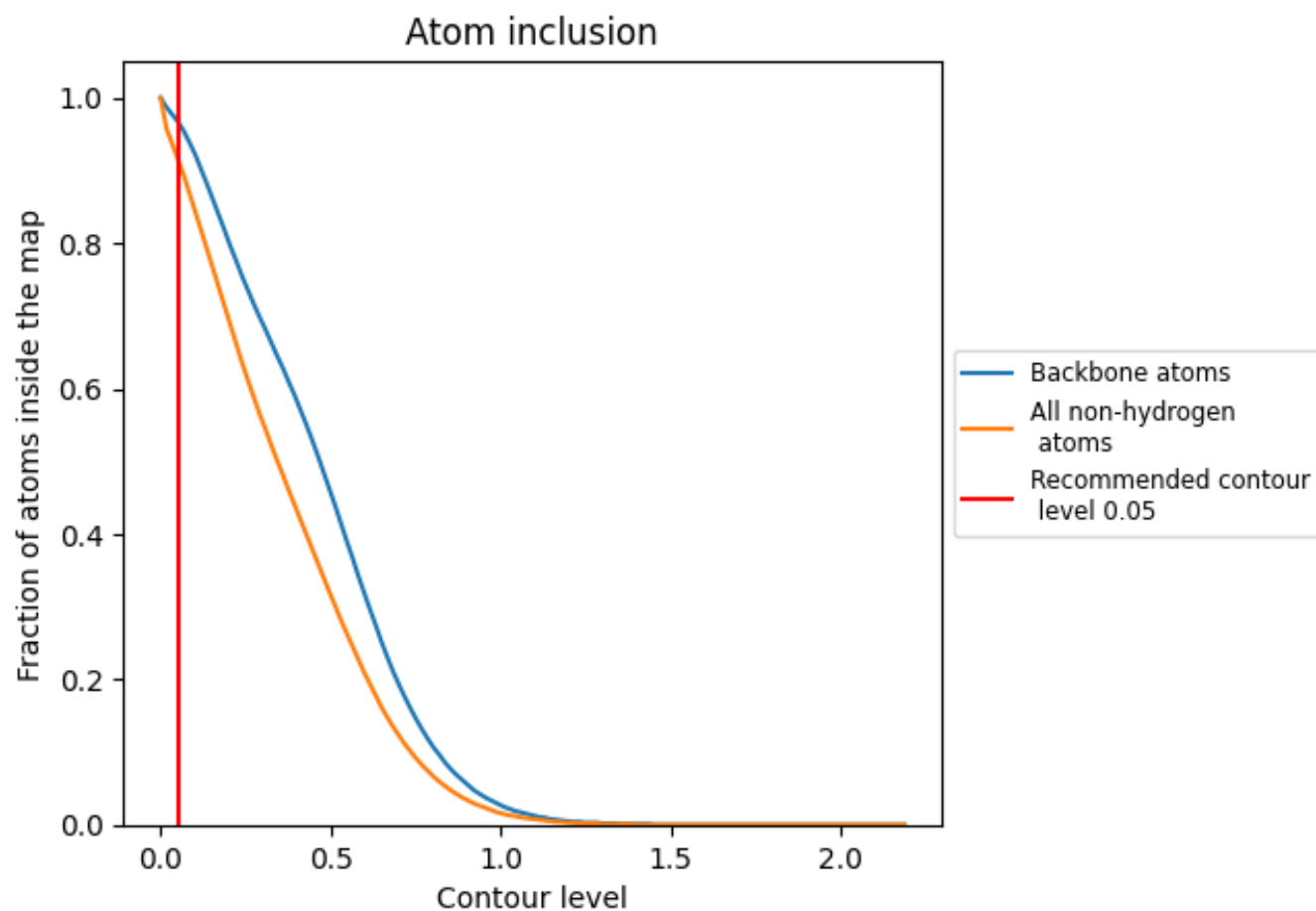
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9170	 0.4120
0	 0.8470	 0.4210
1	 0.8530	 0.4230
10	 0.9180	 0.4590
11	 0.9180	 0.4680
12	 0.9470	 0.4760
13	 0.9350	 0.4780
14	 0.9470	 0.4770
15	 0.9230	 0.4990
16	 0.9410	 0.4740
17	 0.9120	 0.4700
18	 0.9650	 0.4100
19	 0.9230	 0.4330
2	 0.9060	 0.4730
22	 0.9360	 0.4810
23	 0.9420	 0.4320
3	 0.9180	 0.4630
4	 0.8940	 0.4740
5	 0.9180	 0.4600
6	 0.9230	 0.4720
7	 0.9180	 0.4660
8	 0.7880	 0.3050
9	 0.7820	 0.2750
A	 0.6500	 0.2470
A0	 0.9120	 0.4060
A1	 0.9360	 0.3940
A2	 0.9550	 0.4070
A3	 0.9450	 0.3940
A4	 0.9430	 0.4490
A5	 0.9450	 0.4460
A6	 0.9640	 0.4440
A7	 0.9660	 0.4390
A8	 0.9390	 0.4460
A9	 0.9250	 0.4420
B	 0.6980	 0.2810



































































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Chain	Atom inclusion	Q-score
B0	 0.9600	 0.4450
B1	 0.9490	 0.4340
B2	 0.9410	 0.4370
B3	 0.9160	 0.4400
B4	 0.9520	 0.4380
B5	 0.9460	 0.4360
B6	 0.9530	 0.4440
B7	 0.9350	 0.4630
B8	 0.9480	 0.4480
B9	 0.9540	 0.4450
C	 0.8770	 0.3180
C0	 0.9370	 0.3360
C1	 0.8720	 0.3410
C2	 0.8960	 0.3380
C3	 0.9240	 0.3290
C4	 0.9560	 0.3900
C5	 0.9190	 0.3990
C6	 0.9250	 0.3970
C7	 0.9580	 0.3960
C8	 0.9630	 0.4350
C9	 0.9410	 0.4390
D0	 0.9260	 0.4490
D1	 0.9580	 0.4440
D2	 0.9620	 0.4590
D3	 0.9550	 0.4620
D4	 0.9370	 0.4740
D5	 0.9560	 0.4700
D6	 0.9670	 0.4650
D7	 0.9680	 0.4620
D8	 0.9430	 0.4800
D9	 0.9580	 0.4730
E	 0.7780	 0.2920
E0	 0.9600	 0.4670
E1	 0.9550	 0.4580
E2	 0.9310	 0.4700
E3	 0.9370	 0.4690
E4	 0.9690	 0.4580
E5	 0.9610	 0.4560
E6	 0.9500	 0.4700
E7	 0.9450	 0.4740
E8	 0.9480	 0.3900
E9	 0.8830	 0.2960

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Chain	Atom inclusion	Q-score
F	 0.8360	 0.3380
F0	 0.9300	 0.3890
F1	 0.9210	 0.4150
G	 0.8860	 0.3530
H	 0.5310	 0.1180
I	 0.4610	 0.0870
J	 0.5580	 0.1260
K	 0.5050	 0.1020
a	 0.8850	 0.3930
b	 0.9240	 0.3980
c	 0.9140	 0.4570
d	 0.9210	 0.4250
e	 0.9190	 0.4560
f	 0.9420	 0.4500
g	 0.9060	 0.4440
h	 0.9360	 0.4420
i	 0.8730	 0.3100
j	 0.8890	 0.3200
k	 0.8430	 0.3060
l	 0.8140	 0.2870
m	 0.8040	 0.3000
n	 0.7860	 0.3100
o	 0.9360	 0.4220
p	 0.9160	 0.4500
q	 0.9420	 0.4460
r	 0.9260	 0.4640
s	 0.9500	 0.4680
t	 0.9390	 0.4830
u	 0.9400	 0.4460
v	 0.9170	 0.4430
w	 0.9040	 0.3460
x	 0.8780	 0.3570