



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 04:56 PM UTC

PDB ID : 7MIZ / pdb_00007miz
EMDB ID : EMD-23869
Title : Atomic structure of cortical microtubule from *Toxoplasma gondii*
Authors : Wang, X.; Brown, A.; Sibley, L.D.; Zhang, R.
Deposited on : 2021-04-18
Resolution : 3.40 Å(reported)
Based on initial models : 4FYU, 6U42, 3JAS

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

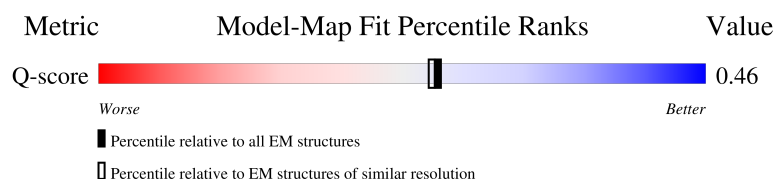
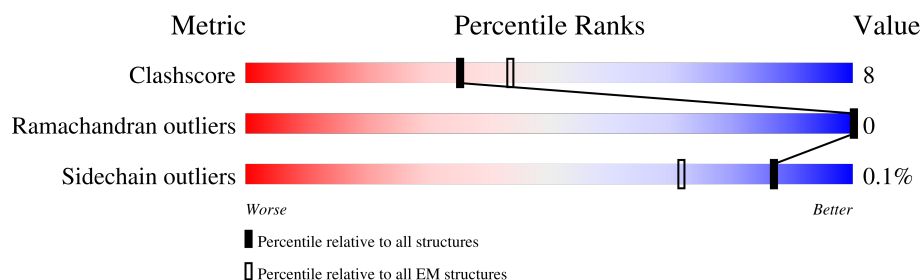
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

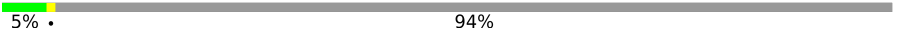
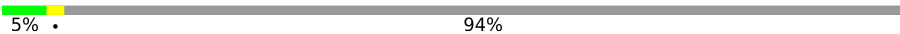
The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



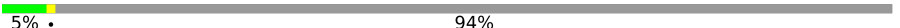
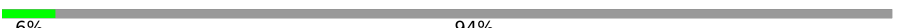
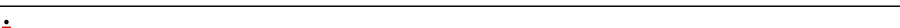
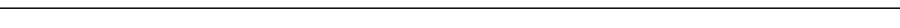
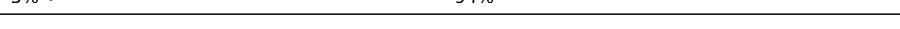
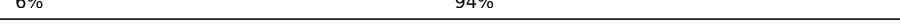
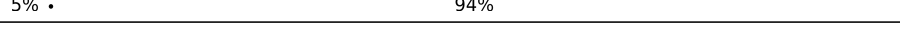
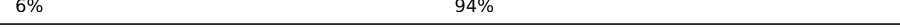
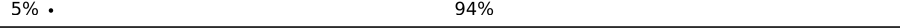
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	351	
1	1	351	
1	10	351	
1	11	351	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	12	351	 5% • 94%
1	13	351	 6% • 94%
1	14	351	 6% • 94%
1	15	351	 6% • 94%
1	16	351	 6% • 94%
1	17	351	 6% • 94%
1	18	351	 6% • 94%
1	19	351	 6% • 94%
1	2	351	 6% • 94%
1	20	351	 6% • 94%
1	21	351	 6% • 94%
1	22	351	 5% • 94%
1	23	351	 5% • 94%
1	3	351	 6% • 94%
1	4	351	 5% • 94%
1	5	351	 6% • 94%
1	6	351	 6% • 94%
1	7	351	 5% • 94%
1	8	351	 6% • 94%
1	9	351	 5% • 94%
2	A0	453	 9% 76% 19% 6%
2	A2	453	 8% 74% 21% 6%
2	A4	453	 78% 16% 6%
2	A6	453	 75% 19% 6%
2	A8	453	 75% 19% 6%

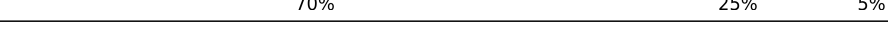
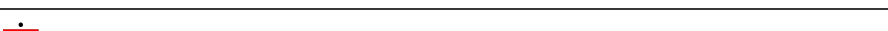
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B0	453	 80%14%6%
2	B2	453	 78%16%6%
2	B4	453	 73%22%6%
2	B6	453	 76%18%6%
2	B8	453	 74%20%6%
2	C0	453	 71%23%6%
2	C2	453	 72%22%6%
2	C4	453	 67%27%6%
2	C6	453	 70%25%6%
2	C8	453	 79%15%6%
2	D0	453	 81%14%6%
2	D2	453	 80%14%6%
2	D4	453	 79%15%6%
2	D6	453	 79%16%6%
2	D8	453	 80%14%6%
2	E0	453	 81%13%6%
2	E2	453	 79%16%6%
2	E4	453	 78%16%6%
2	E6	453	 77%18%6%
2	E8	453	 71%24%6%
2	F0	453	 74%20%6%
3	A1	449	 75%20%5%
3	A3	449	 76%19%5%
3	A5	449	 75%20%5%
3	A7	449	 78%17%5%

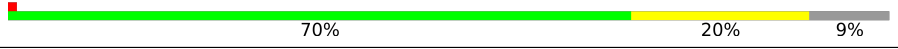
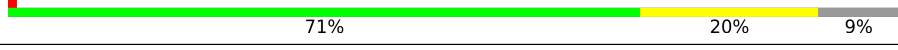
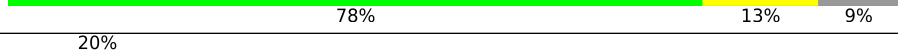
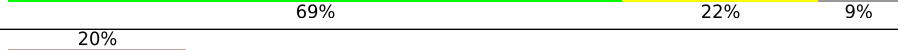
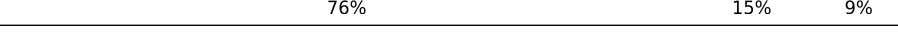
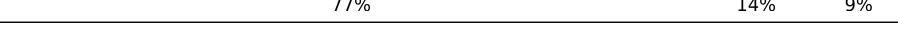
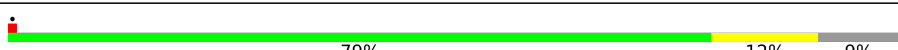
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	A9	449	 74%20%5%
3	B1	449	 77%18%5%
3	B3	449	 78%17%5%
3	B5	449	 77%18%5%
3	B7	449	 77%18%5%
3	B9	449	 78%17%5%
3	C1	449	 72%23%5%
3	C3	449	 70%25%5%
3	C5	449	 72%22%5%
3	C7	449	 72%23%5%
3	C9	449	 76%18%5%
3	D1	449	 77%18%5%
3	D3	449	 76%19%5%
3	D5	449	 70%25%5%
3	D7	449	 73%21%5%
3	D9	449	 77%18%5%
3	E1	449	 81%14%5%
3	E3	449	 79%16%5%
3	E5	449	 72%22%5%
3	E7	449	 76%18%5%
3	E9	449	 72%22%5%
3	F1	449	 72%23%5%
4	a	220	 54%14%32%
4	b	220	 55%13%32%
4	c	220	 71%20%9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	d	220	
4	e	220	
4	f	220	
4	g	220	
4	h	220	
4	i	220	
4	j	220	
4	m	220	
4	n	220	
4	o	220	
4	p	220	
4	q	220	
4	r	220	
4	s	220	
4	t	220	
4	u	220	
4	v	220	
5	k	189	
5	l	189	
5	w	189	
5	x	189	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 214754 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	2	22	Total	C	N	O	S	0	0
			174	114	28	31	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		
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		
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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
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	20	22	Total	C	N	O	S	0	0
			174	114	28	31	1		
1	21	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		

There are 24 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
2	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
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
20	93	ARG	PRO	conflict	UNP A0A7J6K285
21	93	ARG	PRO	conflict	UNP A0A7J6K285
22	93	ARG	PRO	conflict	UNP A0A7J6K285
23	93	ARG	PRO	conflict	UNP A0A7J6K285

- Molecule 2 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	A8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	B8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	C8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	D8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E2	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E4	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E6	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	E8	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		
2	F0	428	Total	C	N	O	S	0	0
			3325	2105	569	625	26		

- Molecule 3 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	A9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	B9	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C1	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C3	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C5	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		
3	C7	426	Total	C	N	O	S	0	0
			3331	2094	569	641	27		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is a protein called PDI family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	150	Total 1198	C 763	N 213	O 217	S 5	0	0
4	b	150	Total 1198	C 763	N 213	O 217	S 5	0	0
4	c	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	d	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	e	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	f	201	Total 1608	C 1021	N 283	O 297	S 7	0	0
4	g	201	Total 1608	C 1021	N 283	O 297	S 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	h	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	i	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	j	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	o	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	p	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	q	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	r	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	s	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	t	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	u	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	v	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	n	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		
4	m	201	Total	C	N	O	S	0	0
			1608	1021	283	297	7		

- Molecule 5 is a protein called PDI family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	k	139	Total	C	N	O	S	0	0
			1140	738	203	195	4		
5	l	139	Total	C	N	O	S	0	0
			1140	738	203	195	4		
5	w	143	Total	C	N	O	S	0	0
			1172	755	207	205	5		
5	x	143	Total	C	N	O	S	0	0
			1172	755	207	205	5		

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	167	SER	-	insertion	UNP A0A7J6K232

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

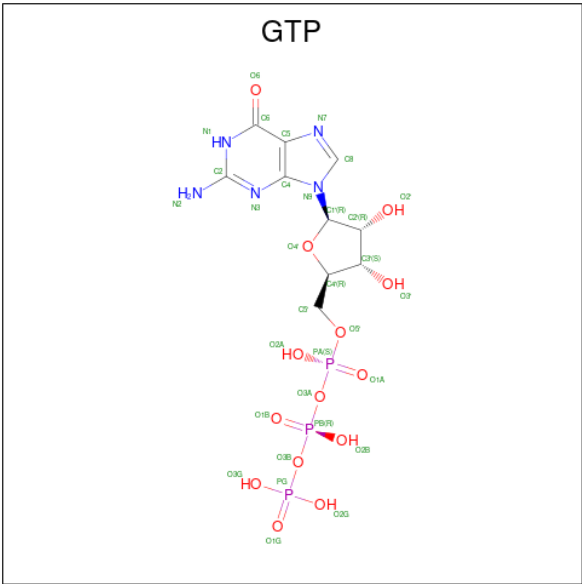
Chain	Residue	Modelled	Actual	Comment	Reference
l	187	GLN	-	insertion	UNP A0A7J6K232
l	188	ASN	-	insertion	UNP A0A7J6K232
l	189	VAL	-	insertion	UNP A0A7J6K232
w	167	SER	-	insertion	UNP A0A7J6K232
w	168	ALA	-	insertion	UNP A0A7J6K232
w	169	GLN	-	insertion	UNP A0A7J6K232
w	170	ARG	-	insertion	UNP A0A7J6K232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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
x	183	LYS	-	insertion	UNP A0A7J6K232
x	184	ARG	-	insertion	UNP A0A7J6K232
x	185	LEU	-	insertion	UNP A0A7J6K232
x	186	PRO	-	insertion	UNP A0A7J6K232
x	187	GLN	-	insertion	UNP A0A7J6K232
x	188	ASN	-	insertion	UNP A0A7J6K232
x	189	VAL	-	insertion	UNP A0A7J6K232

- Molecule 6 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
6	B6	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	B8	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	C0	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	C2	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	C4	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	C6	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	C8	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	D0	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	D2	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	D4	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	D6	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	D8	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E0	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E2	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E4	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E6	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	E8	1	Total	C	N	O	P	0
			32	10	5	14	3	
6	F0	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
7	A0	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

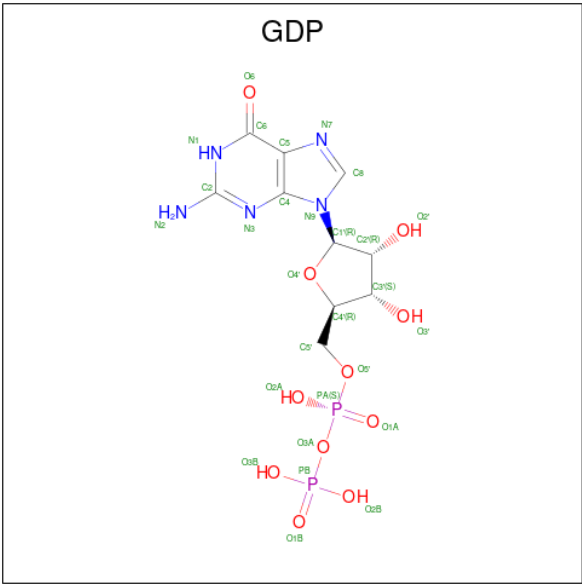
Mol	Chain	Residues	Atoms		AltConf
7	A2	1	Total 1	Mg 1	0
7	A4	1	Total 1	Mg 1	0
7	A6	1	Total 1	Mg 1	0
7	A8	1	Total 1	Mg 1	0
7	B0	1	Total 1	Mg 1	0
7	B2	1	Total 1	Mg 1	0
7	B4	1	Total 1	Mg 1	0
7	B6	1	Total 1	Mg 1	0
7	B8	1	Total 1	Mg 1	0
7	C0	1	Total 1	Mg 1	0
7	C2	1	Total 1	Mg 1	0
7	C4	1	Total 1	Mg 1	0
7	C6	1	Total 1	Mg 1	0
7	C8	1	Total 1	Mg 1	0
7	D0	1	Total 1	Mg 1	0
7	D2	1	Total 1	Mg 1	0
7	D4	1	Total 1	Mg 1	0
7	D6	1	Total 1	Mg 1	0
7	D8	1	Total 1	Mg 1	0
7	E0	1	Total 1	Mg 1	0
7	E2	1	Total 1	Mg 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
7	E4	1	Total	Mg	0
			1	1	
7	E6	1	Total	Mg	0
			1	1	
7	E8	1	Total	Mg	0
			1	1	
7	F0	1	Total	Mg	0
			1	1	

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



Mol	Chain	Residues	Atoms					AltConf
8	A1	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	A3	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	A5	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	A7	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	A9	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	B1	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	B3	1	Total	C	N	O	P	0
			28	10	5	11	2	

Continued on next page...

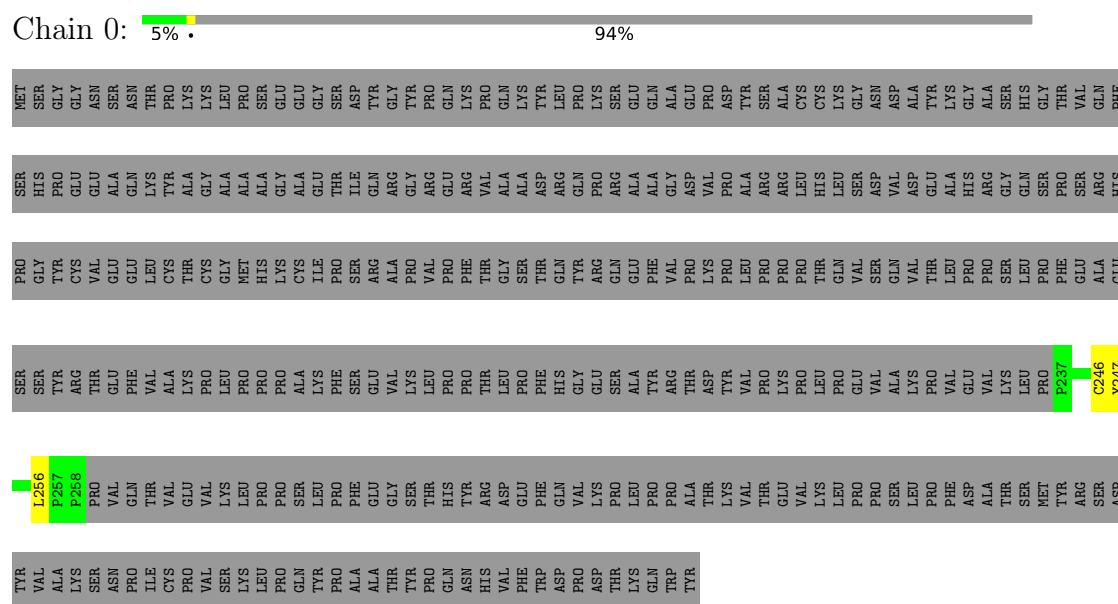
Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
8	B5	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	B7	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	B9	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	C1	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	C3	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	C5	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	C7	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	C9	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	D1	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	D3	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	D5	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	D7	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	D9	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	E1	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	E3	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	E5	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	E7	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	E9	1	Total	C	N	O	P	0
			28	10	5	11	2	
8	F1	1	Total	C	N	O	P	0
			28	10	5	11	2	

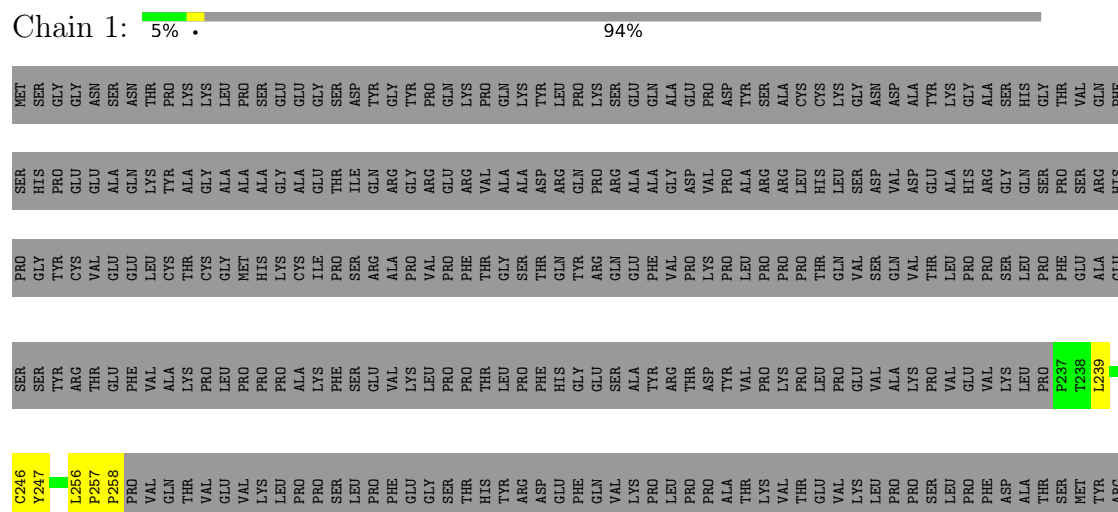
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Microtubule associated protein SPM1



• Molecule 1: Microtubule associated protein SPM1



- Molecule 1: Microtubule associated protein SPM1

Chain 2: 6% 94%

MET	SER	GLY	GLN	ASN	SER	ASN	THR	PRO	LYS	LEU	PRO	SER	GLU	GLY	SER	ASP	TYR	GLY	TYR	PRO	GLN	LYS	GLN	PRO	TYR	LEU	PRO	LYS	GLU	GLN	ALA	ALA	CYS	CYS	LYS	GLY	ASN	ASP	ALA	TYR	LYS	THR	VAL	GLN	PRO
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	HIS	PRO	GLU	GLU	ALA	GLN	LYS	TYR	ALA	ALA	GLY	ALA	ALA	ALA	GLY	GLY	GLU	THR	ILE	GLN	ARG	GLY	GLY	ARG	GLU	ARG	VAL	ALA	ALA	ALA	ASP	ASP	ARG	GLN	PRO	ALA	ALA	ALA	GLY	GLY	ASP	VAL	PRO	VAL	ARG	ARG	LEU	HIS	LEU	SER	SER	ASP	VAL	ASP	GLU	ALA	ALA	ALA	HIS	GLY	ARG	SER	SER	PRO	GLN	SER	ARG	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

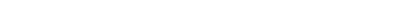
PRO	GLY	TYR	CYS	VAL	GLU	GLU	LEU	CYS	THR	GLY	MET	HIS	LYS	CYS	ILE	PRO	SER	ARG	ALA	PRO	PRO	PRO	PRO	THR	GLY	SER	THR	SER	GLN	TYR	ARG	GLU	GLN	PHE	VAL	PRO	PRO	LYS	PRO	PRO	LEU	PRO	PRO	PRO	THR	GLN	GLN	SER	SER	GLN	VAL	THR	LEU	THR	PRO	PRO	SER	PRO	PRO	PHE	GLU	ALA	GLN
-----	-----	-----	-----	-----	-----	-----	-----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

SER	SER	ARG	THR	GLU	PHE	VAL	LYS	PRO	LEU	PRO	PRO	PRO	LYS	PHE	SER	GLU	VAL	LYS	LEU	PRO	PRO	THR	LEU	PRO	PHE	HIS	GLY	GLU	SER	ALA	TYR	ARG	THR	ASP	TYR	VAL	PRO	LYS	PRO	LEU	PRO	PRO	GLU	VAL	ALA	LYS	VAL	VAL	GLU	VAL	LYS	LEU	PRO	P237	Q244
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------

[illegible]

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
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 1: Microtubule associated protein SPM1

Chain 3:  6% 94%

MET	SER	GLY	GLY	ASN	ASN	THR	THR	PRO	LYS	LYS	LEU	PRO	PRO	SER	GLU	GLY	GLY	SER	ASP	TYR	TYR	TYR	PRO	PRO	GLN	LYS	LYS	LEU	PRO	LYS	SER	GLU	GLN	GLN	ALA	ALA	CYS	CYS	LYS	LYS	GLY	GLY	ASN	ASP	ALA	ALA	TYR	LYS	TYR	GLY	GLY	SER	SER	HIS	GLY	THR	VAL	GLN	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER	HIS	PRO	HIS	GLU	GLY	ALA	ALA	GLN	LYS	TYR	ALA	ALA	GLY	GLY	ALA	ALA	GLU	THR	ILE	GLN	ARG	GLY	ARG	GLY	ARG	GLY	ASP	ASP	GLN	GLN	PRO	PRO	VAL	ASP	GLY	ARG	ARG	LEU	HIS	HIS	LEU	SER	SER	ASP	VAL	ASP	GLU	ALA	GLY	HIS	HIS	ARG	GLY	GLN	PRO	PRO	SER	SER	SER	ARG	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

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

[illegible]

R248	E249	E250	F251	F252	F253	F254	F255	F256	F257	F258	F259	F260	F261	F262	F263	F264	F265	F266	F267	F268	F269	F270	F271	F272	F273	F274	F275	F276	F277	F278	F279	F280	F281	F282	F283	F284	F285	F286	F287	F288	F289	F290	F291	F292	F293	F294	F295	F296	F297	F298	F299	F300	F301	F302	F303	F304	F305	F306	F307	F308	F309	F310	F311	F312	F313	F314	F315	F316	F317	F318	F319	F320	F321	F322	F323	F324	F325	F326	F327	F328	F329	F330	F331	F332	F333	F334	F335	F336	F337	F338	F339	F340	F341	F342	F343	F344	F345	F346	F347	F348	F349	F350	F351	F352	F353	F354	F355	F356	F357	F358	F359	F360	F361	F362	F363	F364	F365	F366	F367	F368	F369	F370	F371	F372	F373	F374	F375	F376	F377	F378	F379	F380	F381	F382	F383	F384	F385	F386	F387	F388	F389	F390	F391	F392	F393	F394	F395	F396	F397	F398	F399	F400	F401	F402	F403	F404	F405	F406	F407	F408	F409	F410	F411	F412	F413	F414	F415	F416	F417	F418	F419	F420	F421	F422	F423	F424	F425	F426	F427	F428	F429	F430	F431	F432	F433	F434	F435	F436	F437	F438	F439	F440	F441	F442	F443	F444	F445	F446	F447	F448	F449	F450	F451	F452	F453	F454	F455	F456	F457	F458	F459	F460	F461	F462	F463	F464	F465	F466	F467	F468	F469	F470	F471	F472	F473	F474	F475	F476	F477	F478	F479	F480	F481	F482	F483	F484	F485	F486	F487	F488	F489	F490	F491	F492	F493	F494	F495	F496	F497	F498	F499	F500	F501	F502	F503	F504	F505	F506	F507	F508	F509	F510	F511	F512	F513	F514	F515	F516	F517	F518	F519	F520	F521	F522	F523	F524	F525	F526	F527	F528	F529	F530	F531	F532	F533	F534	F535	F536	F537	F538	F539	F540	F541	F542	F543	F544	F545	F546	F547	F548	F549	F550	F551	F552	F553	F554	F555	F556	F557	F558	F559	F560	F561	F562	F563	F564	F565	F566	F567	F568	F569	F570	F571	F572	F573	F574	F575	F576	F577	F578	F579	F580	F581	F582	F583	F584	F585	F586	F587	F588	F589	F590	F591	F592	F593	F594	F595	F596	F597	F598	F599	F600	F601	F602	F603	F604	F605	F606	F607	F608	F609	F610	F611	F612	F613	F614	F615	F616	F617	F618	F619	F620	F621	F622	F623	F624	F625	F626	F627	F628	F629	F630	F631	F632	F633	F634	F635	F636	F637	F638	F639	F640	F641	F642	F643	F644	F645	F646	F647	F648	F649	F650	F651	F652	F653	F654	F655	F656	F657	F658	F659	F660	F661	F662	F663	F664	F665	F666	F667	F668	F669	F670	F671	F672	F673	F674	F675	F676	F677	F678	F679	F680	F681	F682	F683	F684	F685	F686	F687	F688	F689	F690	F691	F692	F693	F694	F695	F696	F697	F698	F699	F700	F701	F702	F703	F704	F705	F706	F707	F708	F709	F710	F711	F712	F713	F714	F715	F716	F717	F718	F719	F720	F721	F722	F723	F724	F725	F726	F727	F728	F729	F730	F731	F732	F733	F734	F735	F736	F737	F738	F739	F740	F741	F742	F743	F744	F745	F746	F747	F748	F749	F750	F751	F752	F753	F754	F755	F756	F757	F758
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

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
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Molecule 1: Microtubule associated protein SPM1

Chain 4: 5% 94%

MET	SER	Gly	Gly	ASN	ASN	THR	PRO	Lys	Lys	Leu	Pro	Pro	SER	Gly	Gly	Tyr	ASP	SER	LEU	Pro	Lys	Gln	Lys	Pro	Pro	Gln	Lys	Tyr	Tyr	LEU	Pro	Lys	Gly	Glu	SER	Glu	Gln	ALA	ALA	CYS	CYS	Lys	Lys	Gly	Gly	ASN	ASP	ASP	ALA	ALA	Lys	Tyr	Lys	Val	Thr	Gln	Phe
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

[illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 5: 6% 94%

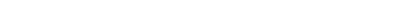
[illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 6: 6% 94%

[illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 7:  5% . 94%

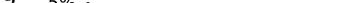
[illegible][illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 8: 6% 94%

[illegible][illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 9:  5% 94%

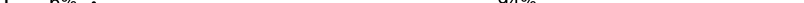
[illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 10: 5% . 94%

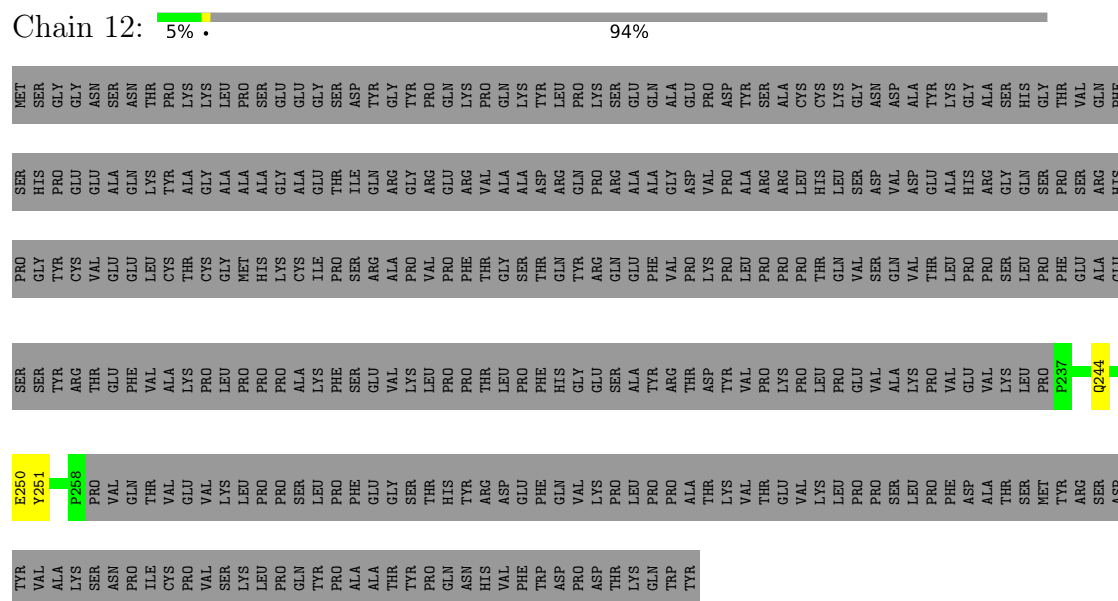
[illegible]

- Molecule 1: Microtubule associated protein SPM1

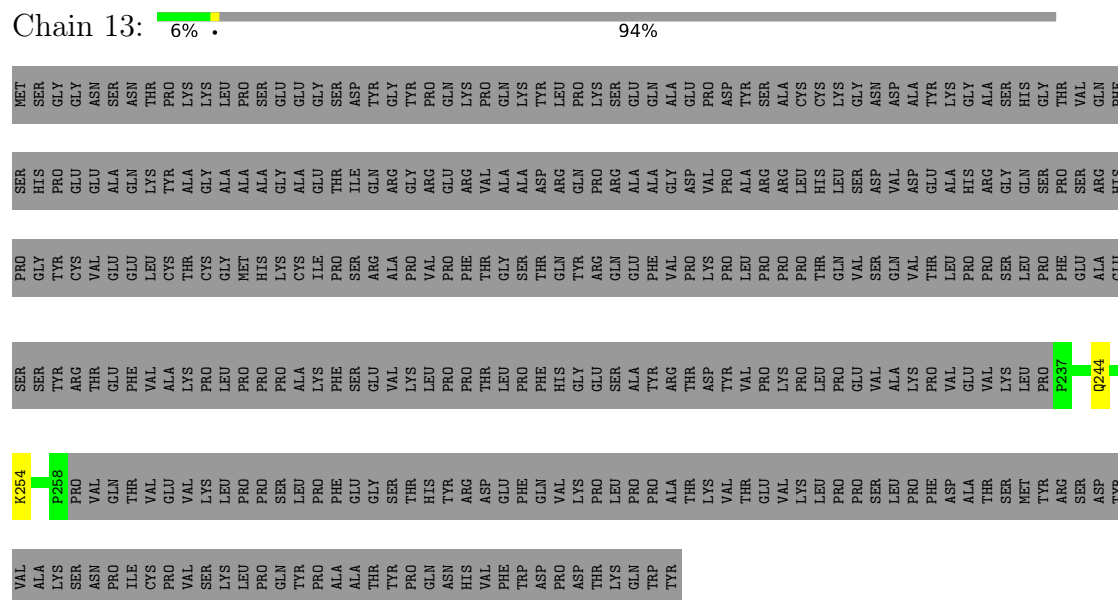
Chain 11:  6% 94%

[illegible]

- Molecule 1: Microtubule associated protein SPM1



- Molecule 1: Microtubule associated protein SPM1



- Molecule 1: Microtubule associated protein SPM1



[illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 15: 6% . 94%

[illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 16: 6% . 94%

[illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 17: 6% 94%

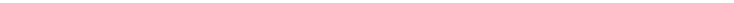
[illegible]

- Molecule 1: Microtubule associated protein SPM1

Chain 18: 6% 94%

[illegible]

- Molecule 1: Microtubule associated protein SPM1

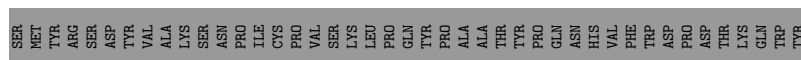
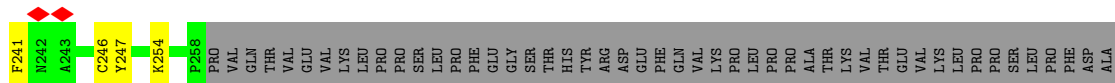
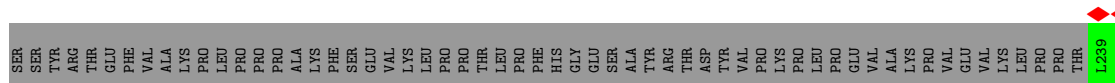
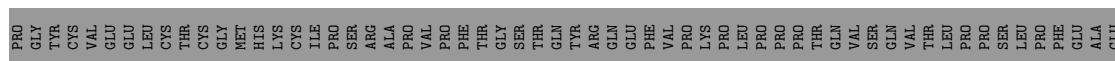
Chain 19:  6% 94%

MET	SER.	GLY	ASN	SER.	ASN	THR.	LYS	LEU	PRO	SER.	GLU	GLY	GLY	TYR.	TYR.	GLY	TYR.	PRO	GLN	LYS	PRO	GLN	LYS	GLY	GLU	GLU	ALA	ALA	CYS	CYS	LYS	GLY	GLY	ASN	ASP	ALA	ALA	TYR.	LYS	LYS	VAL	THR	GLN	PHE.
-----	------	-----	-----	------	-----	------	-----	-----	-----	------	-----	-----	-----	------	------	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----	-----	------

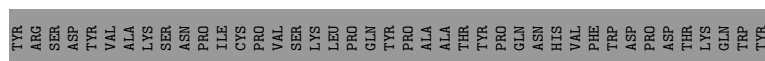
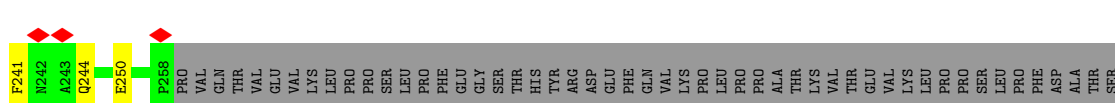
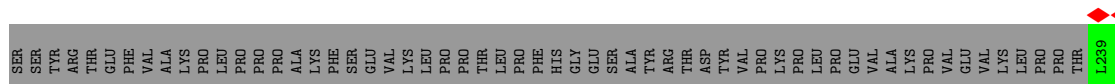
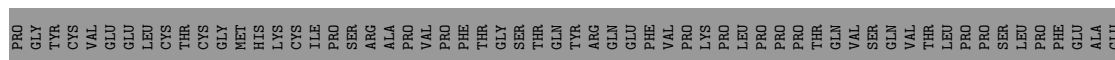


SER	ASP	TYR	VAL	ALA	LYS	SER	ASN	PRO	ILE	CYS	PRO	VAL	SER	LYS	LEU	PRO	GLN	TYR	PRO	ALA	ALA	THR	TYR	PRO	GLN	ASN	HIS	VAL	PHE	TRP	ASP	PRO	ASP	THR	LYS	GLN	TRP	TYR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

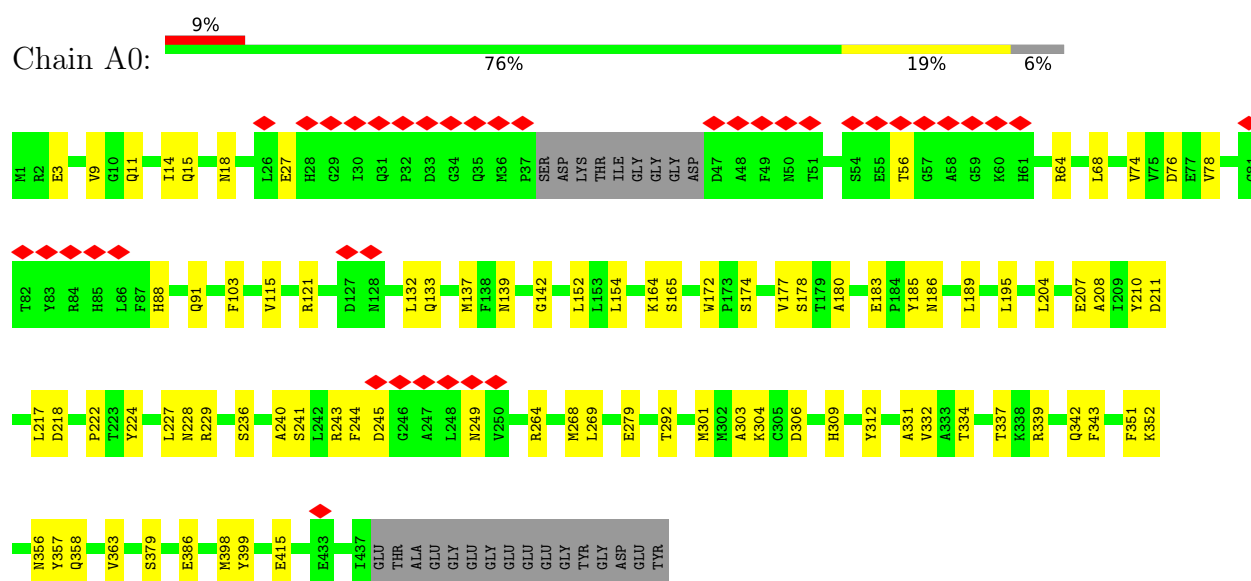
- Molecule 1: Microtubule associated protein SPM1



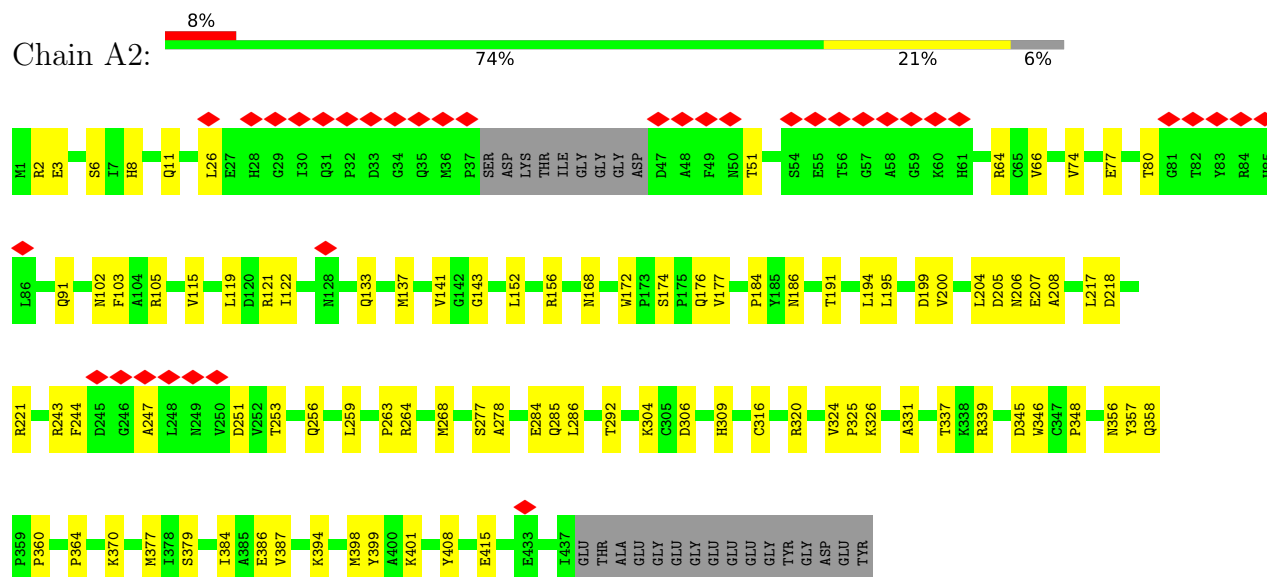
- Molecule 1: Microtubule associated protein SPM1



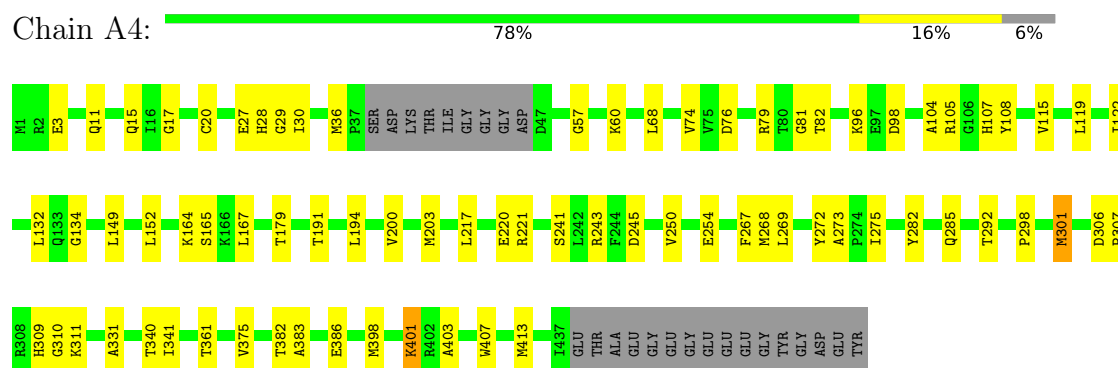
- Molecule 2: Tubulin alpha chain



- Molecule 2: Tubulin alpha chain

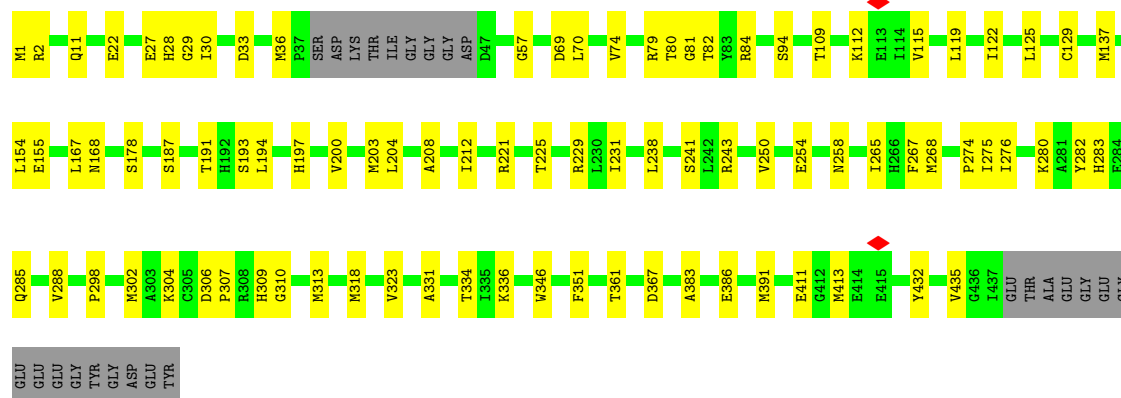


- Molecule 2: Tubulin alpha chain



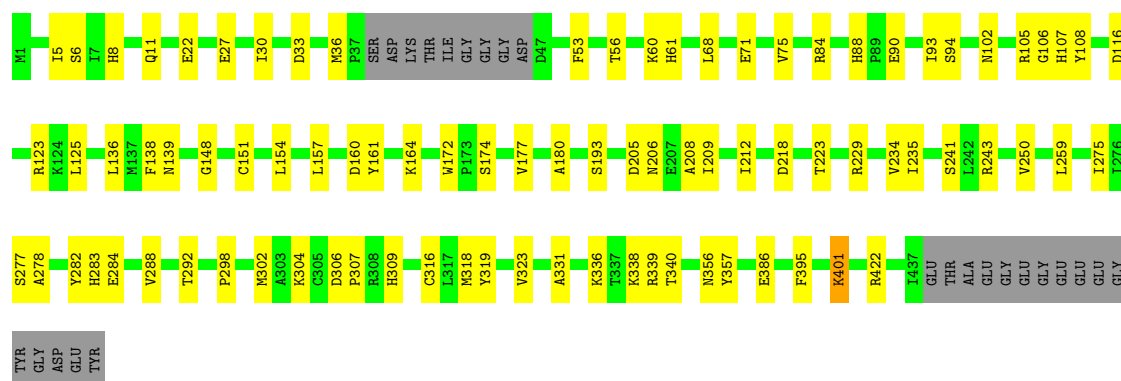
- Molecule 2: Tubulin alpha chain

Chain A6:  75% 19% 6%



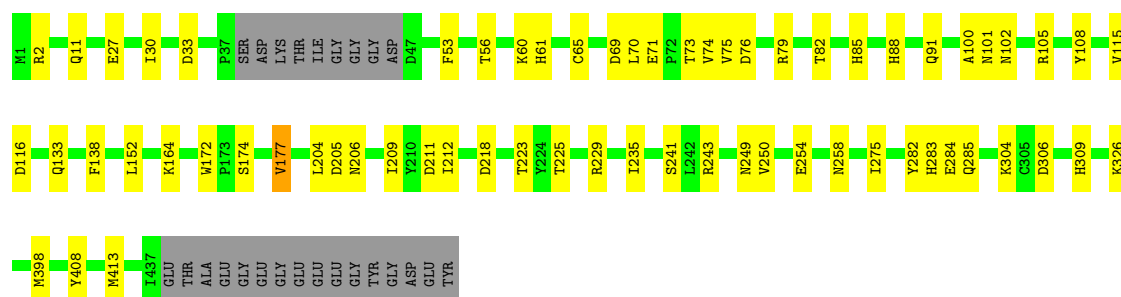
- Molecule 2: Tubulin alpha chain

Chain A8:  75% 19% 6%



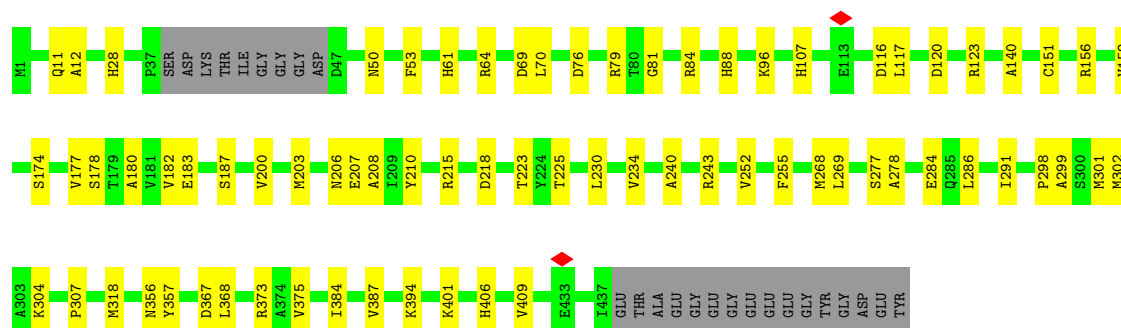
- Molecule 2: Tubulin alpha chain

Chain B0:  80% 14% 6%



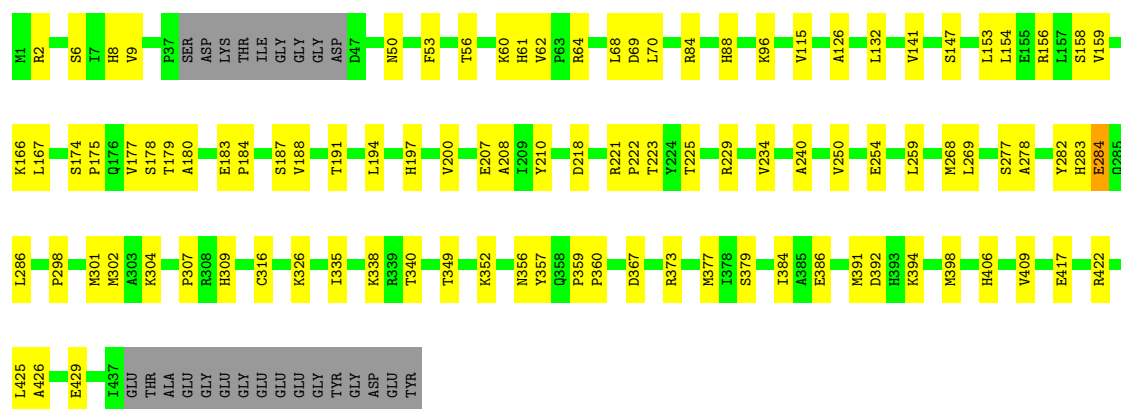
- Molecule 2: Tubulin alpha chain

Chain B2:  78% 16% 6%



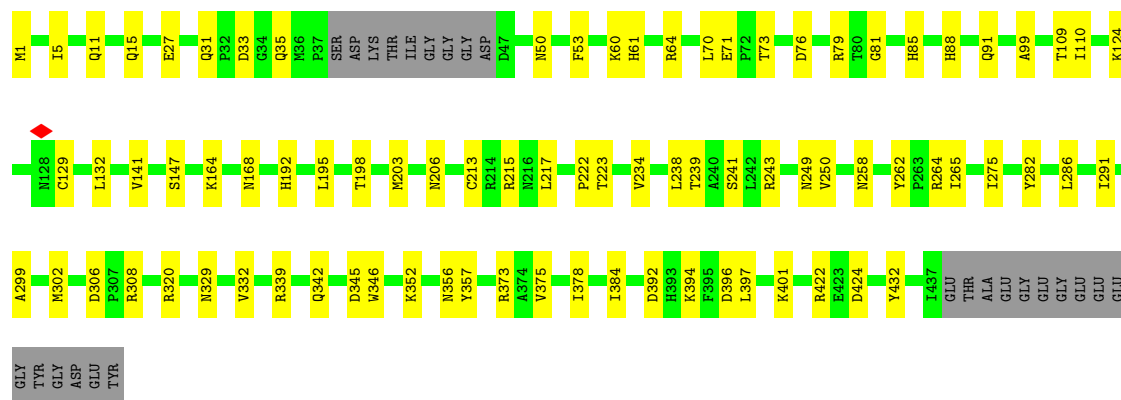
• Molecule 2: Tubulin alpha chain

Chain B4: 73% 22% 6%



• Molecule 2: Tubulin alpha chain

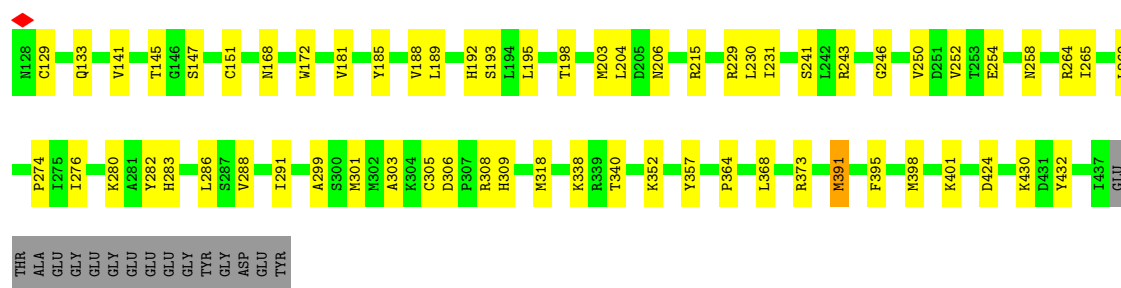
Chain B6: 76% 18% 6%



• Molecule 2: Tubulin alpha chain

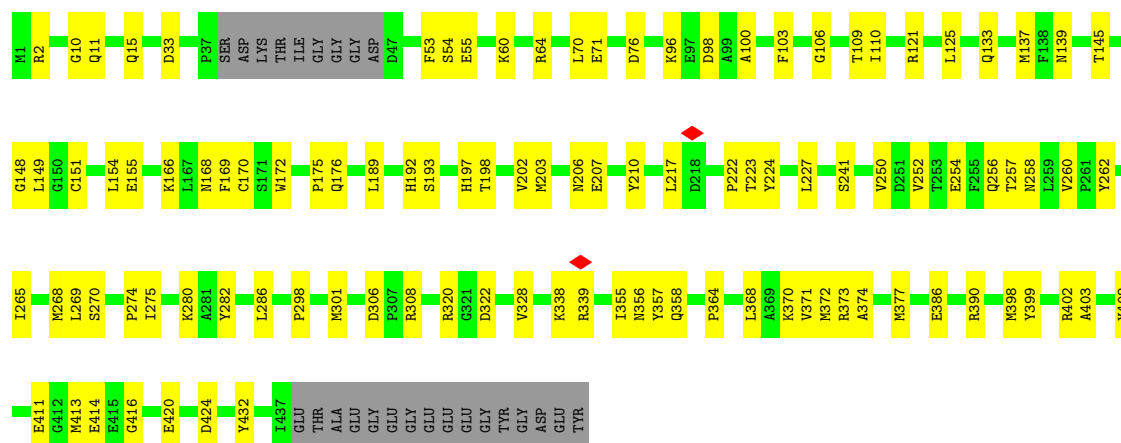
Chain B8: 74% 20% 6%





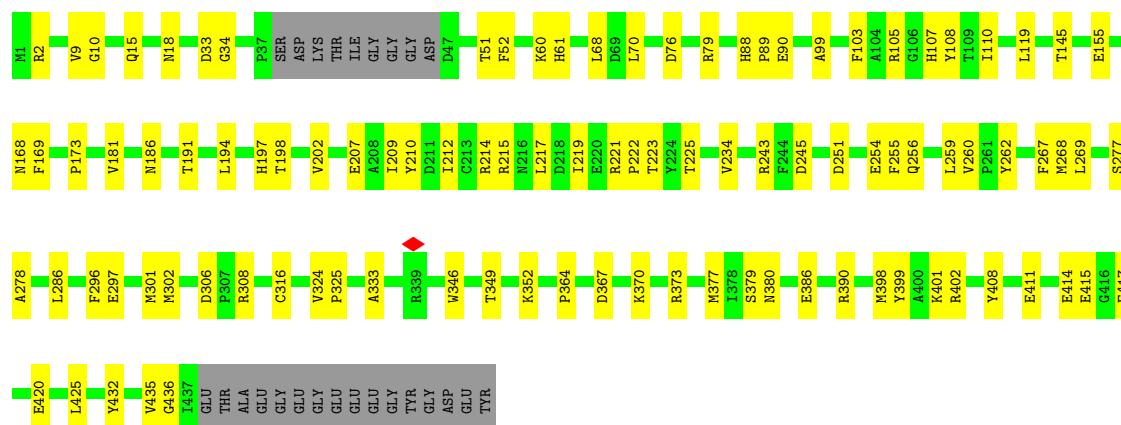
• Molecule 2: Tubulin alpha chain

Chain C0: 71% 23% 6%



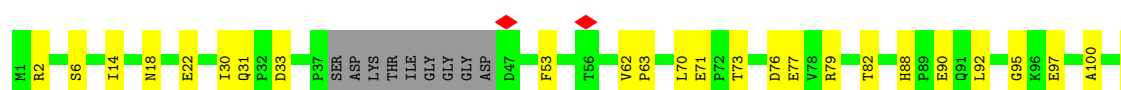
• Molecule 2: Tubulin alpha chain

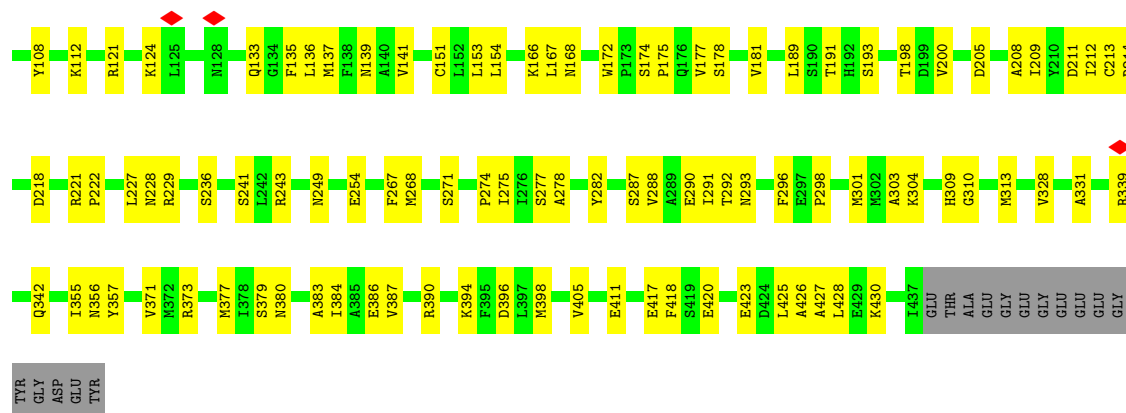
Chain C2: 72% 22% 6%



• Molecule 2: Tubulin alpha chain

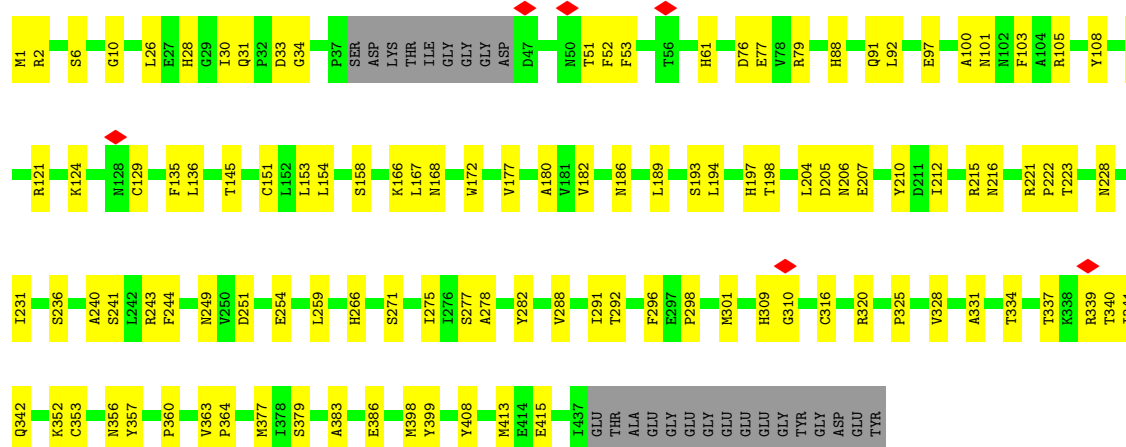
Chain C4: 67% 27% 6%





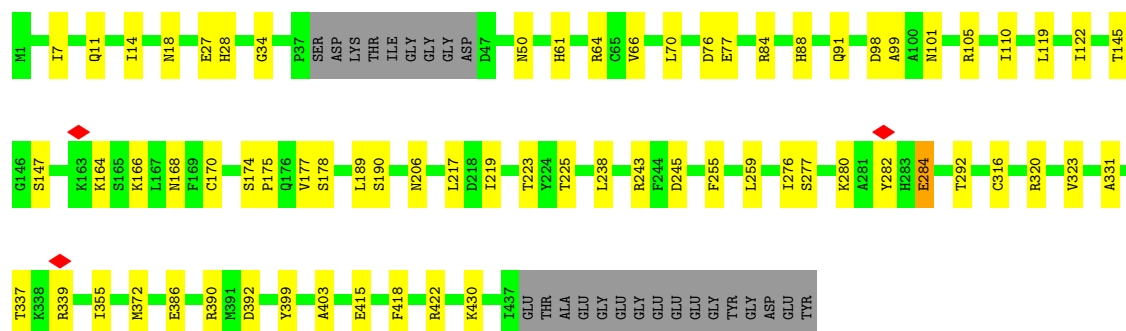
- Molecule 2: Tubulin alpha chain

Chain C6: 70% 25% 6%



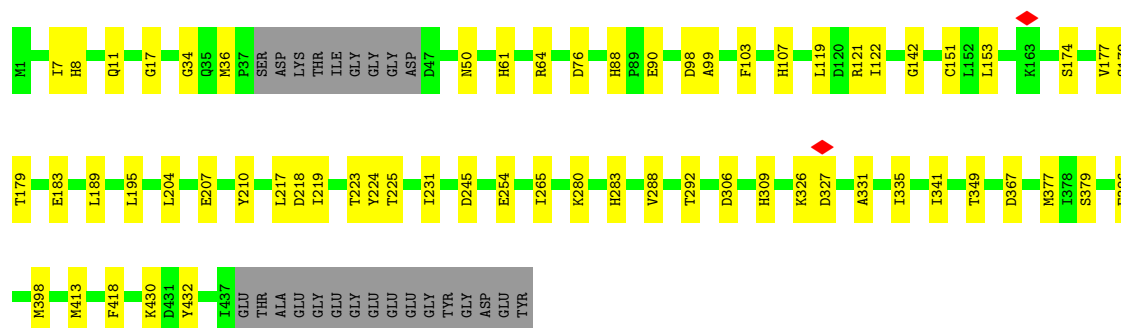
- Molecule 2: Tubulin alpha chain

Chain C8: 79% 15% 6%



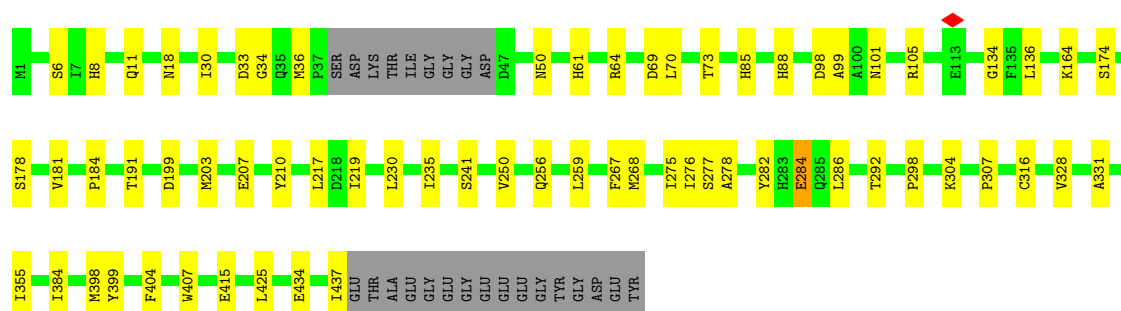
- Molecule 2: Tubulin alpha chain

Chain D0: 81% 14% 6%



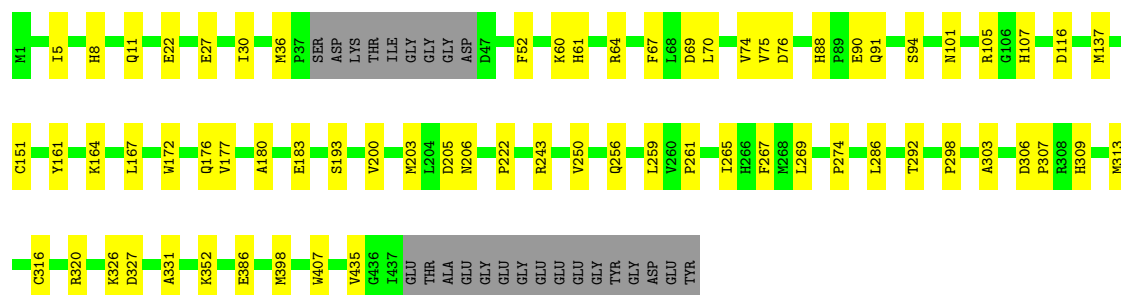
• Molecule 2: Tubulin alpha chain

Chain D2: 80% 14% 6%



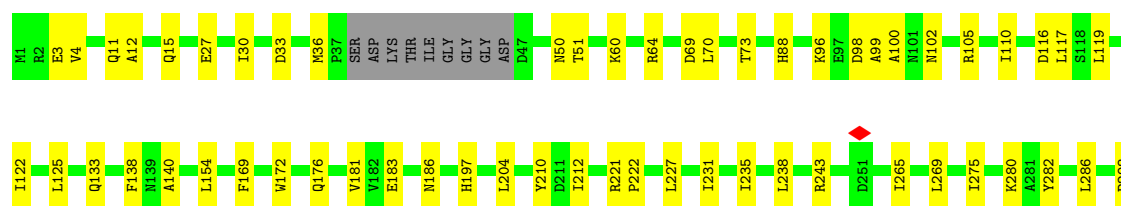
• Molecule 2: Tubulin alpha chain

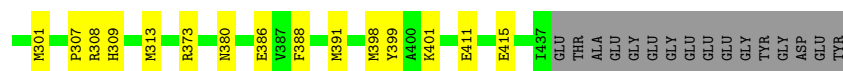
Chain D4: 79% 15% 6%



• Molecule 2: Tubulin alpha chain

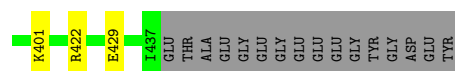
Chain D6: 79% 16% 6%





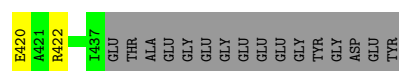
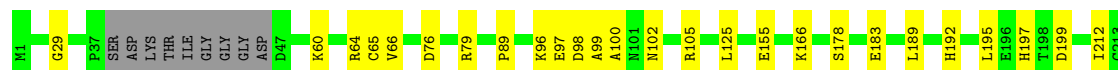
• Molecule 2: Tubulin alpha chain

Chain D8: 80% 14% 6%



• Molecule 2: Tubulin alpha chain

Chain E0: 81% 13% 6%



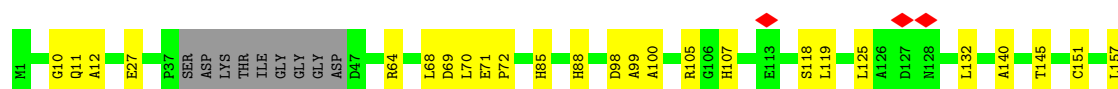
• Molecule 2: Tubulin alpha chain

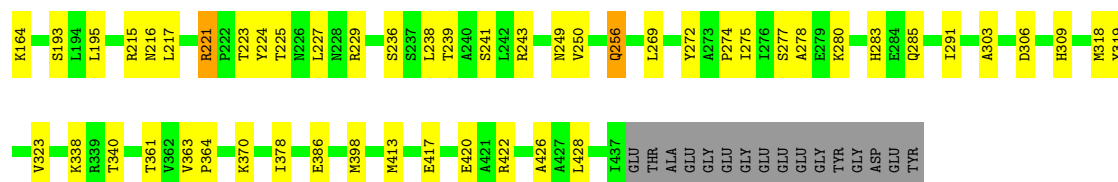
Chain E2: 79% 16% 6%



• Molecule 2: Tubulin alpha chain

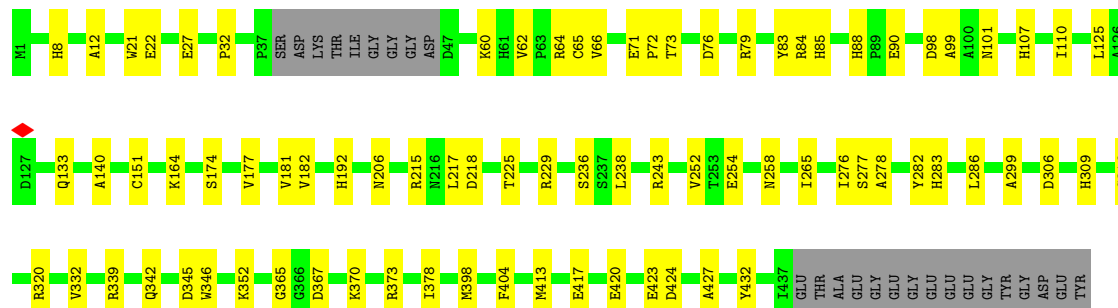
Chain E4: 78% 16% 6%





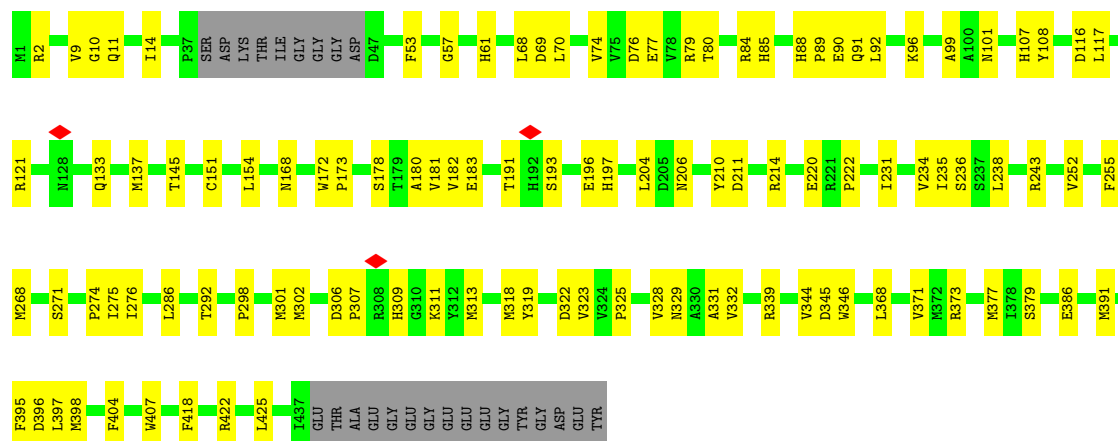
• Molecule 2: Tubulin alpha chain

Chain E6: 77% 18% 6%



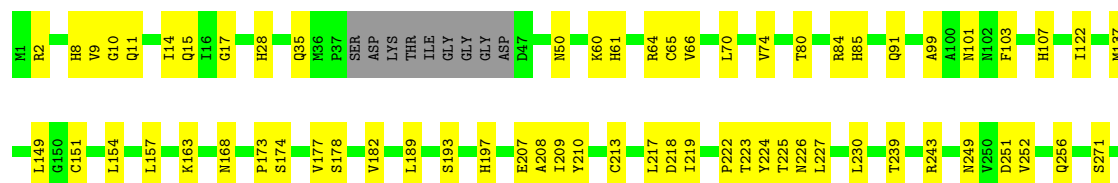
• Molecule 2: Tubulin alpha chain

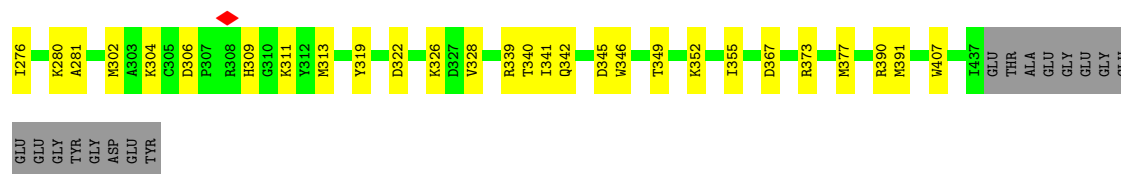
Chain E8: 71% 24% 6%



• Molecule 2: Tubulin alpha chain

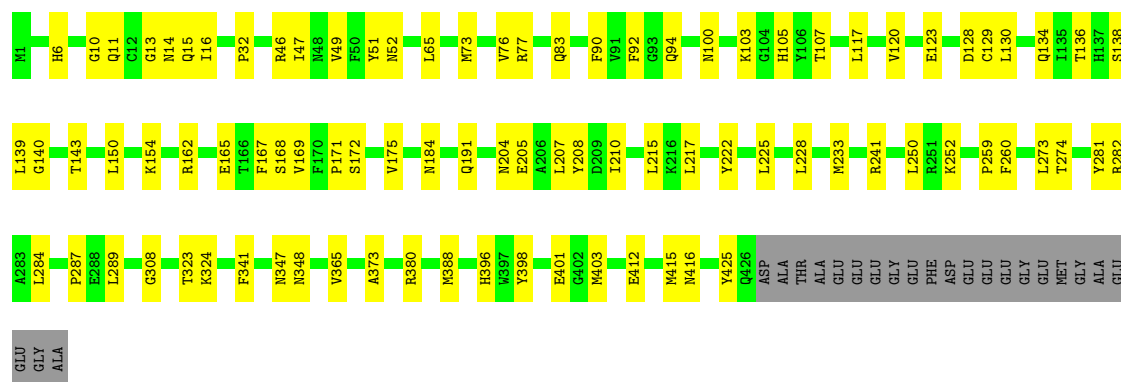
Chain F0: 74% 20% 6%





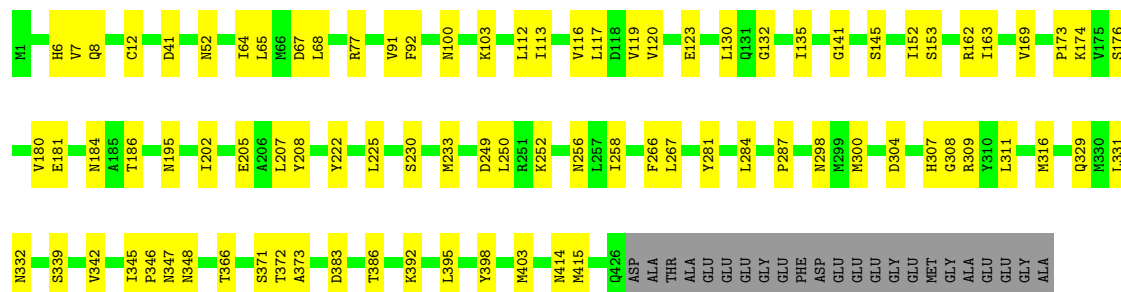
- Molecule 3: Tubulin beta chain

Chain A1: 75% 20% 5%



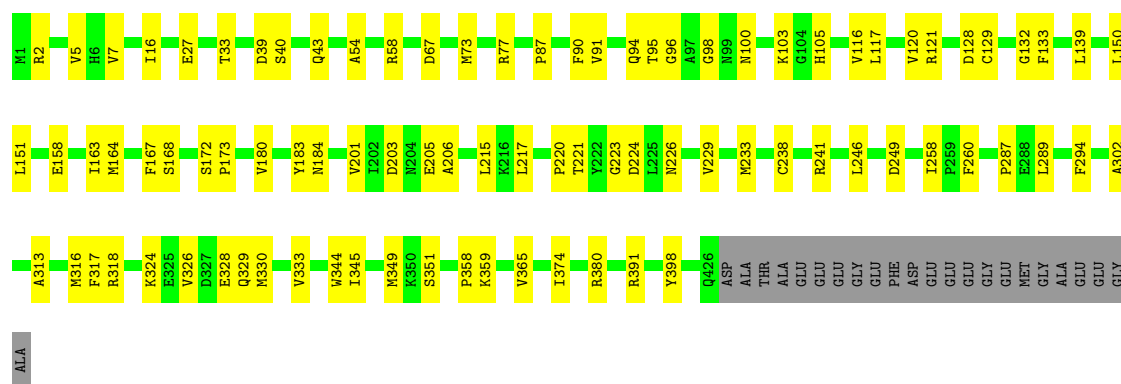
- Molecule 3: Tubulin beta chain

Chain A3: 76% 19% 5%

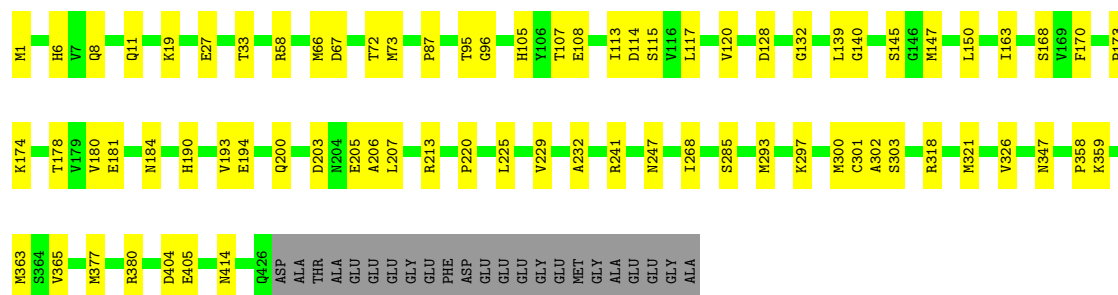


- Molecule 3: Tubulin beta chain

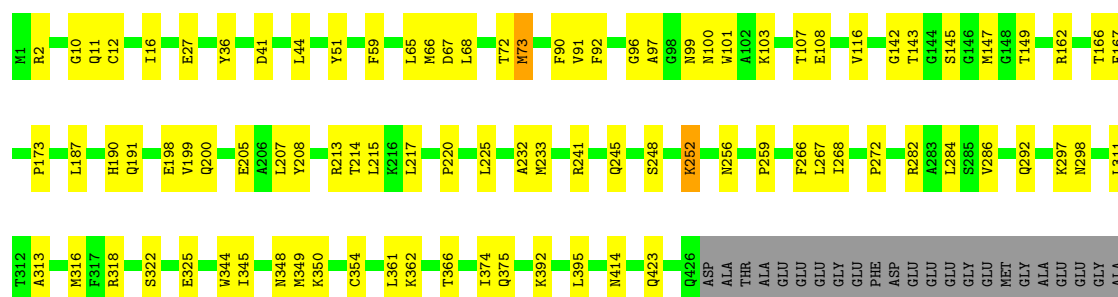
Chain A5: 75% 20% 5%



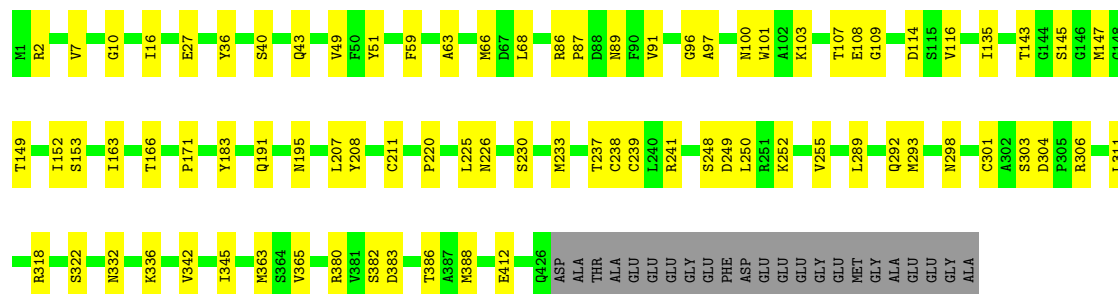
• Molecule 3: Tubulin beta chain

Chain A7:  78% 17% 5%

• Molecule 3: Tubulin beta chain

Chain A9:  74% 20% 5%

• Molecule 3: Tubulin beta chain

Chain B1:  77% 18% 5%

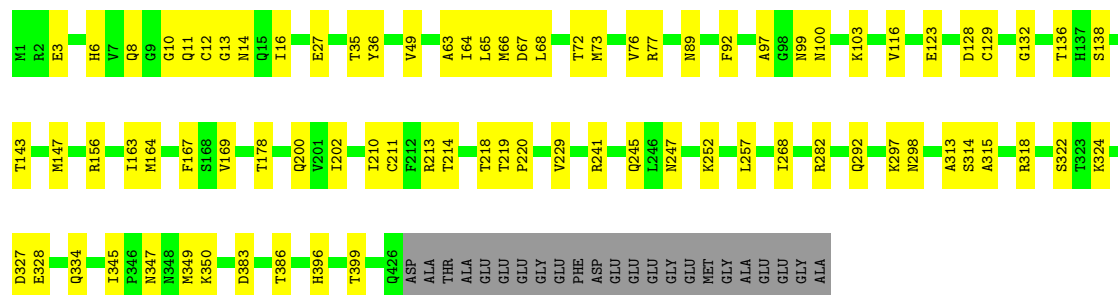
• Molecule 3: Tubulin beta chain

Chain B3:  78% 17% 5%



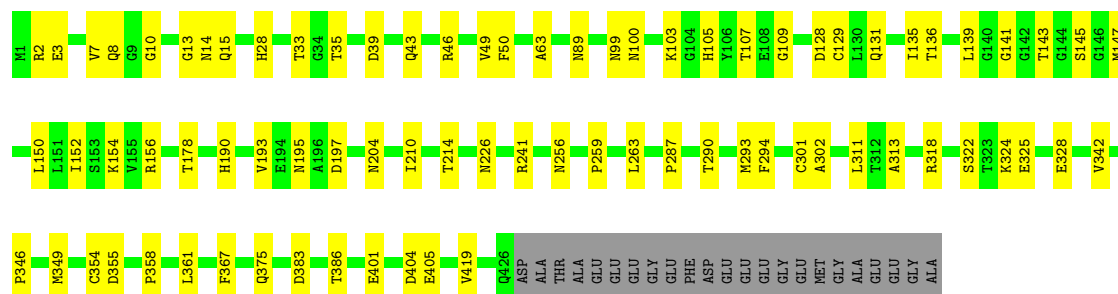
- Molecule 3: Tubulin beta chain

Chain B5: 77% 18% 5%



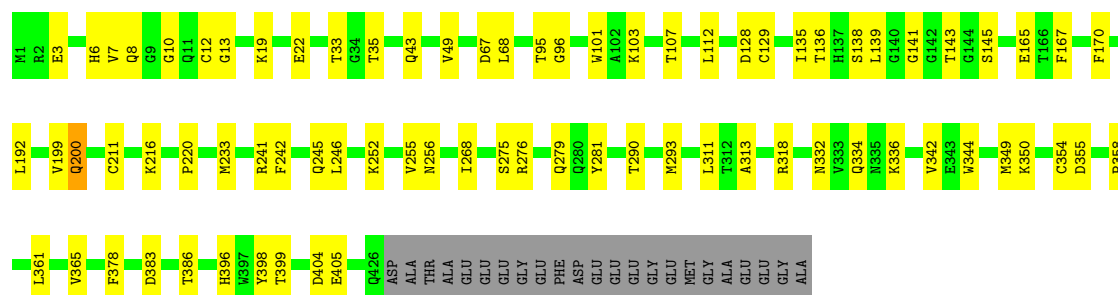
- Molecule 3: Tubulin beta chain

Chain B7: 77% 18% 5%



- Molecule 3: Tubulin beta chain

Chain B9: 78% 17% 5%

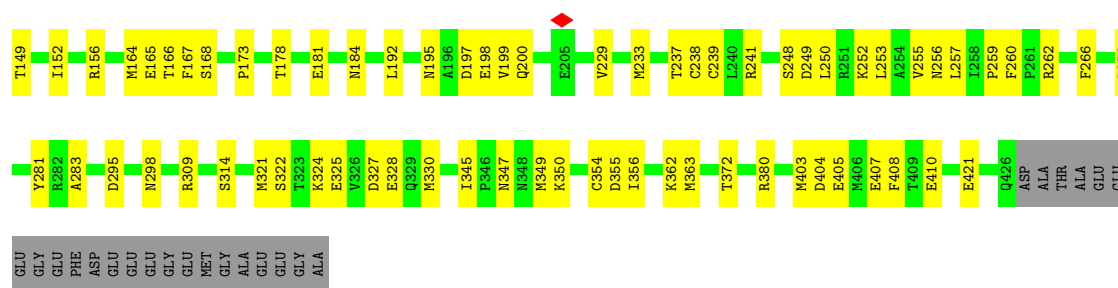


- Molecule 3: Tubulin beta chain

Chain C1: 72% 23% 5%

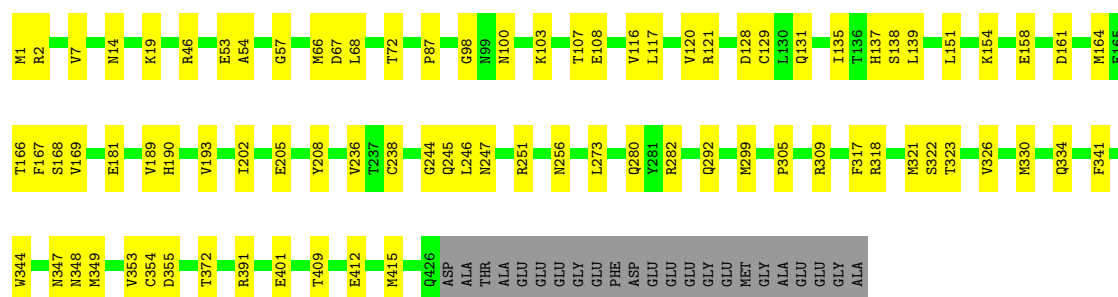






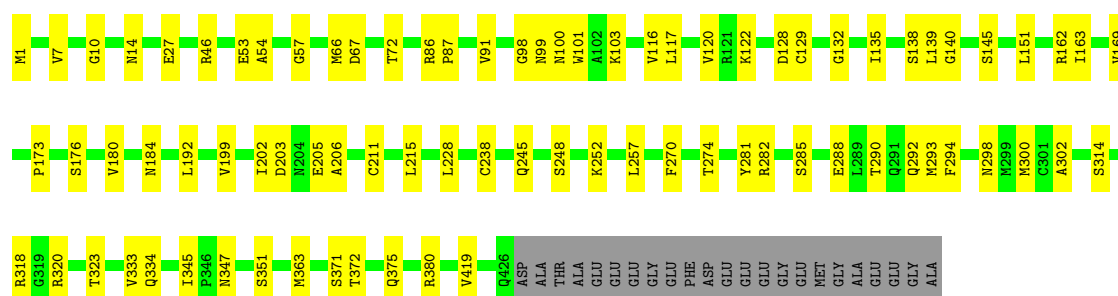
- Molecule 3: Tubulin beta chain

Chain C9: 76% 18% 5%



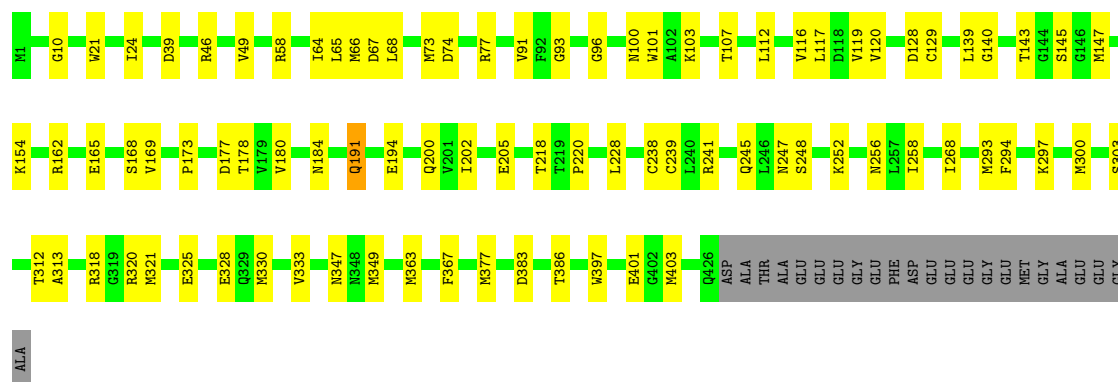
- Molecule 3: Tubulin beta chain

Chain D1: 77% 18% 5%



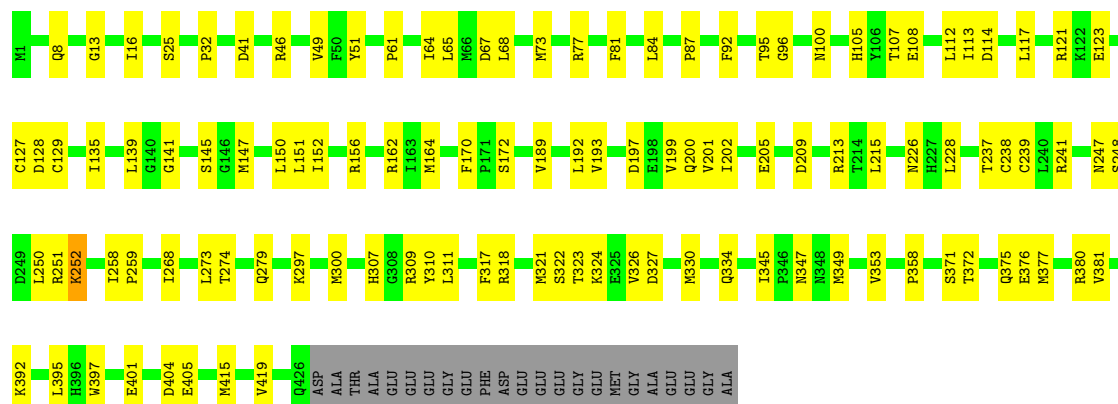
- Molecule 3: Tubulin beta chain

Chain D3: 76% 19% 5%



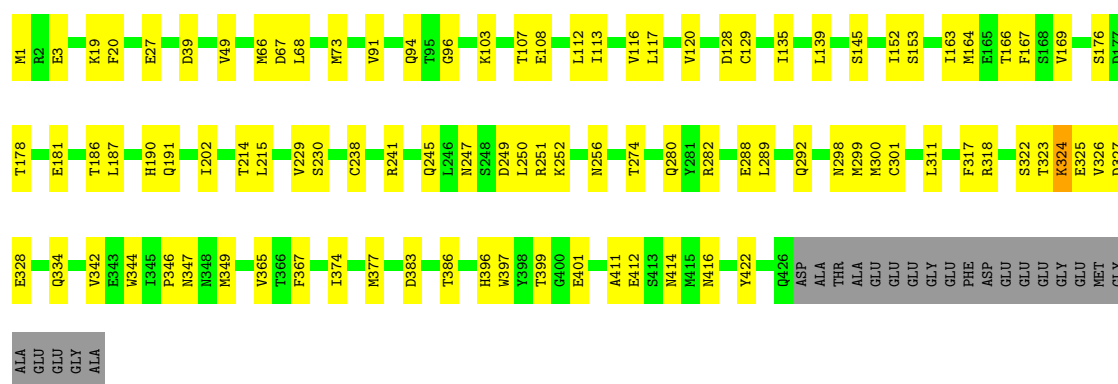
- Molecule 3: Tubulin beta chain

Chain D5:  70% 25% 5%



- Molecule 3: Tubulin beta chain

Chain D7:  73% 21% 5%



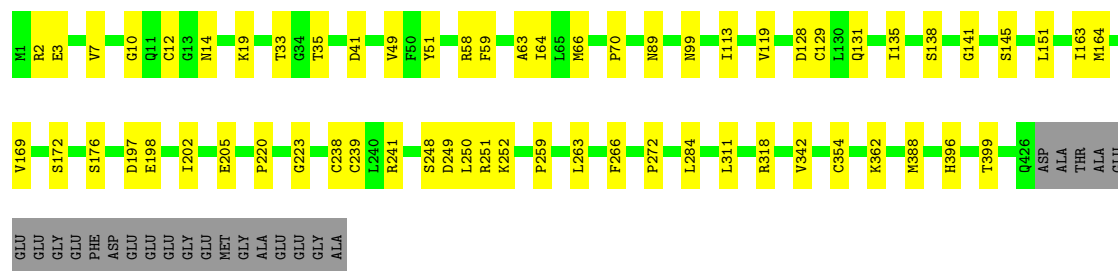
- Molecule 3: Tubulin beta chain

Chain D9:  77% 18% 5%



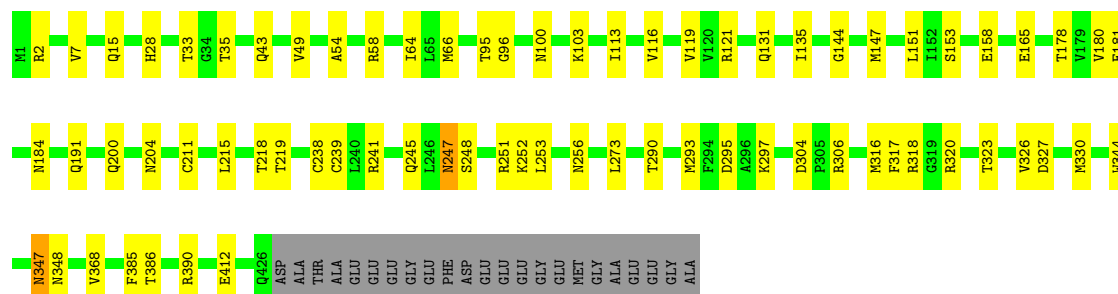
- Molecule 3: Tubulin beta chain

Chain E1:  81% 14% 5%



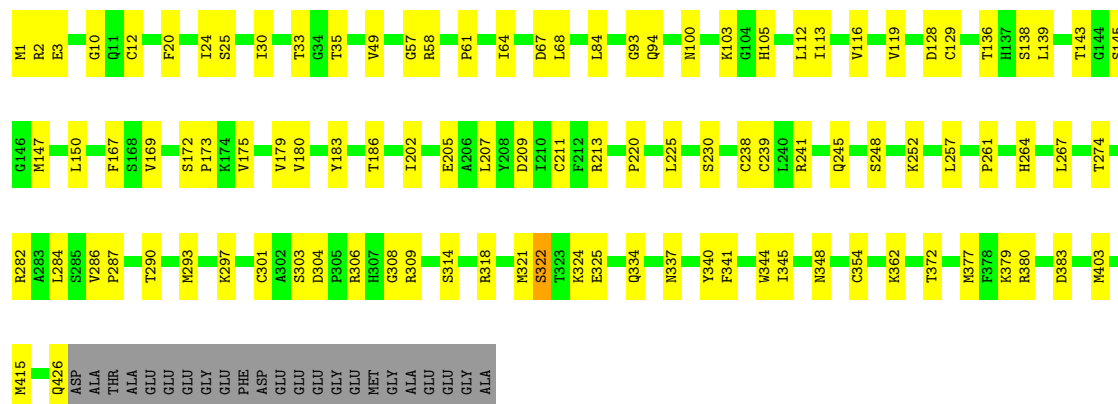
- Molecule 3: Tubulin beta chain

Chain E3: 79% 16% 5%



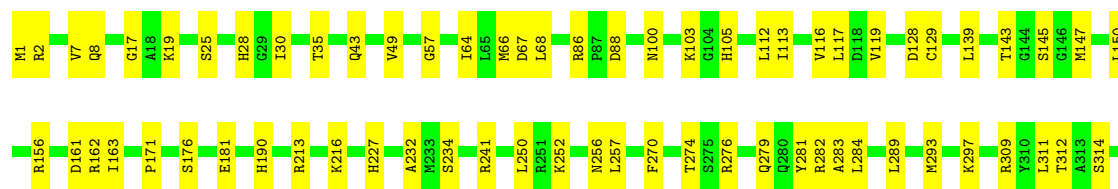
- Molecule 3: Tubulin beta chain

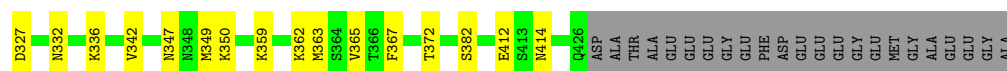
Chain E5: 72% 22% 5%



- Molecule 3: Tubulin beta chain

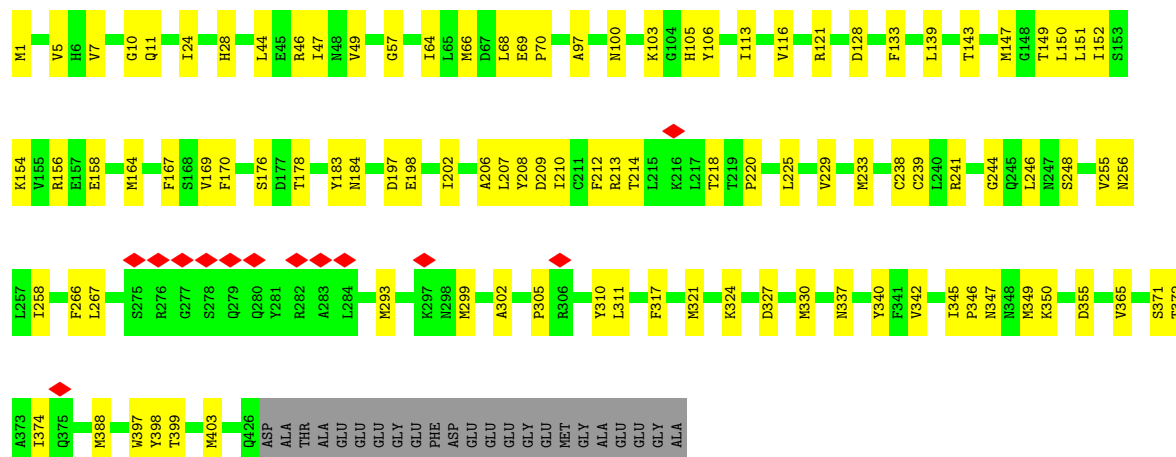
Chain E7: 76% 18% 5%





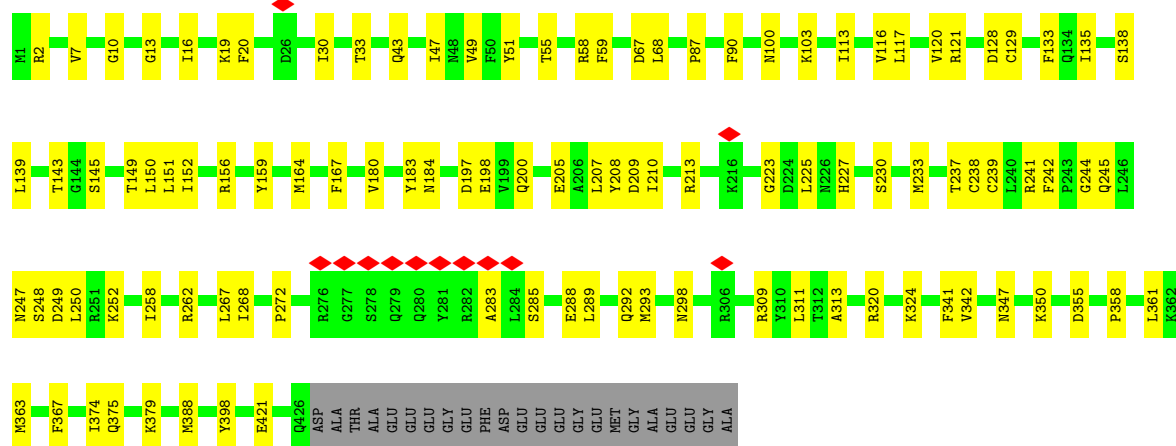
• Molecule 3: Tubulin beta chain

Chain E9: 72% 22% 5%



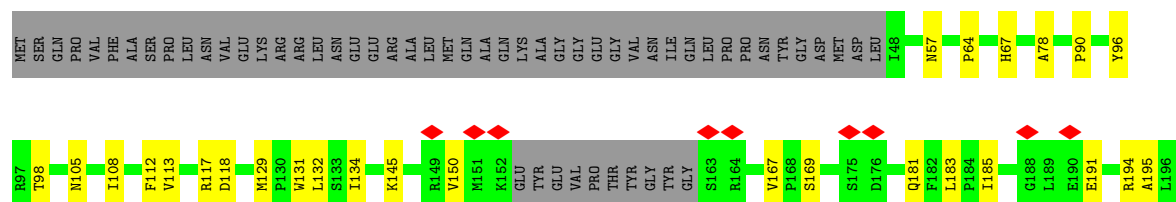
• Molecule 3: Tubulin beta chain

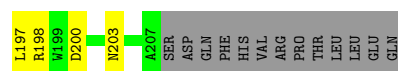
Chain F1: 72% 23% 5%



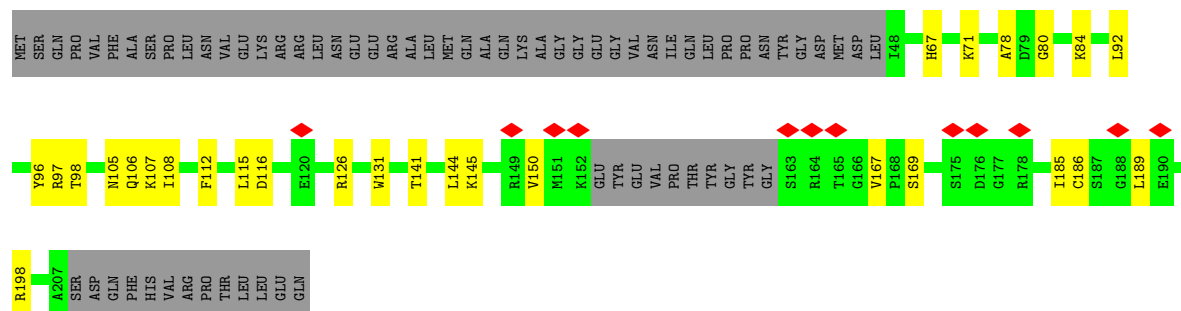
• Molecule 4: PDI family protein

Chain a: 54% 14% 32%

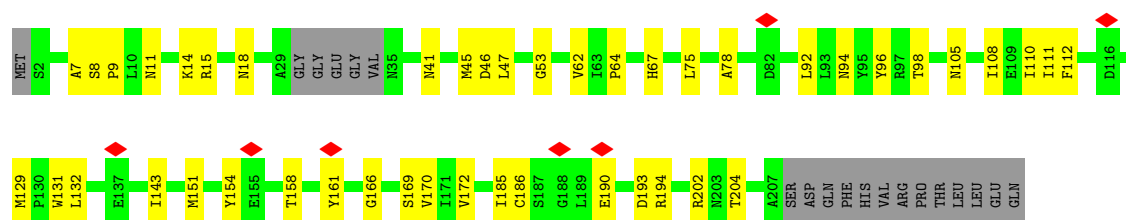




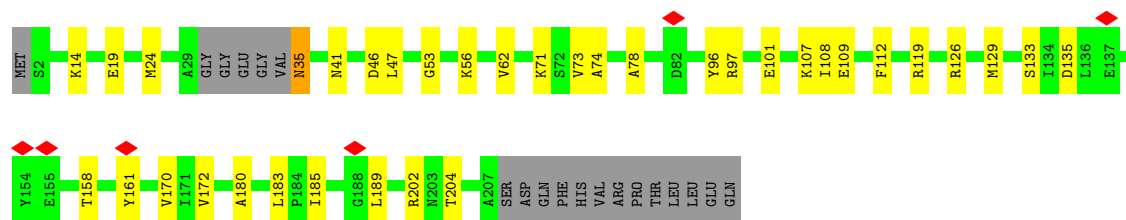
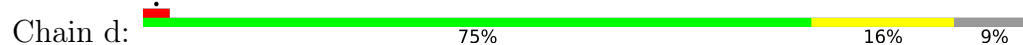
- Molecule 4: PDI family protein



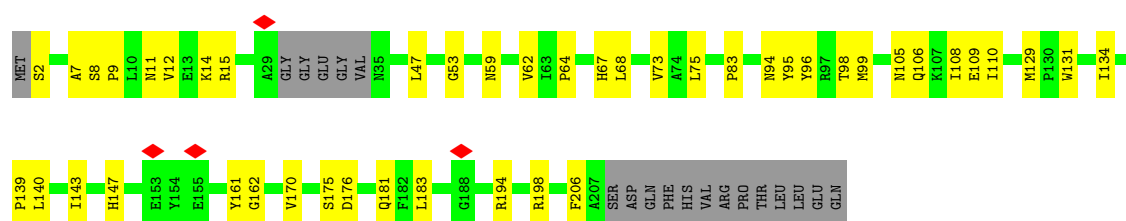
- Molecule 4: PDI family protein



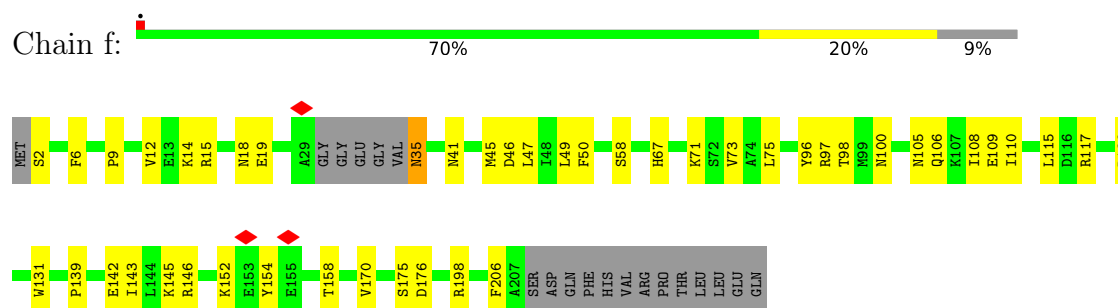
- Molecule 4: PDI family protein



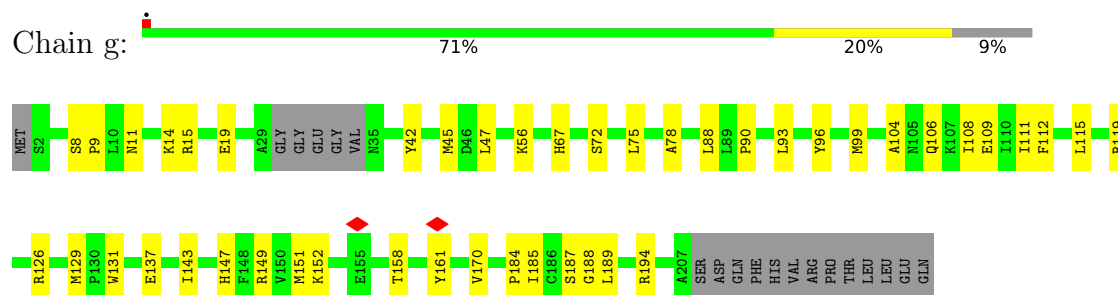
- Molecule 4: PDI family protein



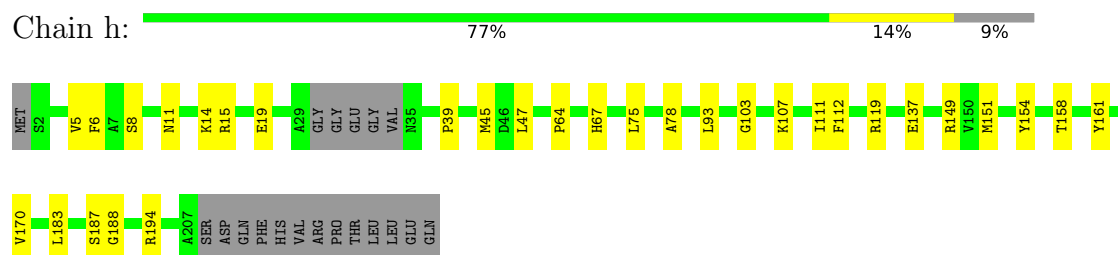
- Molecule 4: PDI family protein



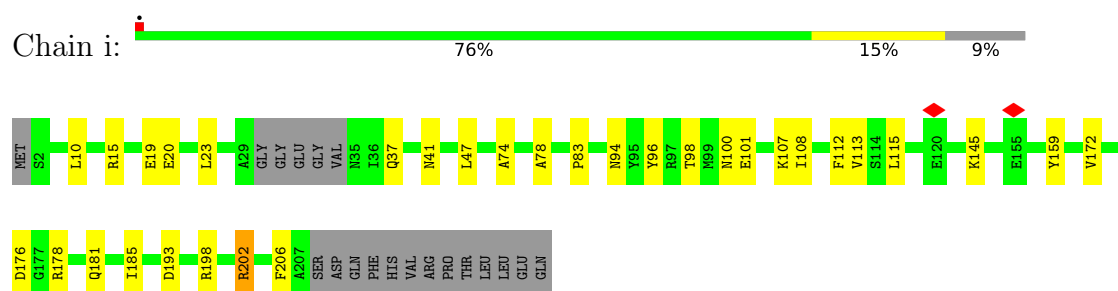
- Molecule 4: PDI family protein



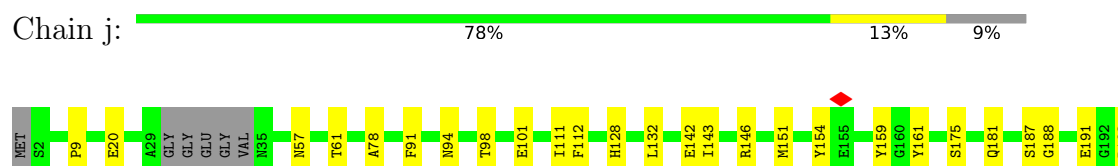
- Molecule 4: PDI family protein

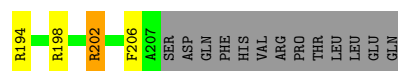


- Molecule 4: PDI family protein

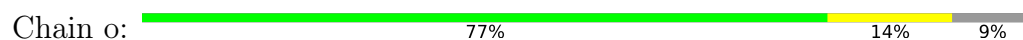


- Molecule 4: PDI family protein

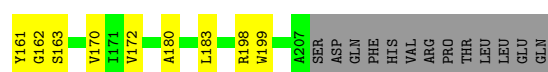
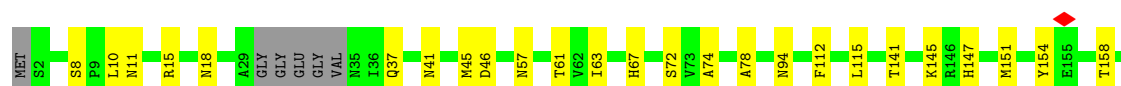
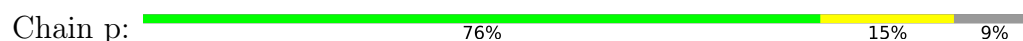




- Molecule 4: PDI family protein



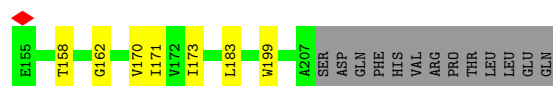
- Molecule 4: PDI family protein



- Molecule 4: PDI family protein

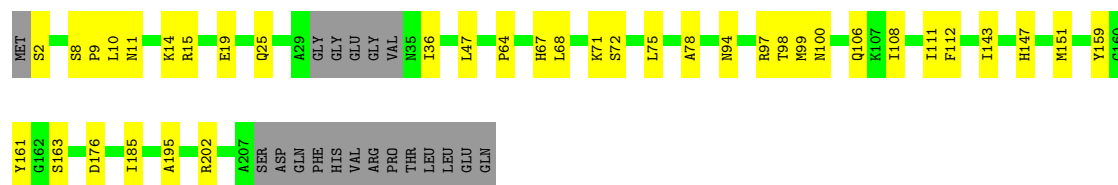


- Molecule 4: PDI family protein



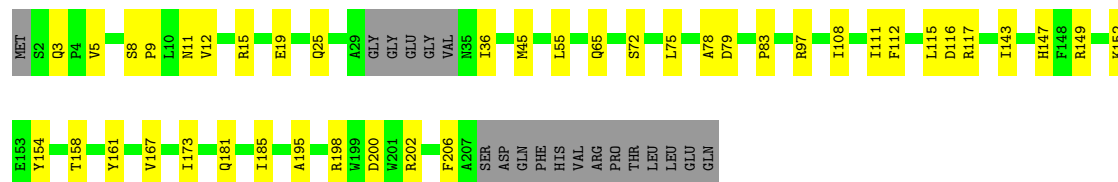
- Molecule 4: PDI family protein





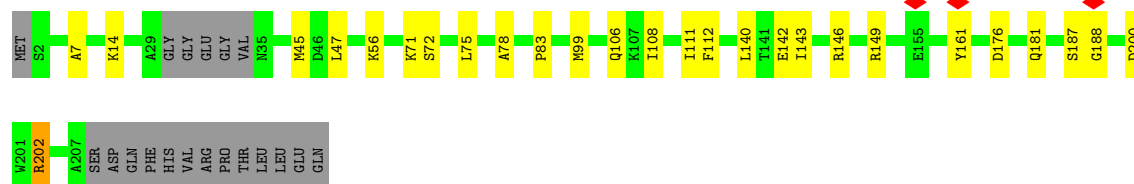
- Molecule 4: PDI family protein

Chain t: 73% 19% 9%



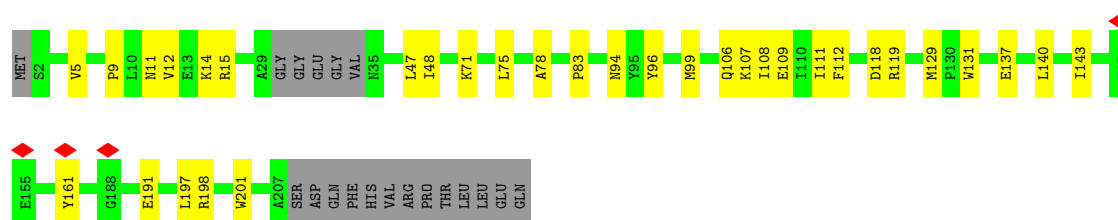
- Molecule 4: PDI family protein

Chain u: 79% 12% 9%



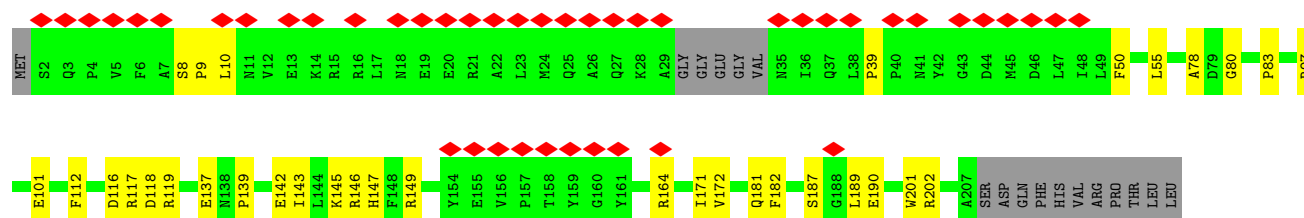
- Molecule 4: PDI family protein

Chain v: 76% 15% 9%



- Molecule 4: PDI family protein

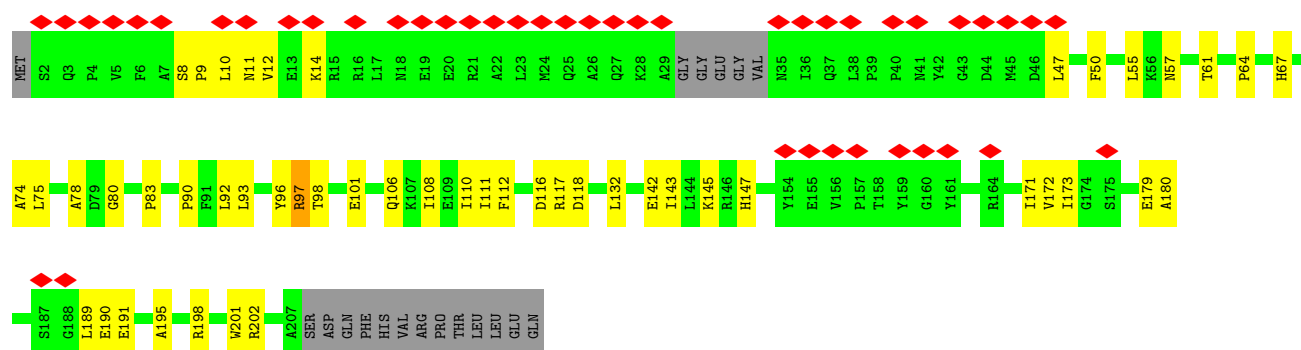
Chain n: 20% 76% 15% 9%



GLU
GLN

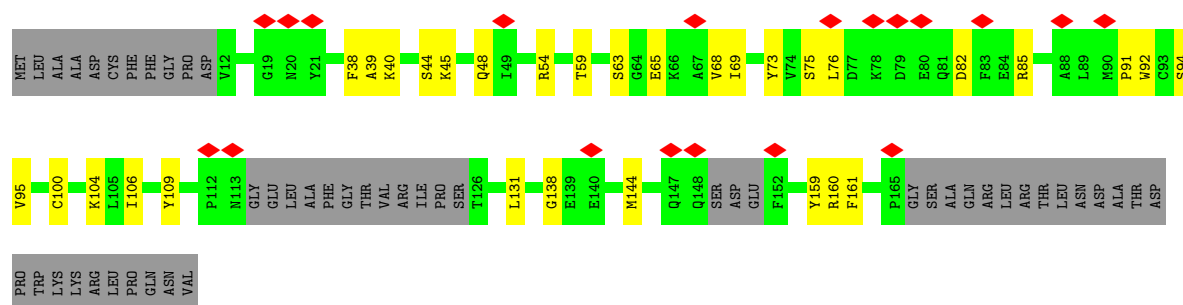
- Molecule 4: PDI family protein

Chain m: 



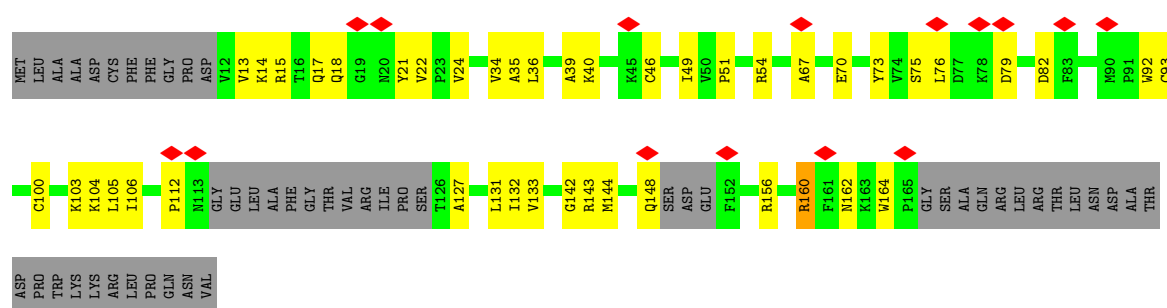
- Molecule 5: PDI family protein

Chain k: 



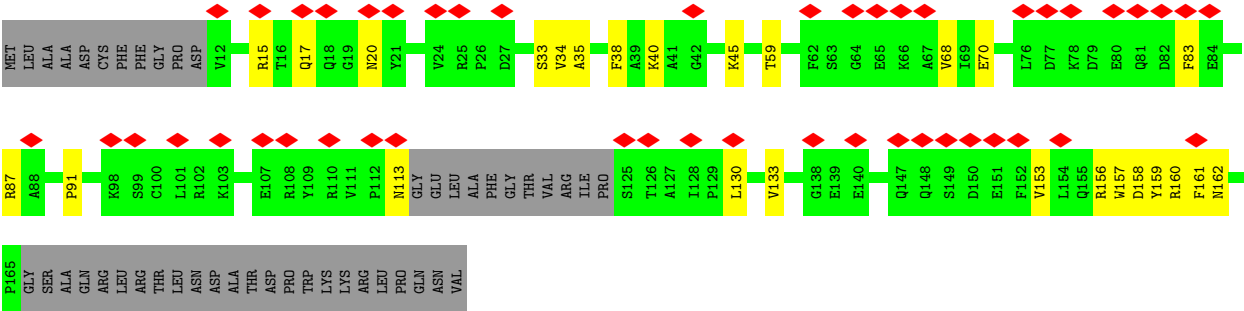
- Molecule 5: PDI family protein

Chain l: 

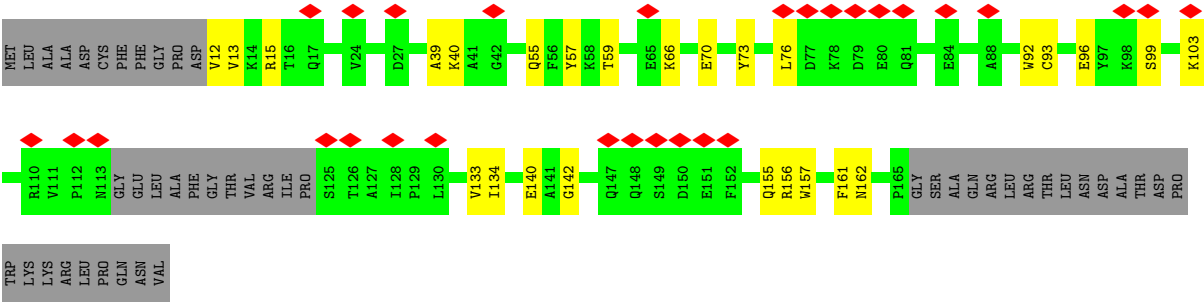


- Molecule 5: PDI family protein

Chain w: 



• Molecule 5: PDI family protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	220139	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF amplitude correction was performed as part of the 3D reconstruction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	63.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.228	Depositor
Minimum map value	0.000	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	438.4, 438.4, 438.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.096, 1.096, 1.096	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.32	0/181	0.42	0/248
1	1	0.28	0/181	0.44	0/248
1	10	0.36	0/181	0.54	0/248
1	11	0.38	0/181	0.49	0/248
1	12	0.32	0/181	0.45	0/248
1	13	0.34	0/181	0.44	0/248
1	14	0.30	0/181	0.36	0/248
1	15	0.37	0/181	0.37	0/248
1	16	0.24	0/181	0.35	0/248
1	17	0.32	0/181	0.40	0/248
1	18	0.27	0/181	0.40	0/248
1	19	0.40	0/181	0.48	0/248
1	2	0.40	0/181	0.54	0/248
1	20	0.27	0/181	0.61	0/248
1	21	0.26	0/181	0.49	0/248
1	22	0.27	0/166	0.43	0/227
1	23	0.29	0/166	0.42	0/227
1	3	0.40	0/181	0.49	0/248
1	4	0.33	0/181	0.45	0/248
1	5	0.35	0/181	0.45	0/248
1	6	0.33	0/181	0.41	0/248
1	7	0.32	0/181	0.42	0/248
1	8	0.37	0/181	0.66	0/248
1	9	0.32	0/181	0.58	0/248
2	A0	0.35	0/3398	0.57	2/4606 (0.0%)
2	A2	0.31	0/3398	0.56	2/4606 (0.0%)
2	A4	0.45	0/3398	0.61	1/4606 (0.0%)
2	A6	0.40	0/3398	0.60	0/4606
2	A8	0.43	0/3398	0.58	0/4606
2	B0	0.42	0/3398	0.59	3/4606 (0.1%)
2	B2	0.46	0/3398	0.60	2/4606 (0.0%)
2	B4	0.45	0/3398	0.59	1/4606 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	B6	0.46	0/3398	0.59	0/4606
2	B8	0.47	0/3398	0.61	1/4606 (0.0%)
2	C0	0.38	0/3398	0.58	0/4606
2	C2	0.38	0/3398	0.63	0/4606
2	C4	0.37	0/3398	0.66	0/4606
2	C6	0.38	0/3398	0.76	2/4606 (0.0%)
2	C8	0.37	0/3398	0.58	1/4606 (0.0%)
2	D0	0.43	0/3398	0.58	0/4606
2	D2	0.36	0/3398	0.56	0/4606
2	D4	0.43	0/3398	0.56	0/4606
2	D6	0.34	0/3398	0.53	0/4606
2	D8	0.44	0/3398	0.56	1/4606 (0.0%)
2	E0	0.29	0/3398	0.50	0/4606
2	E2	0.37	0/3398	0.56	1/4606 (0.0%)
2	E4	0.31	0/3398	0.58	2/4606 (0.0%)
2	E6	0.38	0/3398	0.54	0/4606
2	E8	0.31	0/3398	0.55	0/4606
2	F0	0.38	0/3398	0.59	0/4606
3	A1	0.40	0/3404	0.64	1/4606 (0.0%)
3	A3	0.32	0/3404	0.59	0/4606
3	A5	0.43	0/3404	0.63	0/4606
3	A7	0.37	0/3404	0.59	0/4606
3	A9	0.45	0/3404	0.66	2/4606 (0.0%)
3	B1	0.39	0/3404	0.60	0/4606
3	B3	0.47	0/3404	0.63	3/4606 (0.1%)
3	B5	0.42	0/3404	0.58	0/4606
3	B7	0.47	0/3404	0.62	0/4606
3	B9	0.43	0/3404	0.62	0/4606
3	C1	0.41	0/3404	0.64	0/4606
3	C3	0.39	0/3404	0.64	0/4606
3	C5	0.38	0/3404	0.65	0/4606
3	C7	0.38	0/3404	0.65	0/4606
3	C9	0.46	0/3404	0.61	0/4606
3	D1	0.43	0/3404	0.58	0/4606
3	D3	0.43	0/3404	0.61	0/4606
3	D5	0.43	0/3404	0.61	1/4606 (0.0%)
3	D7	0.44	0/3404	0.63	1/4606 (0.0%)
3	D9	0.44	0/3404	0.60	0/4606
3	E1	0.34	0/3404	0.53	0/4606
3	E3	0.39	0/3404	0.59	3/4606 (0.1%)
3	E5	0.33	0/3404	0.59	0/4606
3	E7	0.39	0/3404	0.57	0/4606
3	E9	0.34	0/3404	0.61	0/4606

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	F1	0.38	0/3404	0.64	0/4606
4	a	0.39	0/1225	0.61	0/1654
4	b	0.31	0/1225	0.54	0/1654
4	c	0.44	0/1645	0.63	0/2225
4	d	0.38	0/1645	0.62	0/2225
4	e	0.44	0/1645	0.63	2/2225 (0.1%)
4	f	0.41	0/1645	0.57	0/2225
4	g	0.43	0/1645	0.59	0/2225
4	h	0.42	0/1645	0.57	0/2225
4	i	0.41	0/1645	0.64	1/2225 (0.0%)
4	j	0.41	0/1645	0.63	1/2225 (0.0%)
4	m	0.35	0/1645	0.59	1/2225 (0.0%)
4	n	0.35	0/1645	0.60	0/2225
4	o	0.41	0/1645	0.60	0/2225
4	p	0.41	0/1645	0.57	0/2225
4	q	0.38	0/1645	0.57	0/2225
4	r	0.43	0/1645	0.57	0/2225
4	s	0.35	0/1645	0.59	0/2225
4	t	0.41	0/1645	0.59	0/2225
4	u	0.28	0/1645	0.55	1/2225 (0.0%)
4	v	0.38	0/1645	0.65	0/2225
5	k	0.26	0/1168	0.59	0/1578
5	l	0.29	0/1168	0.71	1/1578 (0.1%)
5	w	0.25	0/1201	0.56	0/1623
5	x	0.27	0/1201	0.52	0/1623
All	All	0.39	0/217964	0.60	37/295182 (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	A2	0	1
2	A4	0	2
2	A8	0	1
2	B4	0	1
2	B6	0	1
2	C8	0	1
2	D2	0	1
3	A1	0	1
3	B3	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B9	0	1
3	E5	0	2
5	1	0	1
All	All	0	14

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C6	30	ILE	CA-C-N	19.77	148.56	120.49
2	C6	30	ILE	C-N-CA	19.77	148.56	120.49
3	B3	303	SER	CA-C-N	6.72	130.61	121.20
3	B3	303	SER	C-N-CA	6.72	130.61	121.20
3	A9	252	LYS	CA-CB-CG	6.19	126.48	114.10

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A1	191	GLN	Peptide
2	A2	401	LYS	Peptide
2	A4	254	GLU	Peptide
2	A4	401	LYS	Peptide
2	A8	401	LYS	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	3	0
1	1	174	0	171	5	0
1	10	174	0	171	3	0
1	11	174	0	171	3	0
1	12	174	0	171	4	0
1	13	174	0	171	2	0
1	14	174	0	171	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	15	174	0	171	2	0
1	16	174	0	171	2	0
1	17	174	0	171	2	0
1	18	174	0	171	1	0
1	19	174	0	171	2	0
1	2	174	0	171	2	0
1	20	174	0	171	2	0
1	21	174	0	171	3	0
1	22	160	0	156	3	0
1	23	160	0	156	3	0
1	3	174	0	171	2	0
1	4	174	0	171	3	0
1	5	174	0	171	3	0
1	6	174	0	171	1	0
1	7	174	0	171	3	0
1	8	174	0	171	1	0
1	9	174	0	171	2	0
2	A0	3325	0	3251	59	0
2	A2	3325	0	3252	61	0
2	A4	3325	0	3252	50	0
2	A6	3325	0	3252	60	0
2	A8	3325	0	3252	59	0
2	B0	3325	0	3252	50	0
2	B2	3325	0	3252	49	0
2	B4	3325	0	3252	69	0
2	B6	3325	0	3252	54	0
2	B8	3325	0	3252	68	0
2	C0	3325	0	3252	78	0
2	C2	3325	0	3252	77	0
2	C4	3325	0	3252	85	0
2	C6	3325	0	3252	75	0
2	C8	3325	0	3252	48	0
2	D0	3325	0	3252	44	0
2	D2	3325	0	3252	46	0
2	D4	3325	0	3252	47	0
2	D6	3325	0	3252	48	0
2	D8	3325	0	3252	46	0
2	E0	3325	0	3252	37	0
2	E2	3325	0	3252	53	0
2	E4	3325	0	3252	59	0
2	E6	3325	0	3252	57	0
2	E8	3325	0	3252	76	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F0	3325	0	3252	70	0
3	A1	3331	0	3207	59	0
3	A3	3331	0	3209	58	0
3	A5	3331	0	3207	58	0
3	A7	3331	0	3207	48	0
3	A9	3331	0	3207	62	0
3	B1	3331	0	3209	52	0
3	B3	3331	0	3207	51	0
3	B5	3331	0	3207	53	0
3	B7	3331	0	3209	52	0
3	B9	3331	0	3209	45	0
3	C1	3331	0	3209	78	0
3	C3	3331	0	3209	77	0
3	C5	3331	0	3209	67	0
3	C7	3331	0	3209	67	0
3	C9	3331	0	3209	62	0
3	D1	3331	0	3209	56	0
3	D3	3331	0	3207	64	0
3	D5	3331	0	3207	72	0
3	D7	3331	0	3207	70	0
3	D9	3331	0	3207	54	0
3	E1	3331	0	3207	42	0
3	E3	3331	0	3209	50	0
3	E5	3331	0	3207	66	0
3	E7	3331	0	3207	56	0
3	E9	3331	0	3207	75	0
3	F1	3331	0	3207	74	0
4	a	1198	0	1194	20	0
4	b	1198	0	1194	21	0
4	c	1608	0	1590	30	0
4	d	1608	0	1590	30	0
4	e	1608	0	1590	31	0
4	f	1608	0	1590	38	0
4	g	1608	0	1590	29	0
4	h	1608	0	1590	28	0
4	i	1608	0	1590	23	0
4	j	1608	0	1590	23	0
4	m	1608	0	1590	33	0
4	n	1608	0	1590	27	0
4	o	1608	0	1590	22	0
4	p	1608	0	1590	28	0
4	q	1608	0	1590	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	r	1608	0	1590	23	0
4	s	1608	0	1590	26	0
4	t	1608	0	1590	29	0
4	u	1608	0	1590	19	0
4	v	1608	0	1590	24	0
5	k	1140	0	1143	22	0
5	l	1140	0	1143	28	0
5	w	1172	0	1171	16	0
5	x	1172	0	1171	19	0
6	A0	32	0	12	2	0
6	A2	32	0	12	0	0
6	A4	32	0	12	0	0
6	A6	32	0	12	0	0
6	A8	32	0	12	1	0
6	B0	32	0	12	1	0
6	B2	32	0	12	1	0
6	B4	32	0	12	0	0
6	B6	32	0	12	2	0
6	B8	32	0	12	1	0
6	C0	32	0	12	2	0
6	C2	32	0	12	1	0
6	C4	32	0	12	1	0
6	C6	32	0	12	3	0
6	C8	32	0	12	1	0
6	D0	32	0	12	0	0
6	D2	32	0	12	0	0
6	D4	32	0	12	1	0
6	D6	32	0	12	0	0
6	D8	32	0	12	1	0
6	E0	32	0	12	0	0
6	E2	32	0	12	1	0
6	E4	32	0	12	0	0
6	E6	32	0	12	3	0
6	E8	32	0	12	2	0
6	F0	32	0	12	1	0
7	A0	1	0	0	0	0
7	A2	1	0	0	0	0
7	A4	1	0	0	0	0
7	A6	1	0	0	0	0
7	A8	1	0	0	0	0
7	B0	1	0	0	0	0
7	B2	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B4	1	0	0	0	0
7	B6	1	0	0	0	0
7	B8	1	0	0	0	0
7	C0	1	0	0	0	0
7	C2	1	0	0	0	0
7	C4	1	0	0	0	0
7	C6	1	0	0	0	0
7	C8	1	0	0	0	0
7	D0	1	0	0	0	0
7	D2	1	0	0	0	0
7	D4	1	0	0	0	0
7	D6	1	0	0	0	0
7	D8	1	0	0	0	0
7	E0	1	0	0	0	0
7	E2	1	0	0	0	0
7	E4	1	0	0	0	0
7	E6	1	0	0	0	0
7	E8	1	0	0	0	0
7	F0	1	0	0	0	0
8	A1	28	0	12	2	0
8	A3	28	0	12	2	0
8	A5	28	0	12	0	0
8	A7	28	0	12	0	0
8	A9	28	0	12	1	0
8	B1	28	0	12	0	0
8	B3	28	0	12	1	0
8	B5	28	0	12	0	0
8	B7	28	0	12	1	0
8	B9	28	0	12	0	0
8	C1	28	0	12	1	0
8	C3	28	0	12	2	0
8	C5	28	0	12	1	0
8	C7	28	0	12	0	0
8	C9	28	0	12	0	0
8	D1	28	0	12	0	0
8	D3	28	0	12	0	0
8	D5	28	0	12	1	0
8	D7	28	0	12	0	0
8	D9	28	0	12	0	0
8	E1	28	0	12	0	0
8	E3	28	0	12	3	0
8	E5	28	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E7	28	0	12	0	0
8	E9	28	0	12	0	0
8	F1	28	0	12	1	0
All	All	214754	0	208289	3323	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 3323 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)
2:C4:282:TYR:HD2	4:m:202:ARG:HD2	1.30	0.93
2:D4:151:CYS:HG	2:D4:193:SER:HG	1.23	0.83
3:A9:248:SER:HA	3:A9:252:LYS:HG2	1.67	0.77
2:C4:398:MET:HE1	3:C5:345:ILE:HG23	1.67	0.77
2:E2:88:HIS:HB3	2:E2:91:GLN:HG2	1.65	0.77

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%)	19 (95%)	1 (5%)	0	100	100
1	1	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	10	20/351 (6%)	16 (80%)	4 (20%)	0	100	100
1	11	20/351 (6%)	17 (85%)	3 (15%)	0	100	100
1	12	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	13	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	14	20/351 (6%)	19 (95%)	1 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	15	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	16	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	17	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	18	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	19	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	2	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	20	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	21	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	22	18/351 (5%)	16 (89%)	2 (11%)	0	100	100
1	23	18/351 (5%)	16 (89%)	2 (11%)	0	100	100
1	3	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	4	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	5	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	6	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	7	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
1	8	20/351 (6%)	18 (90%)	2 (10%)	0	100	100
1	9	20/351 (6%)	19 (95%)	1 (5%)	0	100	100
2	A0	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
2	A2	424/453 (94%)	397 (94%)	27 (6%)	0	100	100
2	A4	424/453 (94%)	398 (94%)	26 (6%)	0	100	100
2	A6	424/453 (94%)	397 (94%)	27 (6%)	0	100	100
2	A8	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
2	B0	424/453 (94%)	406 (96%)	18 (4%)	0	100	100
2	B2	424/453 (94%)	405 (96%)	19 (4%)	0	100	100
2	B4	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
2	B6	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
2	B8	424/453 (94%)	401 (95%)	23 (5%)	0	100	100
2	C0	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
2	C2	424/453 (94%)	400 (94%)	24 (6%)	0	100	100
2	C4	424/453 (94%)	385 (91%)	39 (9%)	0	100	100
2	C6	424/453 (94%)	396 (93%)	28 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C8	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
2	D0	424/453 (94%)	402 (95%)	22 (5%)	0	100	100
2	D2	424/453 (94%)	409 (96%)	15 (4%)	0	100	100
2	D4	424/453 (94%)	407 (96%)	17 (4%)	0	100	100
2	D6	424/453 (94%)	410 (97%)	14 (3%)	0	100	100
2	D8	424/453 (94%)	408 (96%)	16 (4%)	0	100	100
2	E0	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
2	E2	424/453 (94%)	404 (95%)	20 (5%)	0	100	100
2	E4	424/453 (94%)	401 (95%)	23 (5%)	0	100	100
2	E6	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
2	E8	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
2	F0	424/453 (94%)	403 (95%)	21 (5%)	0	100	100
3	A1	424/449 (94%)	391 (92%)	33 (8%)	0	100	100
3	A3	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
3	A5	424/449 (94%)	388 (92%)	36 (8%)	0	100	100
3	A7	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	A9	424/449 (94%)	398 (94%)	26 (6%)	0	100	100
3	B1	424/449 (94%)	400 (94%)	24 (6%)	0	100	100
3	B3	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	B5	424/449 (94%)	400 (94%)	24 (6%)	0	100	100
3	B7	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	B9	424/449 (94%)	405 (96%)	19 (4%)	0	100	100
3	C1	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	C3	424/449 (94%)	396 (93%)	28 (7%)	0	100	100
3	C5	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	C7	424/449 (94%)	394 (93%)	30 (7%)	0	100	100
3	C9	424/449 (94%)	398 (94%)	26 (6%)	0	100	100
3	D1	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	D3	424/449 (94%)	395 (93%)	29 (7%)	0	100	100
3	D5	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
3	D7	424/449 (94%)	401 (95%)	23 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D9	424/449 (94%)	401 (95%)	23 (5%)	0	100	100
3	E1	424/449 (94%)	403 (95%)	21 (5%)	0	100	100
3	E3	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
3	E5	424/449 (94%)	399 (94%)	25 (6%)	0	100	100
3	E7	424/449 (94%)	402 (95%)	22 (5%)	0	100	100
3	E9	424/449 (94%)	395 (93%)	29 (7%)	0	100	100
3	F1	424/449 (94%)	388 (92%)	36 (8%)	0	100	100
4	a	146/220 (66%)	136 (93%)	10 (7%)	0	100	100
4	b	146/220 (66%)	135 (92%)	11 (8%)	0	100	100
4	c	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
4	d	197/220 (90%)	183 (93%)	14 (7%)	0	100	100
4	e	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
4	f	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
4	g	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	h	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
4	i	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
4	j	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	m	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	n	197/220 (90%)	187 (95%)	10 (5%)	0	100	100
4	o	197/220 (90%)	181 (92%)	16 (8%)	0	100	100
4	p	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
4	q	197/220 (90%)	185 (94%)	12 (6%)	0	100	100
4	r	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
4	s	197/220 (90%)	184 (93%)	13 (7%)	0	100	100
4	t	197/220 (90%)	186 (94%)	11 (6%)	0	100	100
4	u	197/220 (90%)	188 (95%)	9 (5%)	0	100	100
4	v	197/220 (90%)	181 (92%)	16 (8%)	0	100	100
5	k	133/189 (70%)	128 (96%)	5 (4%)	0	100	100
5	l	133/189 (70%)	128 (96%)	5 (4%)	0	100	100
5	w	139/189 (74%)	134 (96%)	5 (4%)	0	100	100
5	x	139/189 (74%)	129 (93%)	10 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	26906/37032 (73%)	25394 (94%)	1512 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	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
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	20	20/305 (7%)	20 (100%)	0	100	100
1	21	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%)	20 (100%)	0	100	100
1	6	20/305 (7%)	20 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	A0	359/379 (95%)	359 (100%)	0	100	100
2	A2	359/379 (95%)	359 (100%)	0	100	100
2	A4	359/379 (95%)	358 (100%)	1 (0%)	86	84
2	A6	359/379 (95%)	359 (100%)	0	100	100
2	A8	359/379 (95%)	359 (100%)	0	100	100
2	B0	359/379 (95%)	359 (100%)	0	100	100
2	B2	359/379 (95%)	359 (100%)	0	100	100
2	B4	359/379 (95%)	359 (100%)	0	100	100
2	B6	359/379 (95%)	359 (100%)	0	100	100
2	B8	359/379 (95%)	359 (100%)	0	100	100
2	C0	359/379 (95%)	359 (100%)	0	100	100
2	C2	359/379 (95%)	359 (100%)	0	100	100
2	C4	359/379 (95%)	359 (100%)	0	100	100
2	C6	359/379 (95%)	359 (100%)	0	100	100
2	C8	359/379 (95%)	359 (100%)	0	100	100
2	D0	359/379 (95%)	359 (100%)	0	100	100
2	D2	359/379 (95%)	359 (100%)	0	100	100
2	D4	359/379 (95%)	359 (100%)	0	100	100
2	D6	359/379 (95%)	359 (100%)	0	100	100
2	D8	359/379 (95%)	359 (100%)	0	100	100
2	E0	359/379 (95%)	359 (100%)	0	100	100
2	E2	359/379 (95%)	359 (100%)	0	100	100
2	E4	359/379 (95%)	358 (100%)	1 (0%)	86	84
2	E6	359/379 (95%)	359 (100%)	0	100	100
2	E8	359/379 (95%)	359 (100%)	0	100	100
2	F0	359/379 (95%)	359 (100%)	0	100	100
3	A1	364/381 (96%)	364 (100%)	0	100	100
3	A3	364/381 (96%)	363 (100%)	1 (0%)	86	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A5	364/381 (96%)	364 (100%)	0	100	100
3	A7	364/381 (96%)	363 (100%)	1 (0%)	86	84
3	A9	364/381 (96%)	364 (100%)	0	100	100
3	B1	364/381 (96%)	364 (100%)	0	100	100
3	B3	364/381 (96%)	363 (100%)	1 (0%)	86	84
3	B5	364/381 (96%)	363 (100%)	1 (0%)	86	84
3	B7	364/381 (96%)	363 (100%)	1 (0%)	86	84
3	B9	364/381 (96%)	364 (100%)	0	100	100
3	C1	364/381 (96%)	364 (100%)	0	100	100
3	C3	364/381 (96%)	364 (100%)	0	100	100
3	C5	364/381 (96%)	364 (100%)	0	100	100
3	C7	364/381 (96%)	364 (100%)	0	100	100
3	C9	364/381 (96%)	364 (100%)	0	100	100
3	D1	364/381 (96%)	363 (100%)	1 (0%)	86	84
3	D3	364/381 (96%)	363 (100%)	1 (0%)	86	84
3	D5	364/381 (96%)	364 (100%)	0	100	100
3	D7	364/381 (96%)	364 (100%)	0	100	100
3	D9	364/381 (96%)	364 (100%)	0	100	100
3	E1	364/381 (96%)	364 (100%)	0	100	100
3	E3	364/381 (96%)	363 (100%)	1 (0%)	86	84
3	E5	364/381 (96%)	364 (100%)	0	100	100
3	E7	364/381 (96%)	364 (100%)	0	100	100
3	E9	364/381 (96%)	364 (100%)	0	100	100
3	F1	364/381 (96%)	364 (100%)	0	100	100
4	a	130/190 (68%)	130 (100%)	0	100	100
4	b	130/190 (68%)	130 (100%)	0	100	100
4	c	174/190 (92%)	174 (100%)	0	100	100
4	d	174/190 (92%)	173 (99%)	1 (1%)	78	80
4	e	174/190 (92%)	174 (100%)	0	100	100
4	f	174/190 (92%)	173 (99%)	1 (1%)	78	80
4	g	174/190 (92%)	174 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	h	174/190 (92%)	174 (100%)	0	100	100
4	i	174/190 (92%)	174 (100%)	0	100	100
4	j	174/190 (92%)	174 (100%)	0	100	100
4	m	174/190 (92%)	174 (100%)	0	100	100
4	n	174/190 (92%)	174 (100%)	0	100	100
4	o	174/190 (92%)	174 (100%)	0	100	100
4	p	174/190 (92%)	174 (100%)	0	100	100
4	q	174/190 (92%)	174 (100%)	0	100	100
4	r	174/190 (92%)	174 (100%)	0	100	100
4	s	174/190 (92%)	174 (100%)	0	100	100
4	t	174/190 (92%)	174 (100%)	0	100	100
4	u	174/190 (92%)	174 (100%)	0	100	100
4	v	174/190 (92%)	174 (100%)	0	100	100
5	k	122/164 (74%)	122 (100%)	0	100	100
5	l	122/164 (74%)	122 (100%)	0	100	100
5	w	127/164 (77%)	127 (100%)	0	100	100
5	x	127/164 (77%)	126 (99%)	1 (1%)	73	77
All	All	23164/31536 (74%)	23151 (100%)	13 (0%)	87	89

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D3	191	GLN
3	E3	247	ASN
5	x	162	ASN
4	d	35	ASN
4	f	35	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 234 such sidechains are listed below:

Mol	Chain	Res	Type
3	D1	396	HIS
4	t	37	GLN
3	D9	8	GLN
4	s	37	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	e	106	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
6	GTP	E8	501	7	33,34,34	0.91	2 (6%)	50,54,54	1.64	8 (16%)
8	GDP	E7	501	-	29,30,30	1.21	4 (13%)	45,47,47	1.80	8 (17%)
6	GTP	C8	501	7	33,34,34	0.96	2 (6%)	50,54,54	1.58	8 (16%)
8	GDP	E5	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.82	9 (20%)
8	GDP	D5	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.76	7 (15%)
6	GTP	B4	501	7	33,34,34	1.03	3 (9%)	50,54,54	1.65	8 (16%)
6	GTP	D4	501	7	33,34,34	0.98	2 (6%)	50,54,54	1.63	8 (16%)
6	GTP	A2	501	7	33,34,34	0.92	1 (3%)	50,54,54	1.56	8 (16%)
6	GTP	C6	501	7	33,34,34	0.95	1 (3%)	50,54,54	1.63	9 (18%)
8	GDP	C7	501	-	29,30,30	1.21	4 (13%)	45,47,47	1.79	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GTP	C2	501	7	33,34,34	0.95	1 (3%)	50,54,54	1.58	8 (16%)
8	GDP	A1	501	-	29,30,30	1.23	4 (13%)	45,47,47	1.84	8 (17%)
6	GTP	D0	501	7	33,34,34	0.96	2 (6%)	50,54,54	1.62	8 (16%)
8	GDP	B3	501	-	29,30,30	1.25	4 (13%)	45,47,47	1.78	6 (13%)
8	GDP	C9	501	-	29,30,30	1.19	3 (10%)	45,47,47	1.86	9 (20%)
6	GTP	D8	501	7	33,34,34	0.95	1 (3%)	50,54,54	1.56	8 (16%)
8	GDP	A5	501	-	29,30,30	1.21	4 (13%)	45,47,47	1.75	7 (15%)
8	GDP	A9	501	-	29,30,30	1.22	4 (13%)	45,47,47	1.75	8 (17%)
8	GDP	F1	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.82	8 (17%)
8	GDP	D3	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.81	7 (15%)
8	GDP	C5	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.82	8 (17%)
6	GTP	B0	501	7	33,34,34	0.92	1 (3%)	50,54,54	1.63	8 (16%)
6	GTP	C0	501	7	33,34,34	0.95	2 (6%)	50,54,54	1.61	9 (18%)
8	GDP	C3	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.77	6 (13%)
8	GDP	D9	501	-	29,30,30	1.21	4 (13%)	45,47,47	1.77	6 (13%)
6	GTP	D2	501	7	33,34,34	0.94	1 (3%)	50,54,54	1.63	8 (16%)
8	GDP	B5	501	-	29,30,30	1.24	4 (13%)	45,47,47	1.77	6 (13%)
8	GDP	E9	501	-	29,30,30	1.22	4 (13%)	45,47,47	1.74	6 (13%)
6	GTP	C4	501	7	33,34,34	0.98	2 (6%)	50,54,54	1.61	9 (18%)
6	GTP	D6	501	7	33,34,34	0.87	1 (3%)	50,54,54	1.62	8 (16%)
6	GTP	B2	501	7	33,34,34	1.01	2 (6%)	50,54,54	1.66	8 (16%)
8	GDP	A3	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.70	6 (13%)
6	GTP	A6	501	7	33,34,34	0.94	2 (6%)	50,54,54	1.60	8 (16%)
8	GDP	E1	501	-	29,30,30	1.19	4 (13%)	45,47,47	1.82	7 (15%)
6	GTP	B8	501	7	33,34,34	1.00	2 (6%)	50,54,54	1.63	8 (16%)
6	GTP	E6	501	7	33,34,34	0.94	2 (6%)	50,54,54	1.59	9 (18%)
8	GDP	B7	501	-	29,30,30	1.24	4 (13%)	45,47,47	1.70	6 (13%)
8	GDP	E3	501	-	29,30,30	1.22	4 (13%)	45,47,47	1.78	6 (13%)
8	GDP	D1	501	-	29,30,30	1.22	4 (13%)	45,47,47	1.83	8 (17%)
8	GDP	A7	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.75	6 (13%)
8	GDP	C1	501	-	29,30,30	1.25	4 (13%)	45,47,47	1.78	7 (15%)
6	GTP	A4	501	7	33,34,34	0.99	3 (9%)	50,54,54	1.56	8 (16%)
6	GTP	B6	501	7	33,34,34	1.01	2 (6%)	50,54,54	1.65	8 (16%)
6	GTP	E4	501	7	33,34,34	0.91	1 (3%)	50,54,54	1.59	9 (18%)
8	GDP	B9	501	-	29,30,30	1.22	4 (13%)	45,47,47	1.73	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GDP	B1	501	-	29,30,30	1.21	4 (13%)	45,47,47	1.74	6 (13%)
6	GTP	E2	501	7	33,34,34	0.96	2 (6%)	50,54,54	1.62	8 (16%)
6	GTP	A8	501	7	33,34,34	0.96	1 (3%)	50,54,54	1.65	8 (16%)
6	GTP	E0	501	7	33,34,34	0.91	1 (3%)	50,54,54	1.63	9 (18%)
8	GDP	D7	501	-	29,30,30	1.24	4 (13%)	45,47,47	1.75	6 (13%)
6	GTP	F0	501	7	33,34,34	0.95	2 (6%)	50,54,54	1.63	9 (18%)
6	GTP	A0	501	7	33,34,34	0.93	2 (6%)	50,54,54	1.57	9 (18%)

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
6	GTP	E8	501	7	-	6/22/38/38	0/3/3/3
8	GDP	E7	501	-	-	3/16/32/32	0/3/3/3
6	GTP	C8	501	7	-	3/22/38/38	0/3/3/3
8	GDP	E5	501	-	-	3/16/32/32	0/3/3/3
8	GDP	D5	501	-	-	6/16/32/32	0/3/3/3
6	GTP	B4	501	7	-	4/22/38/38	0/3/3/3
6	GTP	D4	501	7	-	4/22/38/38	0/3/3/3
6	GTP	A2	501	7	-	7/22/38/38	0/3/3/3
6	GTP	C6	501	7	-	4/22/38/38	0/3/3/3
8	GDP	C7	501	-	-	1/16/32/32	0/3/3/3
6	GTP	C2	501	7	-	3/22/38/38	0/3/3/3
8	GDP	A1	501	-	-	6/16/32/32	0/3/3/3
6	GTP	D0	501	7	-	3/22/38/38	0/3/3/3
8	GDP	B3	501	-	-	4/16/32/32	0/3/3/3
8	GDP	C9	501	-	-	3/16/32/32	0/3/3/3
6	GTP	D8	501	7	-	5/22/38/38	0/3/3/3
8	GDP	A5	501	-	-	3/16/32/32	0/3/3/3
8	GDP	A9	501	-	-	5/16/32/32	0/3/3/3
8	GDP	F1	501	-	-	4/16/32/32	0/3/3/3
8	GDP	D3	501	-	-	4/16/32/32	0/3/3/3
8	GDP	C5	501	-	-	6/16/32/32	0/3/3/3
6	GTP	B0	501	7	-	7/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GTP	C0	501	7	-	8/22/38/38	0/3/3/3
8	GDP	C3	501	-	-	4/16/32/32	0/3/3/3
8	GDP	D9	501	-	-	5/16/32/32	0/3/3/3
6	GTP	D2	501	7	-	7/22/38/38	0/3/3/3
8	GDP	B5	501	-	-	2/16/32/32	0/3/3/3
8	GDP	E9	501	-	-	4/16/32/32	0/3/3/3
6	GTP	C4	501	7	-	5/22/38/38	0/3/3/3
6	GTP	D6	501	7	-	7/22/38/38	0/3/3/3
6	GTP	B2	501	7	-	6/22/38/38	0/3/3/3
8	GDP	A3	501	-	-	2/16/32/32	0/3/3/3
6	GTP	A6	501	7	-	6/22/38/38	0/3/3/3
8	GDP	E1	501	-	-	2/16/32/32	0/3/3/3
6	GTP	B8	501	7	-	6/22/38/38	0/3/3/3
6	GTP	E6	501	7	-	5/22/38/38	0/3/3/3
8	GDP	B7	501	-	-	3/16/32/32	0/3/3/3
8	GDP	E3	501	-	-	0/16/32/32	0/3/3/3
8	GDP	D1	501	-	-	3/16/32/32	0/3/3/3
8	GDP	A7	501	-	-	4/16/32/32	0/3/3/3
8	GDP	C1	501	-	-	5/16/32/32	0/3/3/3
6	GTP	A4	501	7	-	4/22/38/38	0/3/3/3
6	GTP	B6	501	7	-	6/22/38/38	0/3/3/3
6	GTP	E4	501	7	-	6/22/38/38	0/3/3/3
8	GDP	B9	501	-	-	3/16/32/32	0/3/3/3
8	GDP	B1	501	-	-	5/16/32/32	0/3/3/3
6	GTP	E2	501	7	-	4/22/38/38	0/3/3/3
6	GTP	A8	501	7	-	4/22/38/38	0/3/3/3
6	GTP	E0	501	7	-	2/22/38/38	0/3/3/3
8	GDP	D7	501	-	-	4/16/32/32	0/3/3/3
6	GTP	F0	501	7	-	7/22/38/38	0/3/3/3
6	GTP	A0	501	7	-	8/22/38/38	0/3/3/3

The worst 5 of 147 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D1	501	GDP	C6-N1	-3.25	1.32	1.38
8	D7	501	GDP	C6-N1	-3.18	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B5	501	GDP	C6-N1	-3.14	1.33	1.38
8	A1	501	GDP	C6-N1	-3.14	1.33	1.38
8	C9	501	GDP	C6-N1	-3.11	1.33	1.38

The worst 5 of 394 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C9	501	GDP	C5-C4-N3	-6.57	117.93	128.39
8	F1	501	GDP	C5-C4-N3	-6.49	118.06	128.39
8	D1	501	GDP	C5-C4-N3	-6.41	118.19	128.39
8	B5	501	GDP	C5-C4-N3	-6.35	118.28	128.39
8	D7	501	GDP	C5-C4-N3	-6.23	118.47	128.39

There are no chirality outliers.

5 of 231 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A0	501	GTP	PB-O3A-PA-O5'
6	A0	501	GTP	C5'-O5'-PA-O3A
6	A0	501	GTP	C5'-O5'-PA-O1A
6	A0	501	GTP	C5'-O5'-PA-O2A
6	A2	501	GTP	C5'-O5'-PA-O3A

There are no ring outliers.

28 monomers are involved in 41 short contacts:

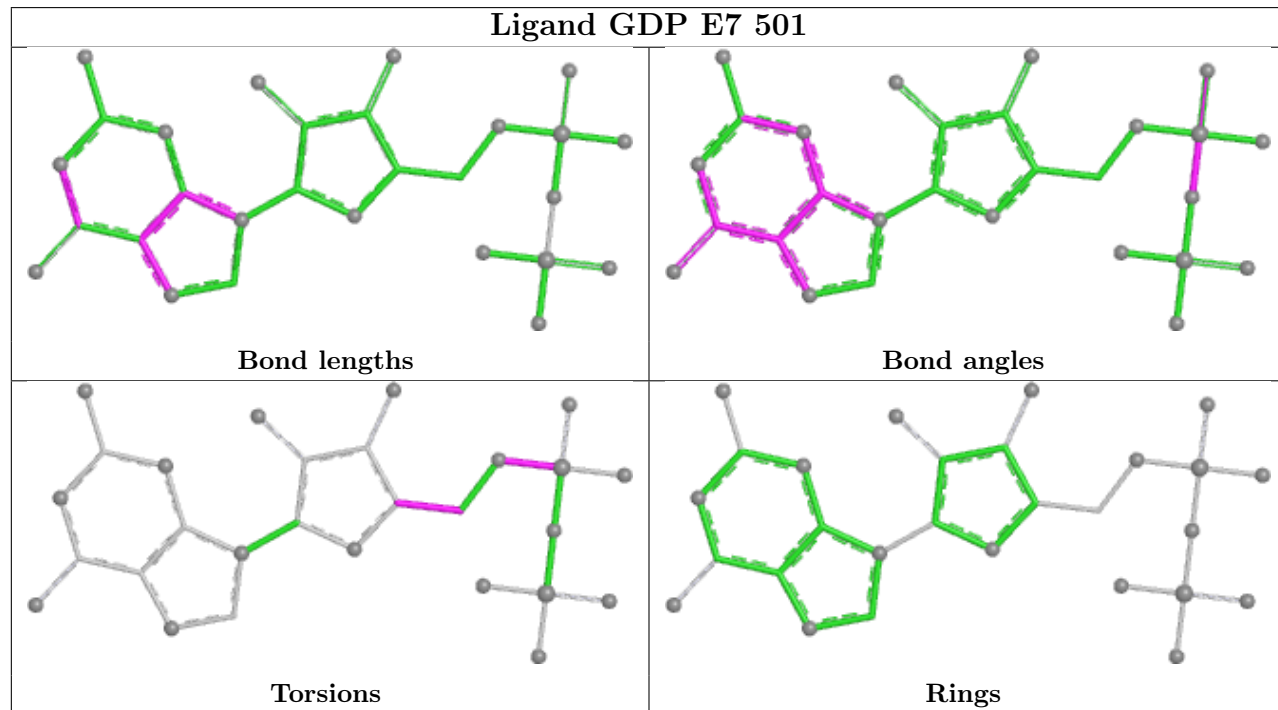
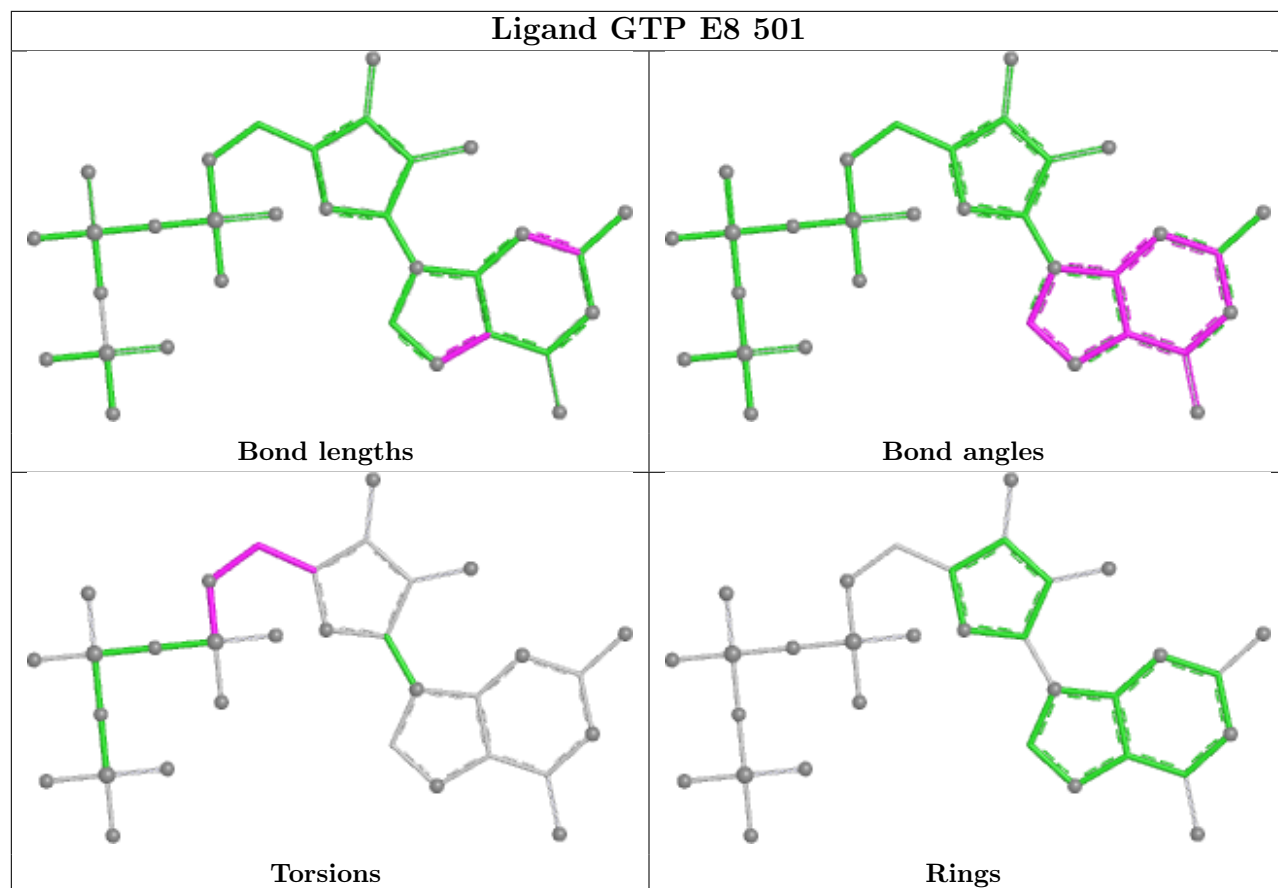
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E8	501	GTP	2	0
6	C8	501	GTP	1	0
8	D5	501	GDP	1	0
6	D4	501	GTP	1	0
6	C6	501	GTP	3	0
6	C2	501	GTP	1	0
8	A1	501	GDP	2	0
8	B3	501	GDP	1	0
6	D8	501	GTP	1	0
8	A9	501	GDP	1	0
8	F1	501	GDP	1	0
8	C5	501	GDP	1	0
6	B0	501	GTP	1	0
6	C0	501	GTP	2	0

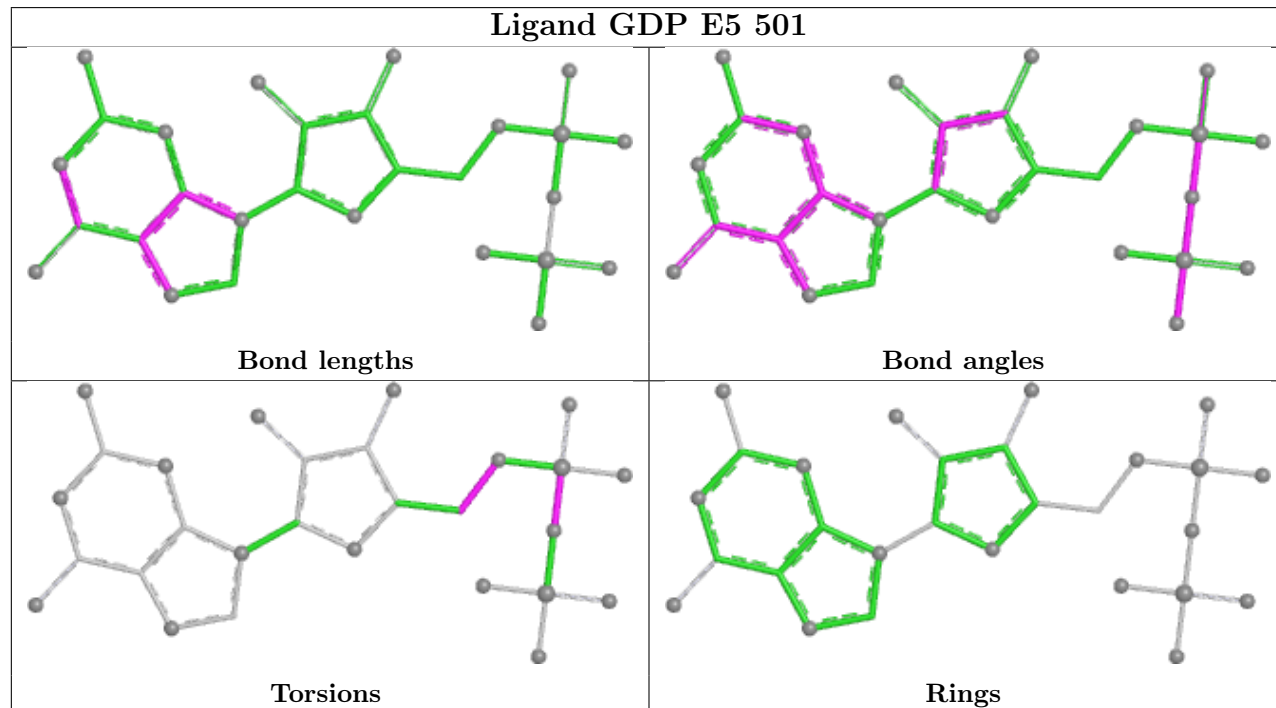
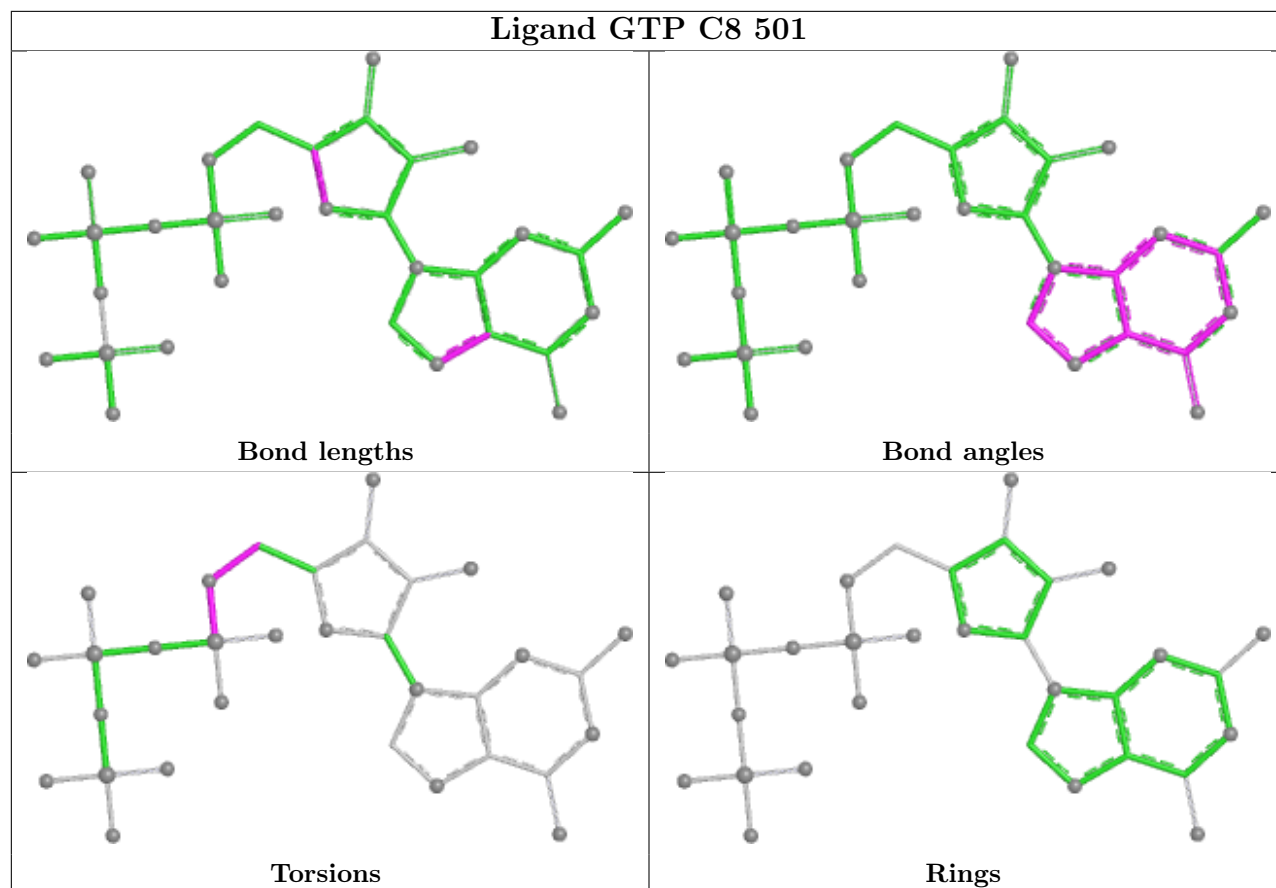
Continued on next page...

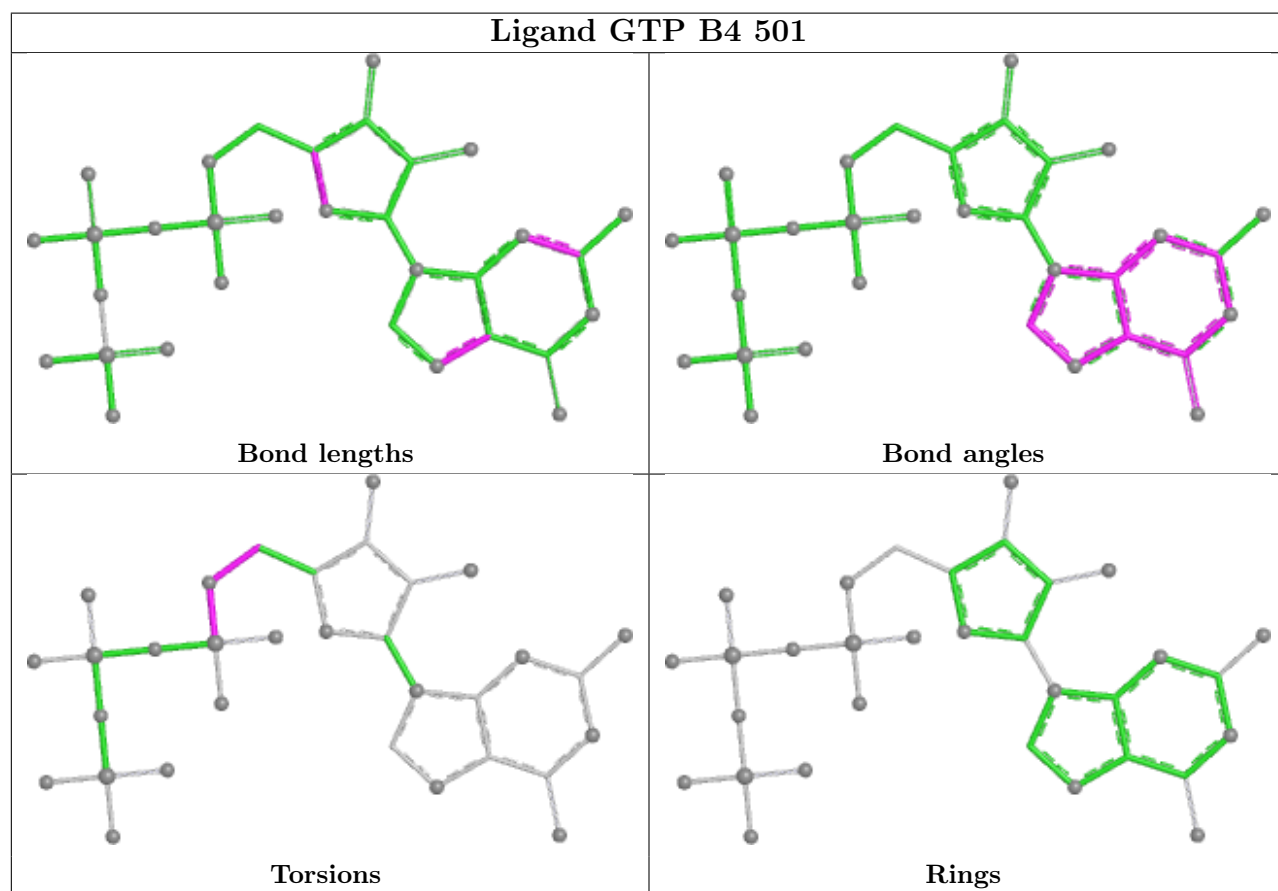
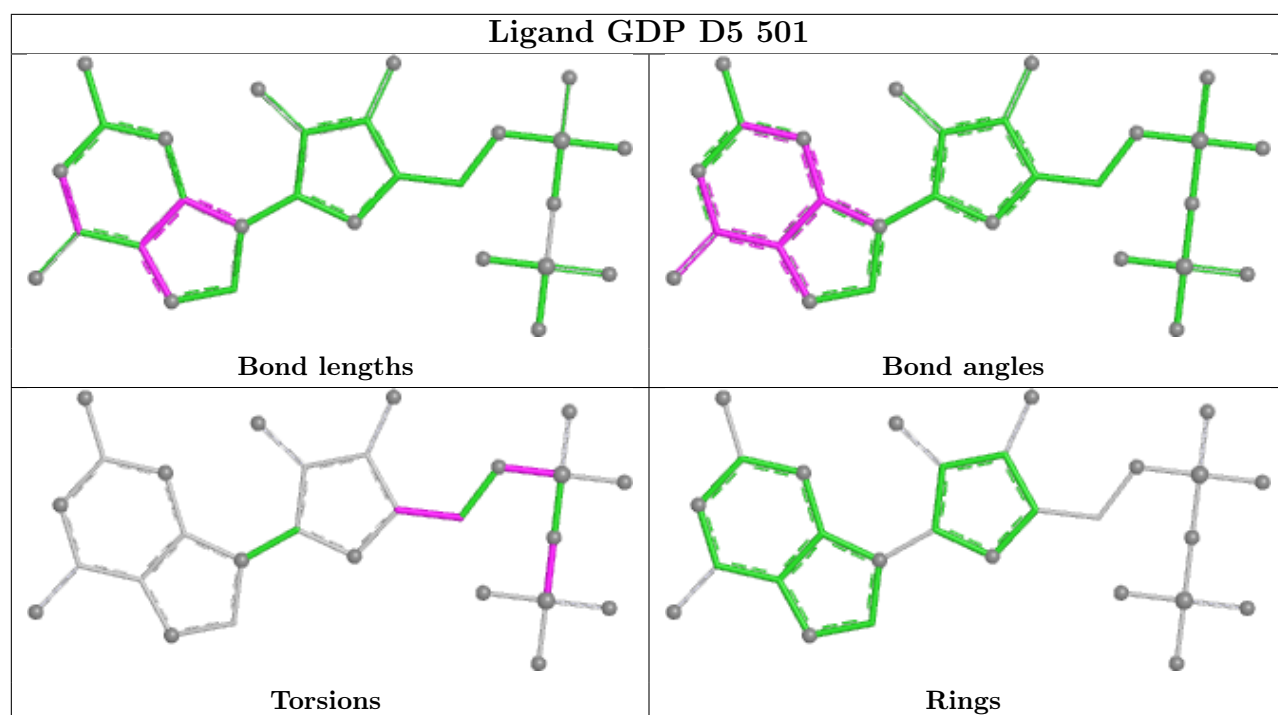
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C3	501	GDP	2	0
6	C4	501	GTP	1	0
6	B2	501	GTP	1	0
8	A3	501	GDP	2	0
6	B8	501	GTP	1	0
6	E6	501	GTP	3	0
8	B7	501	GDP	1	0
8	E3	501	GDP	3	0
8	C1	501	GDP	1	0
6	B6	501	GTP	2	0
6	E2	501	GTP	1	0
6	A8	501	GTP	1	0
6	F0	501	GTP	1	0
6	A0	501	GTP	2	0

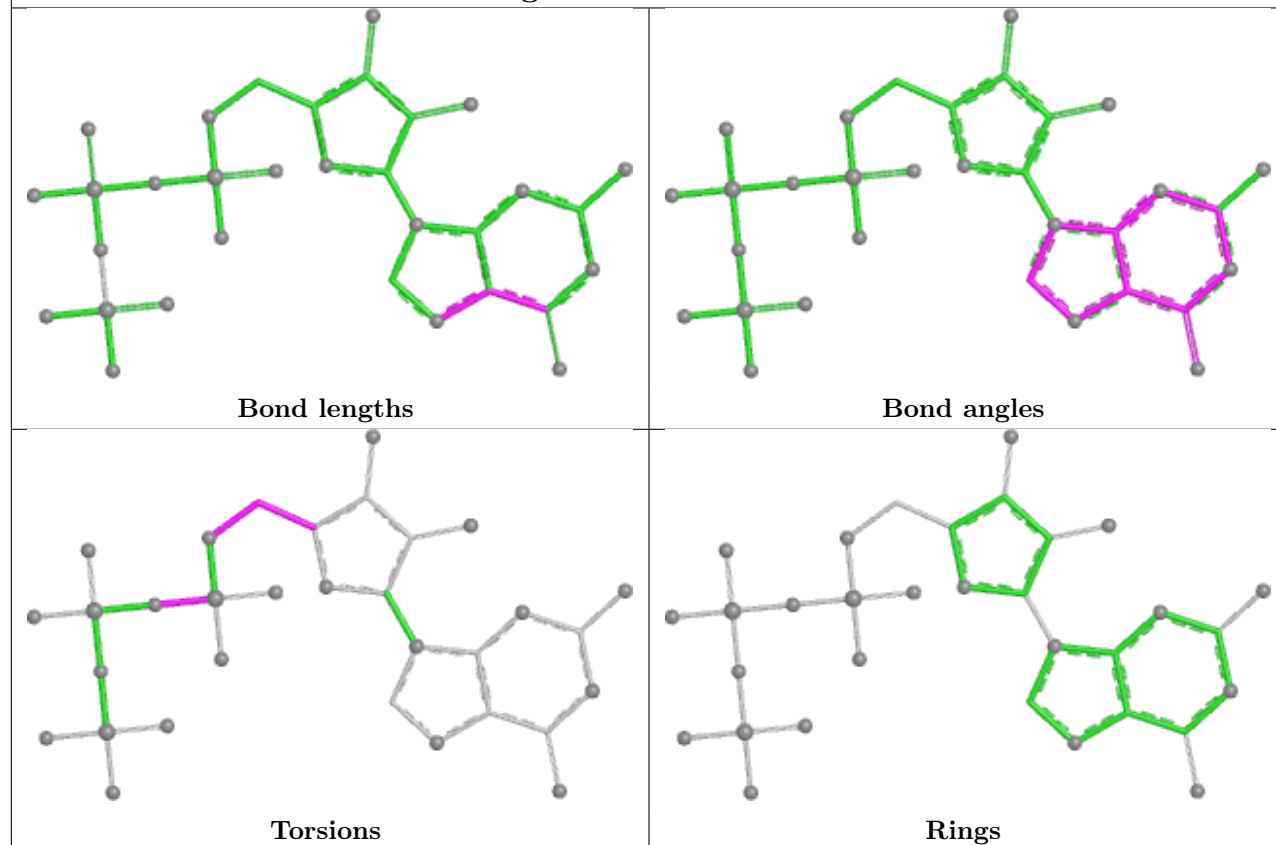
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



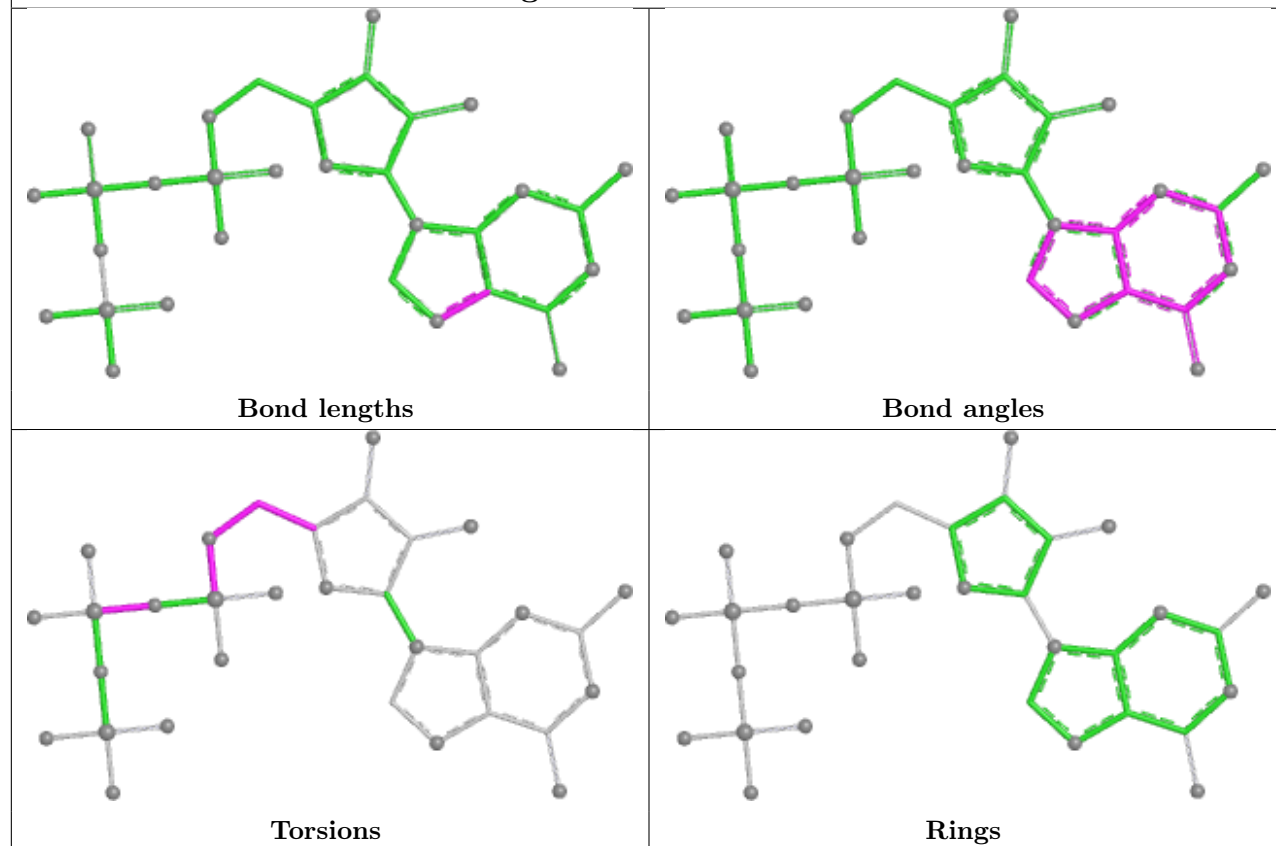


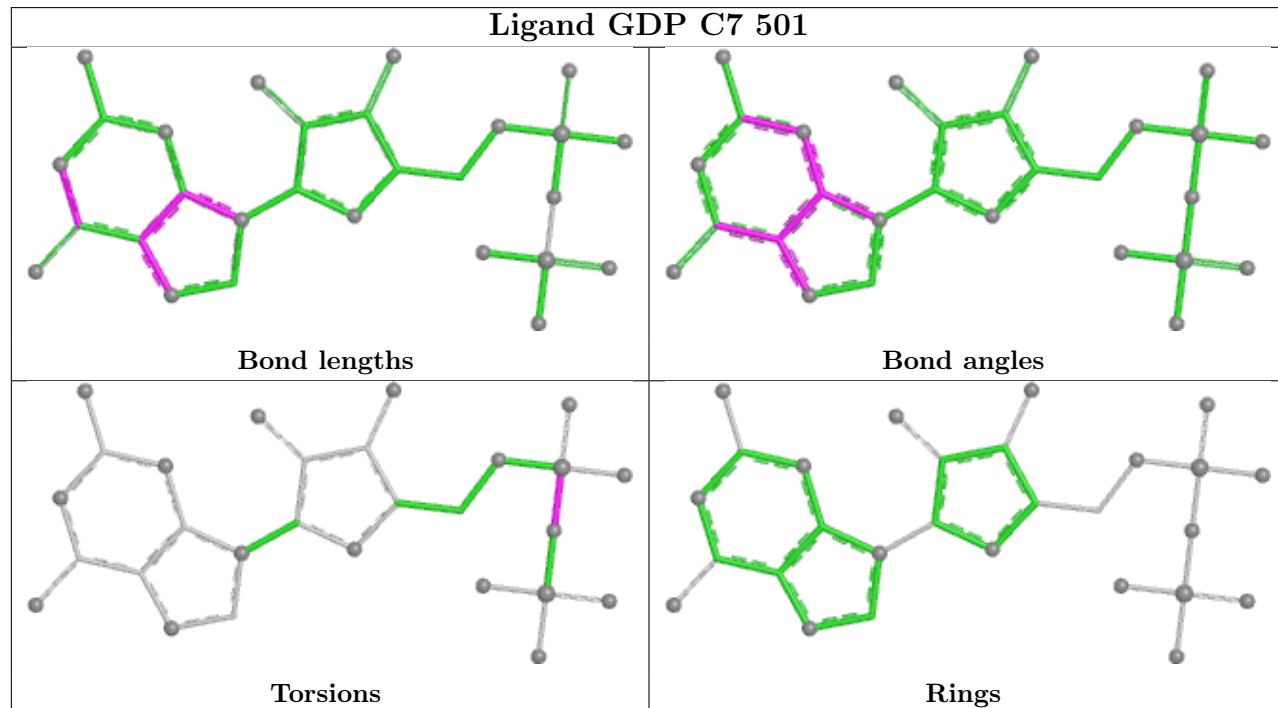
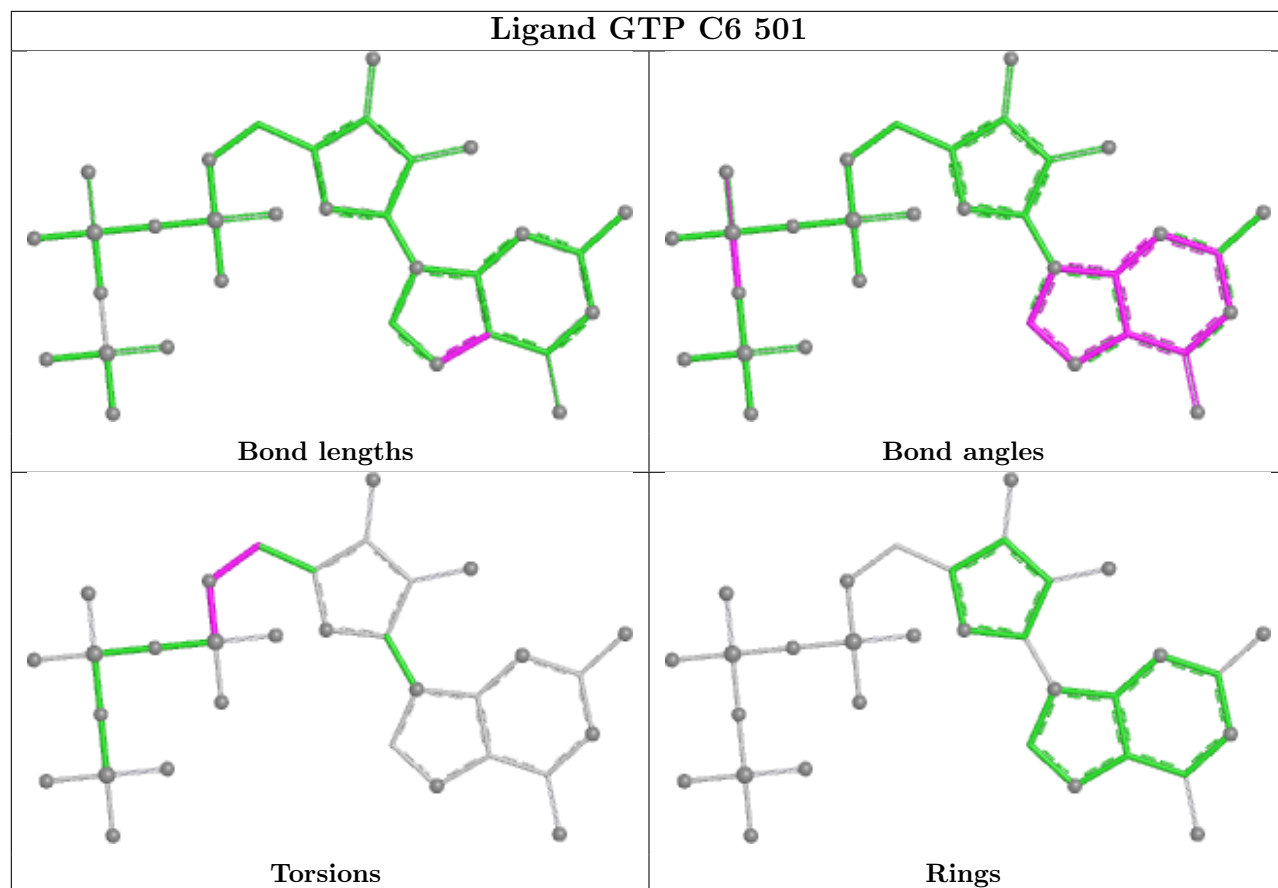


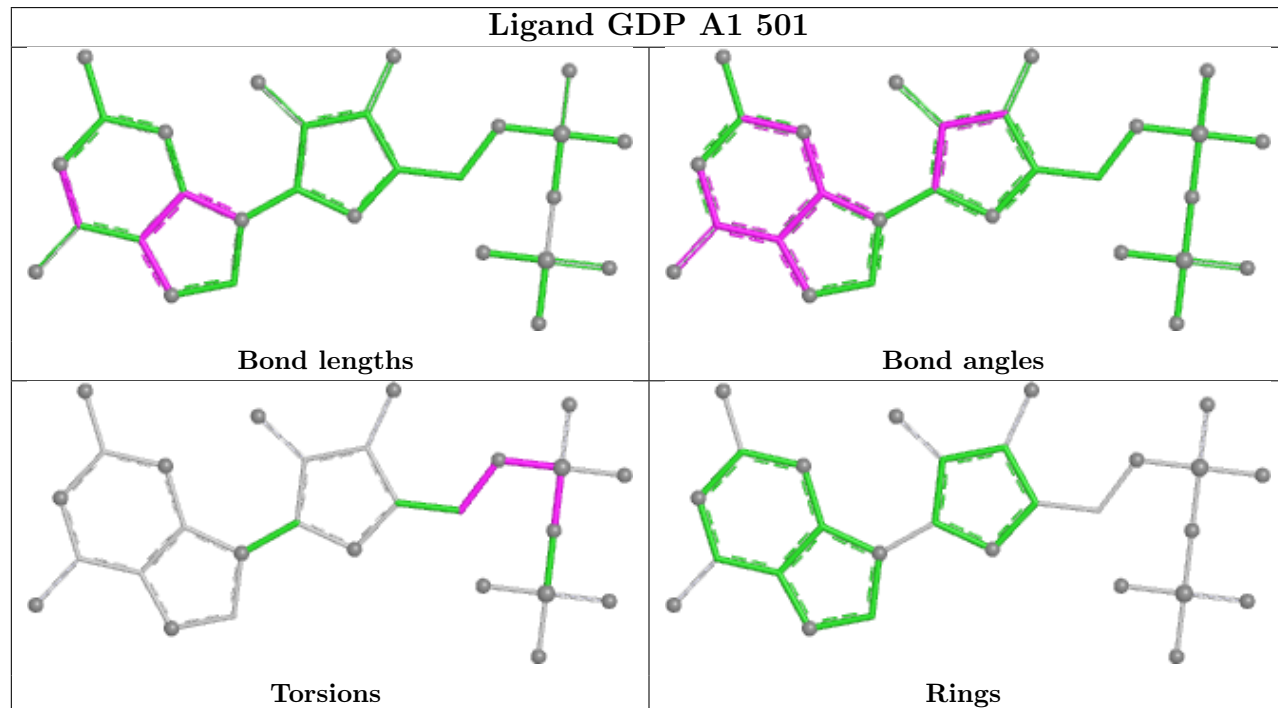
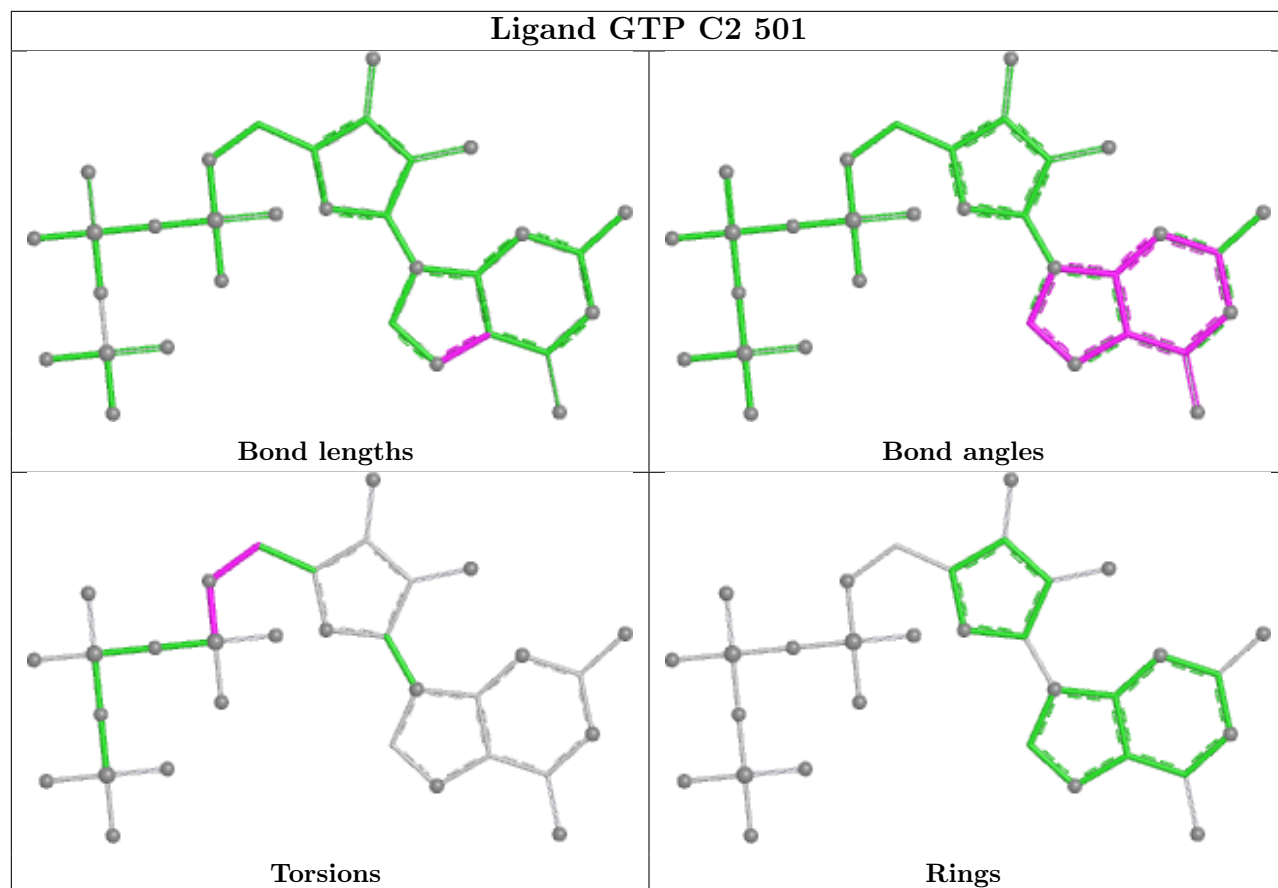
Ligand GTP D4 501

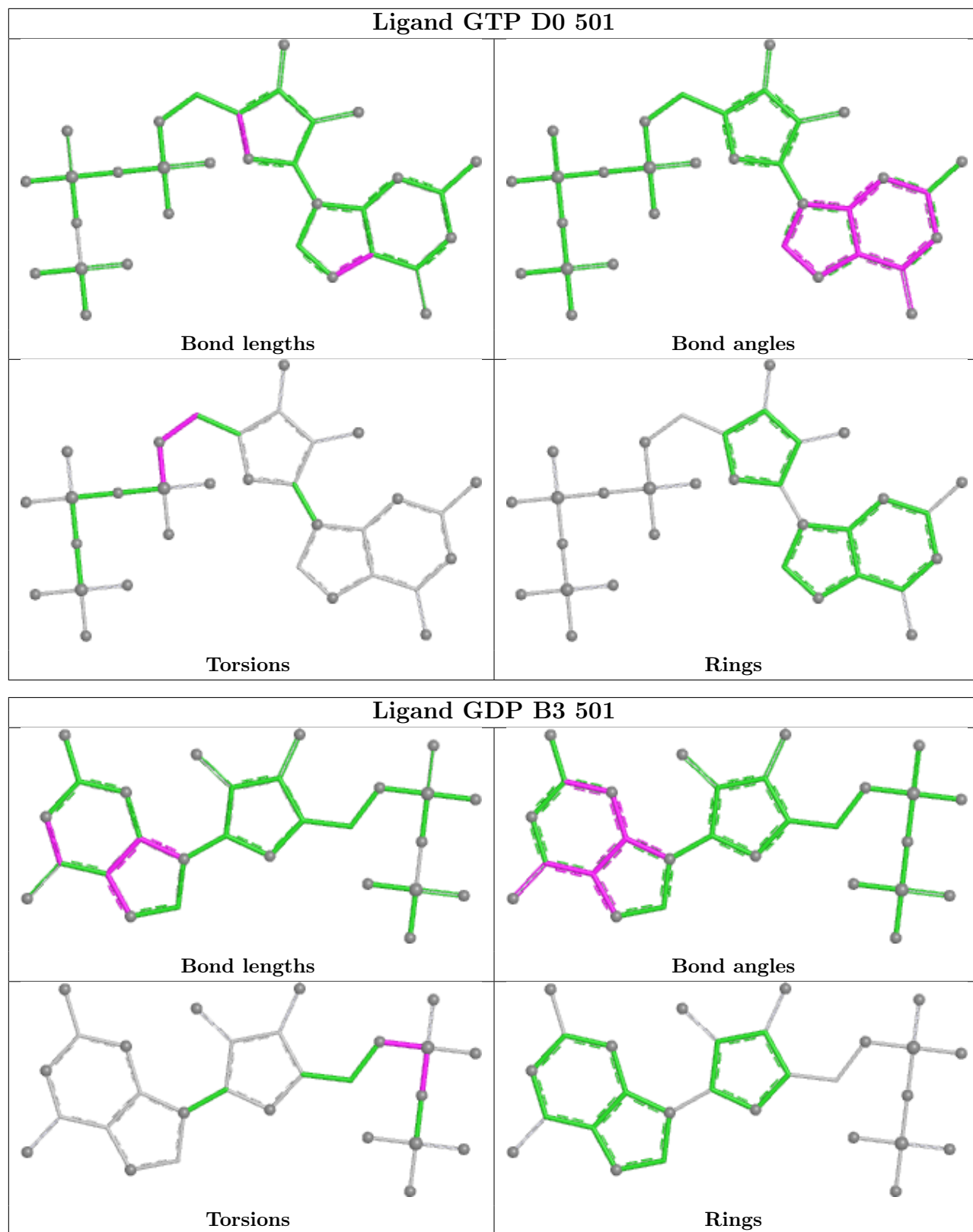


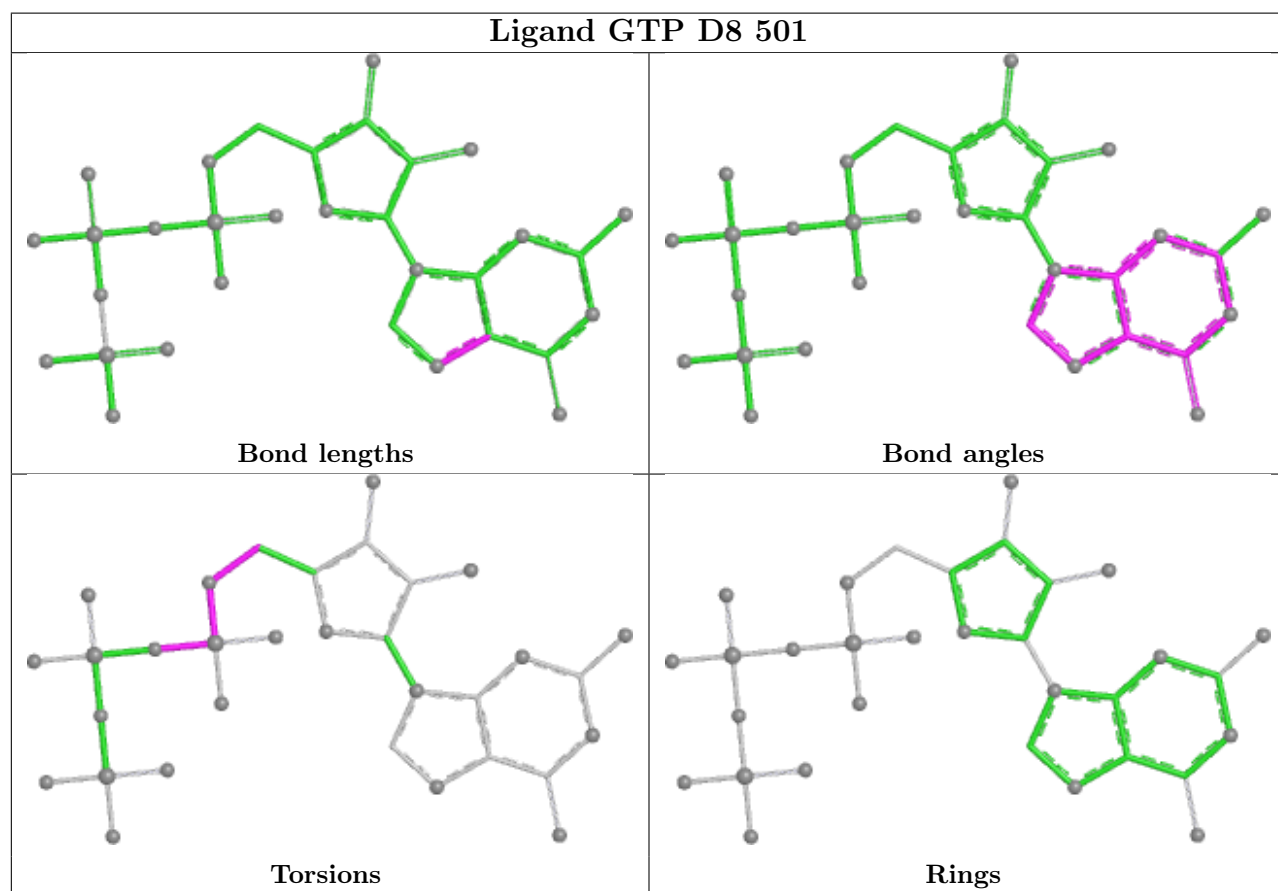
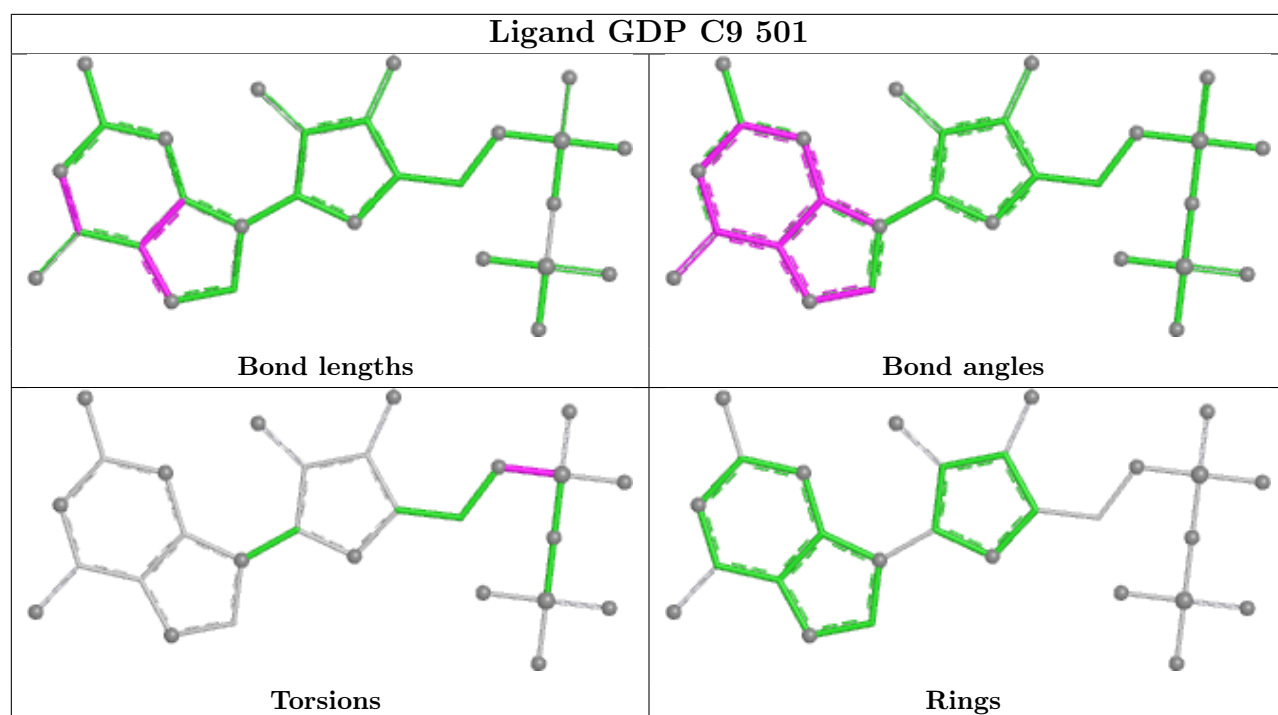
Ligand GTP A2 501

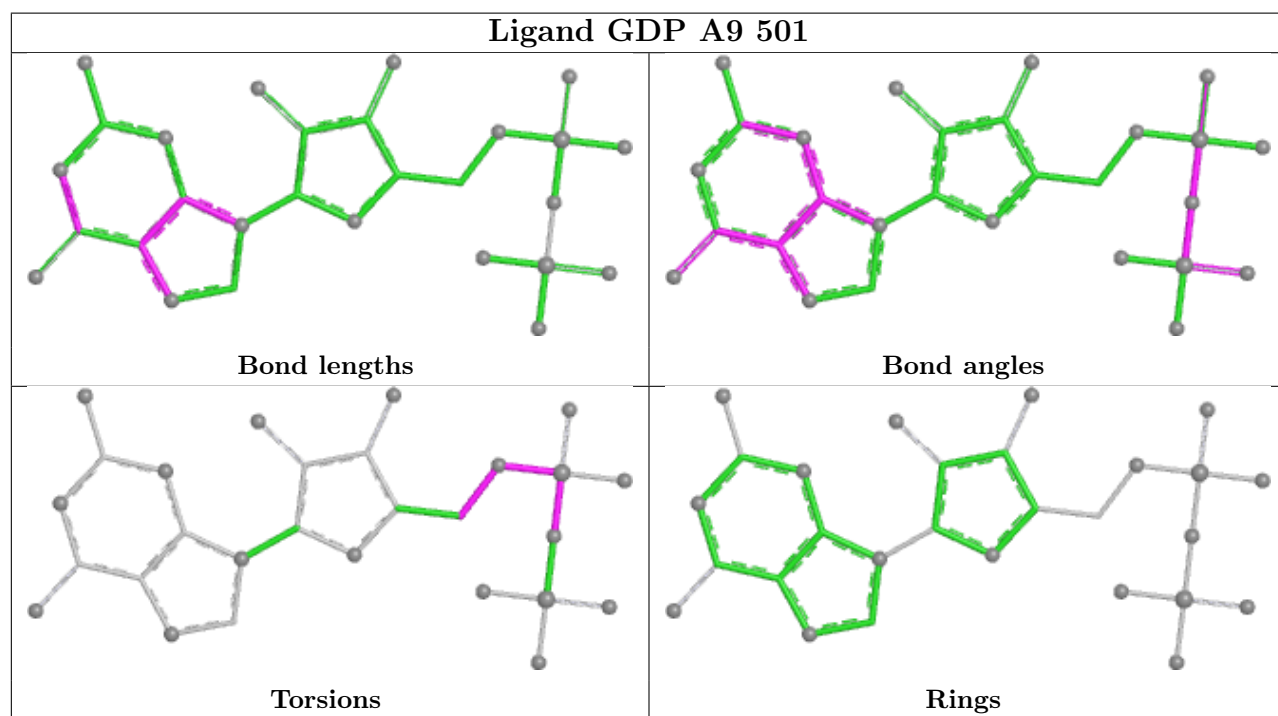
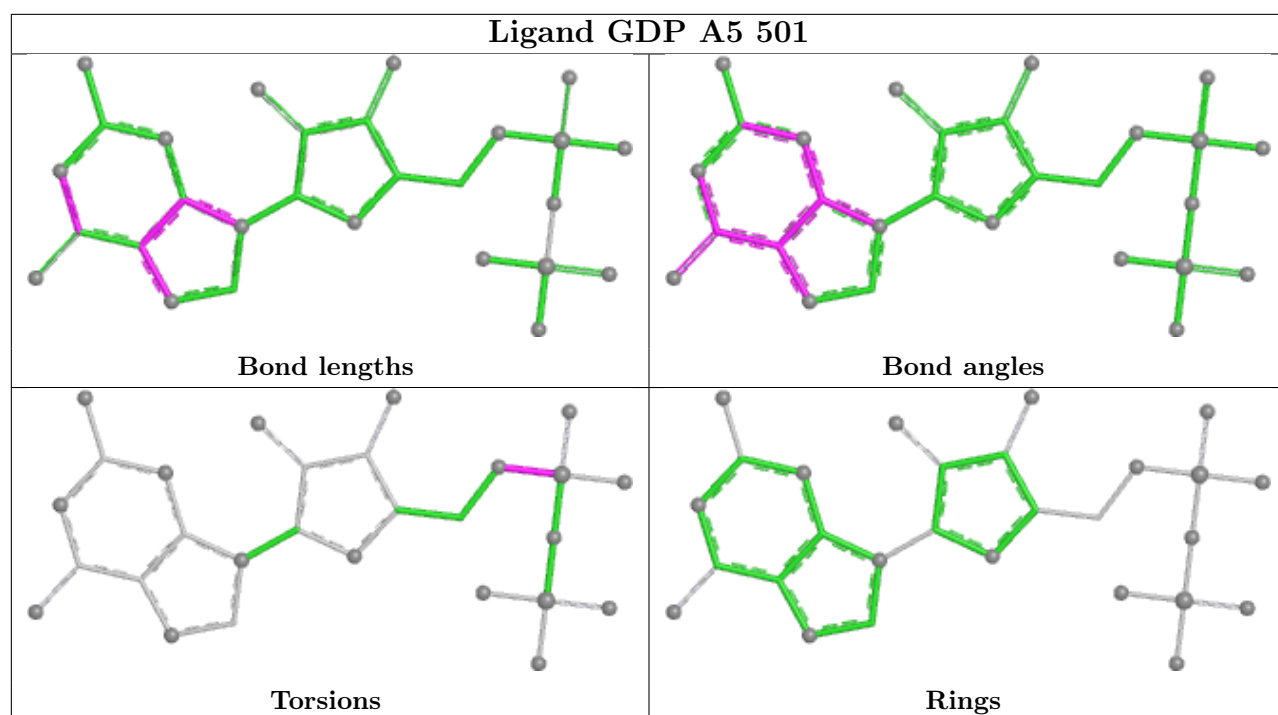


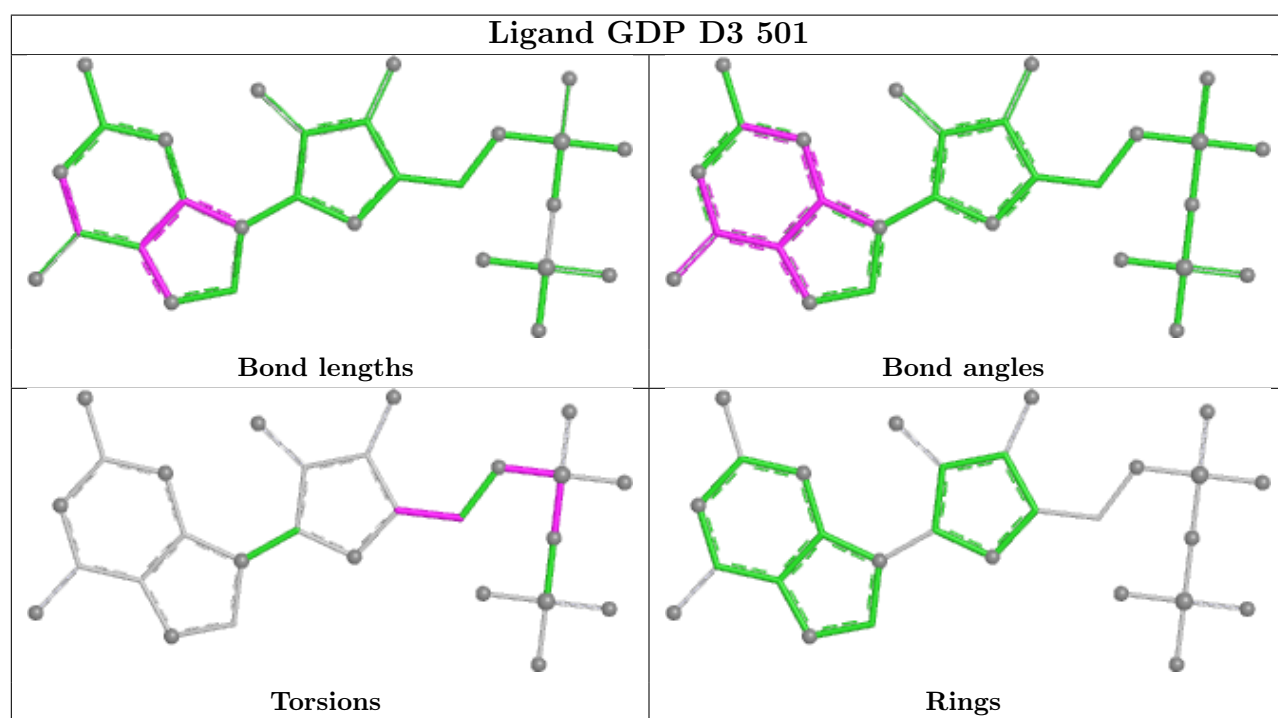
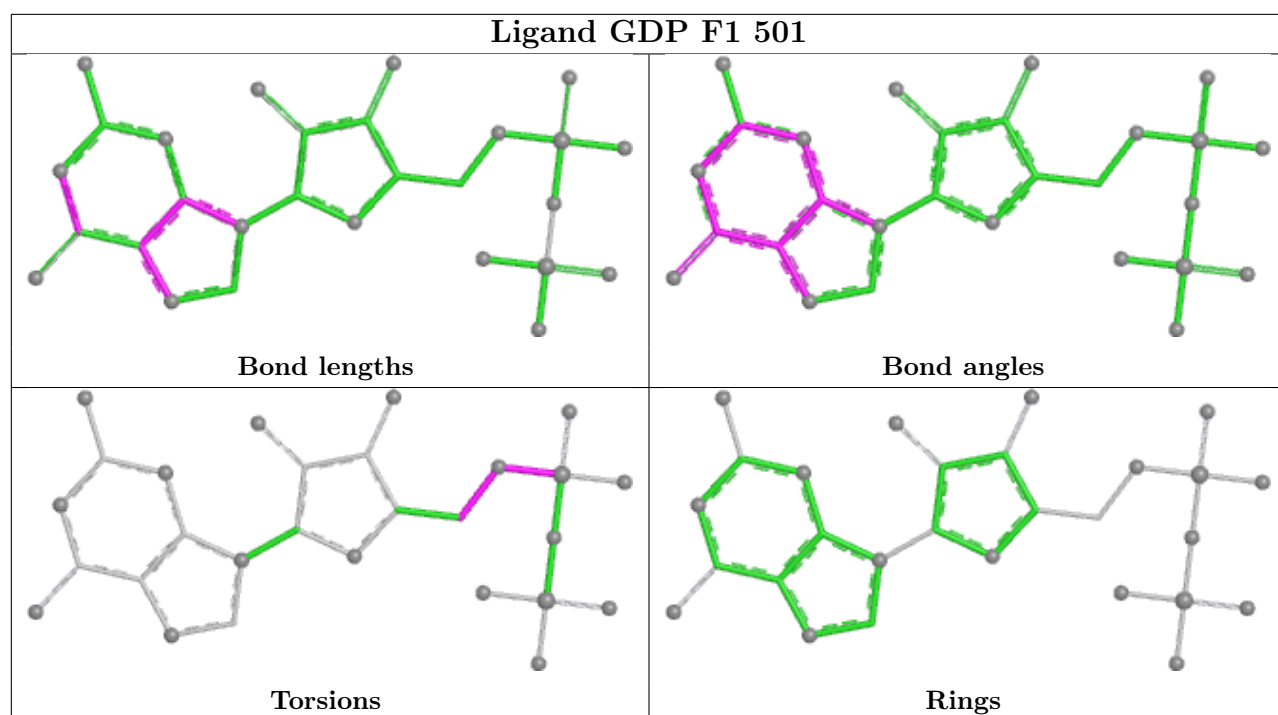


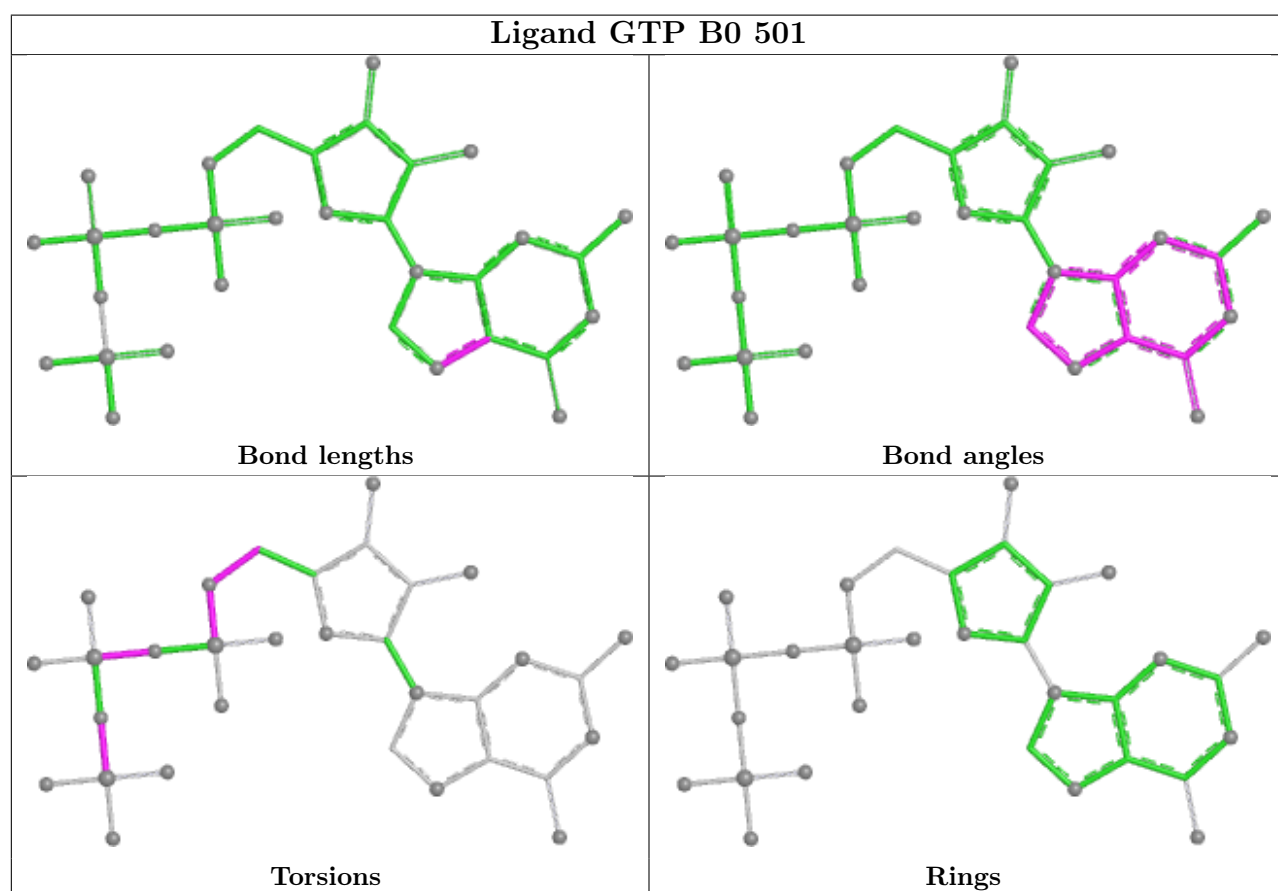
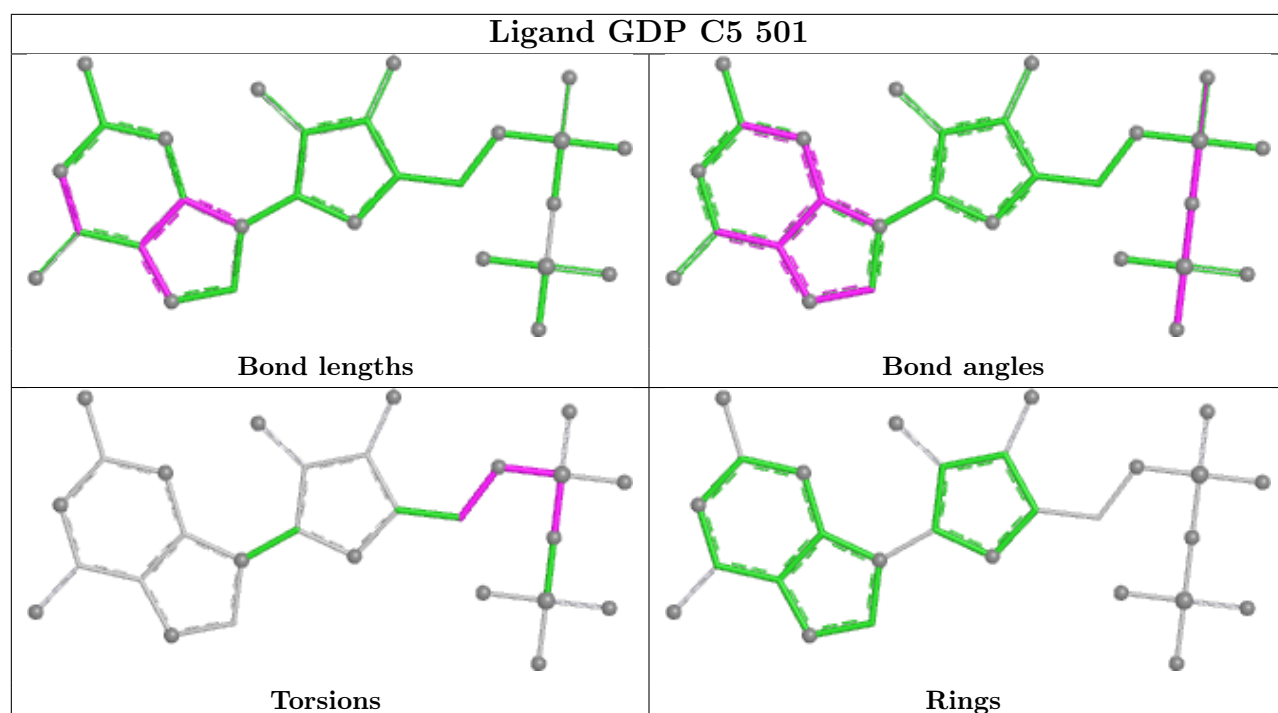


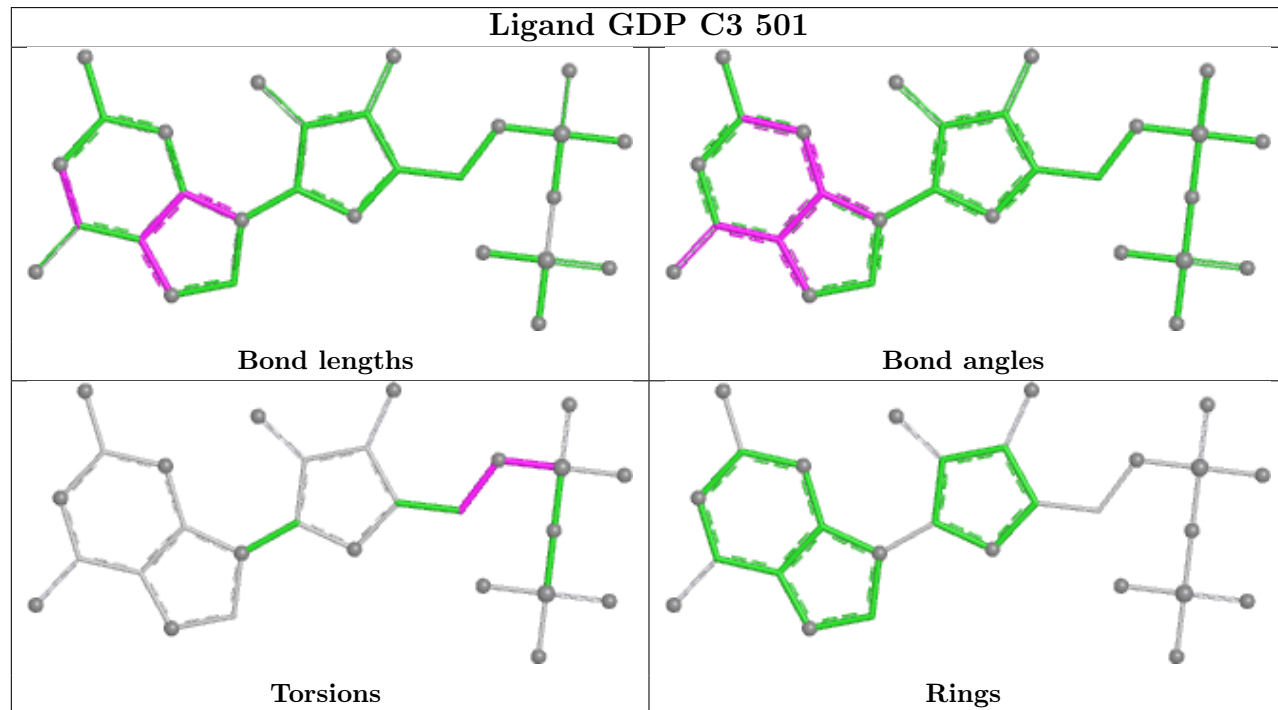
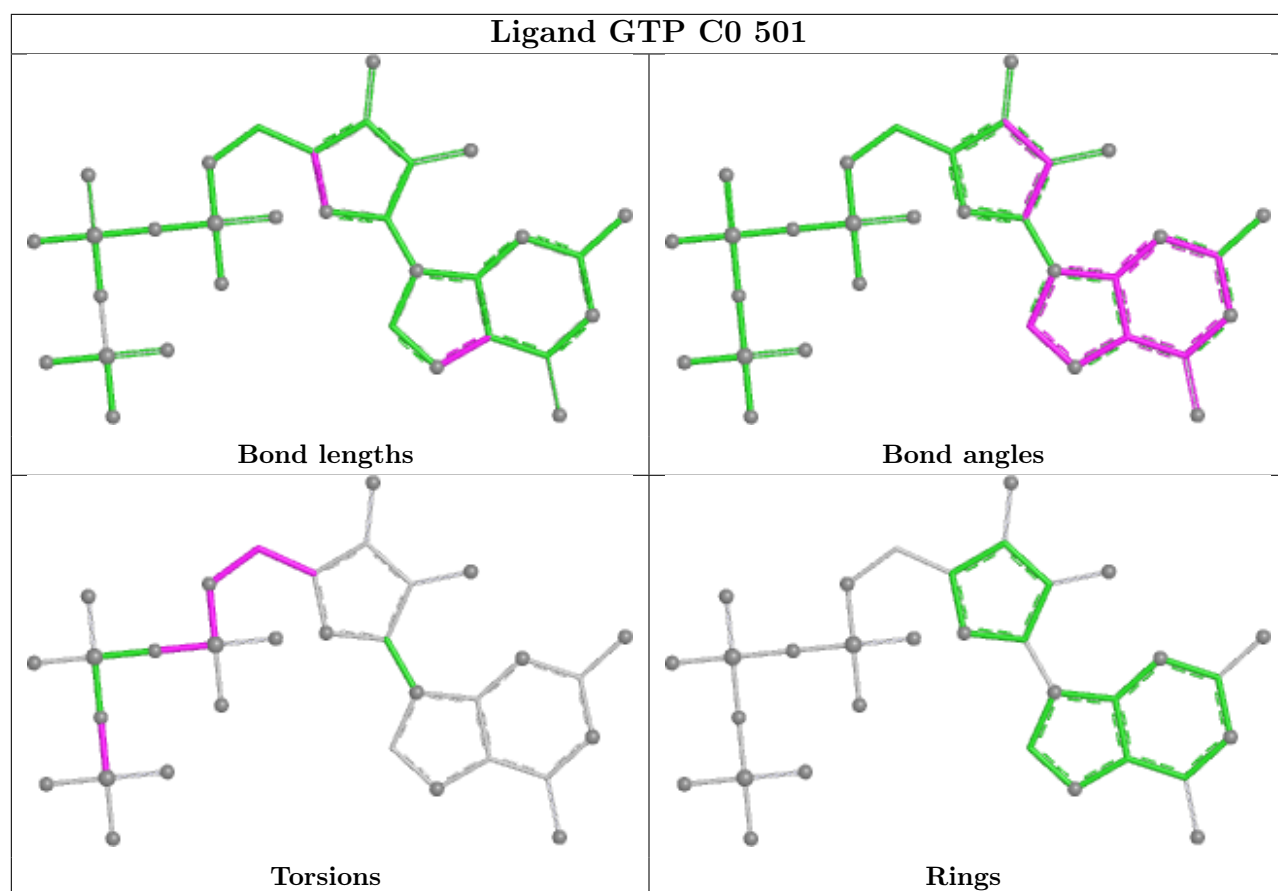


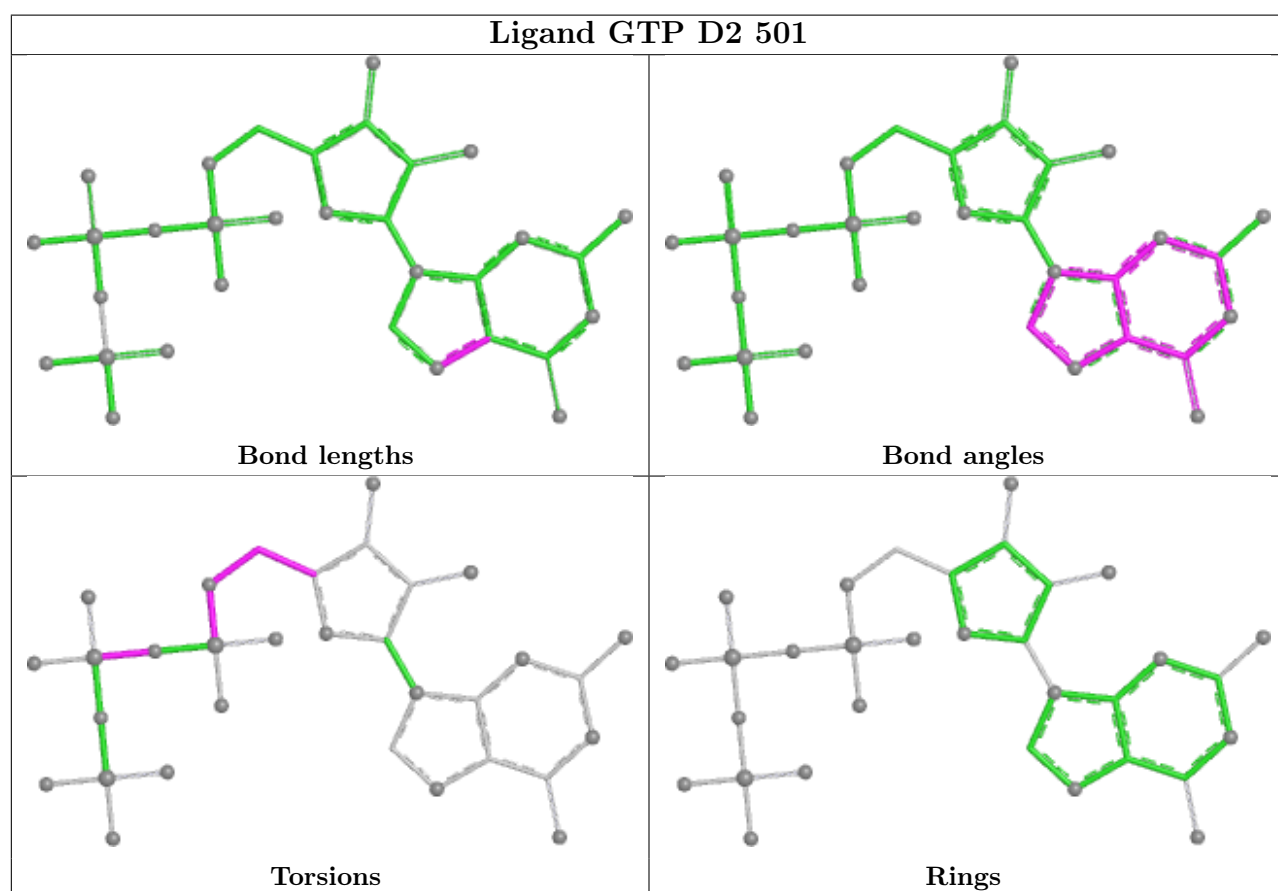
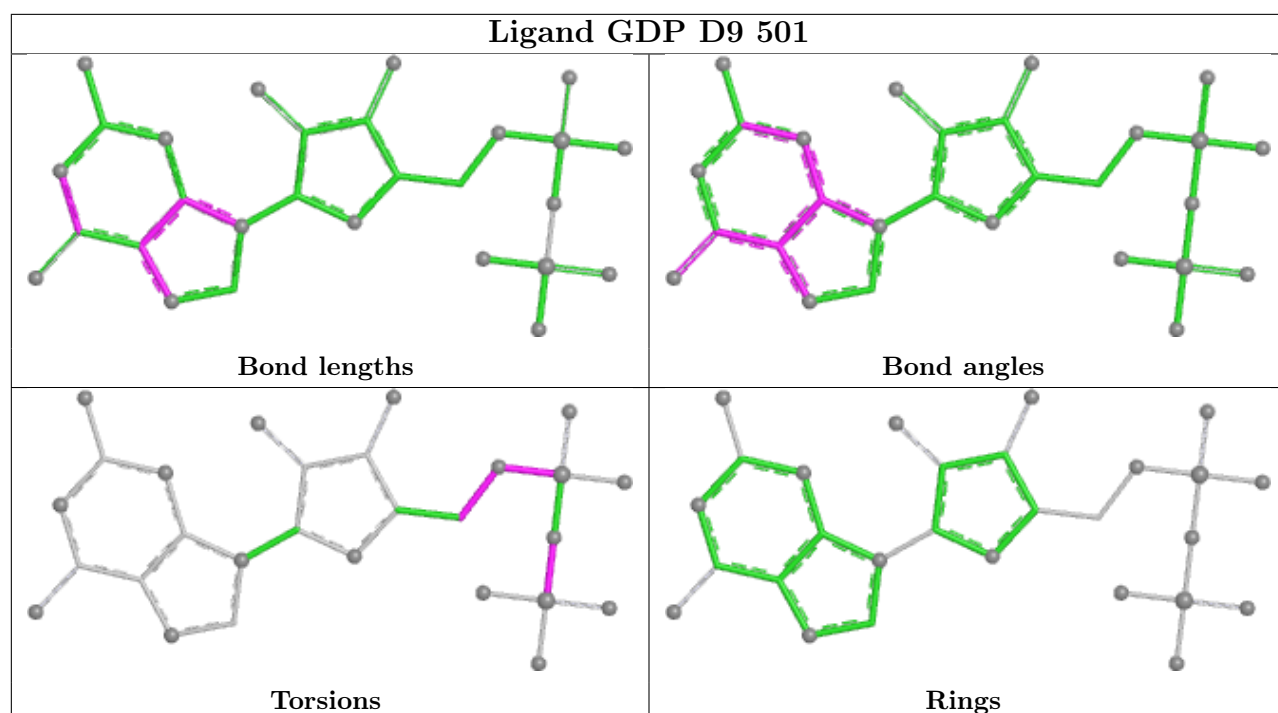


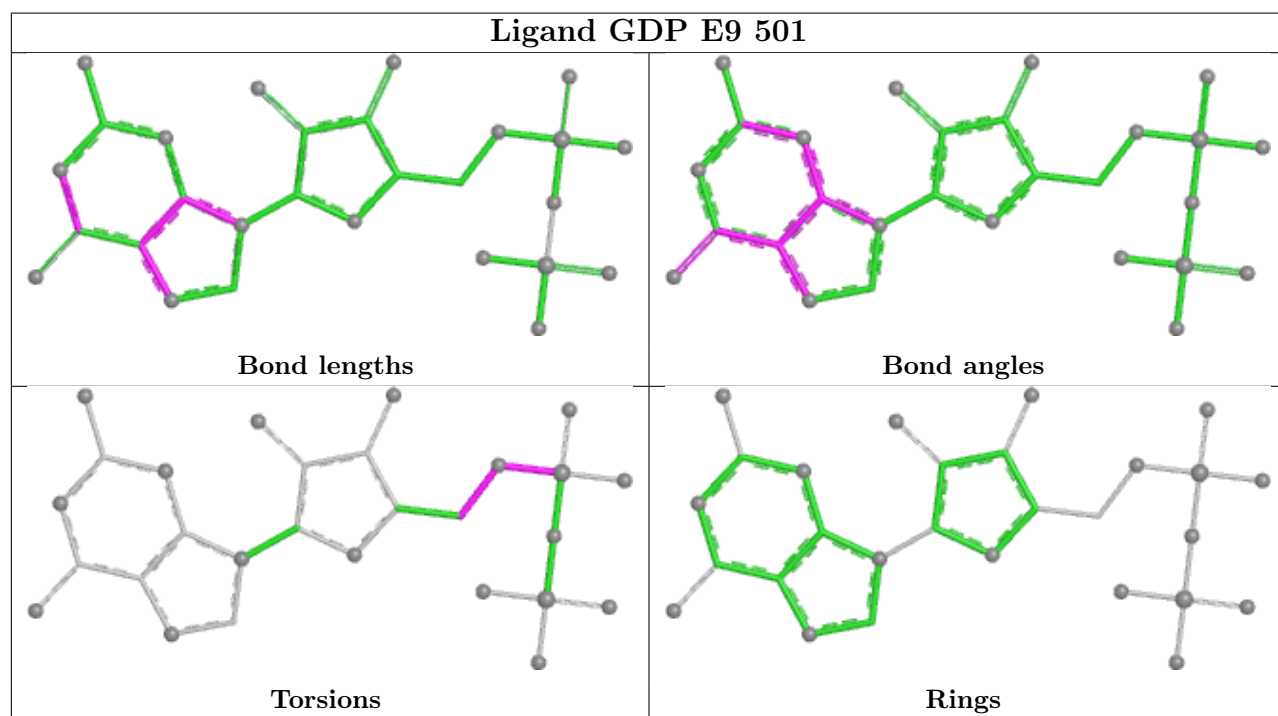
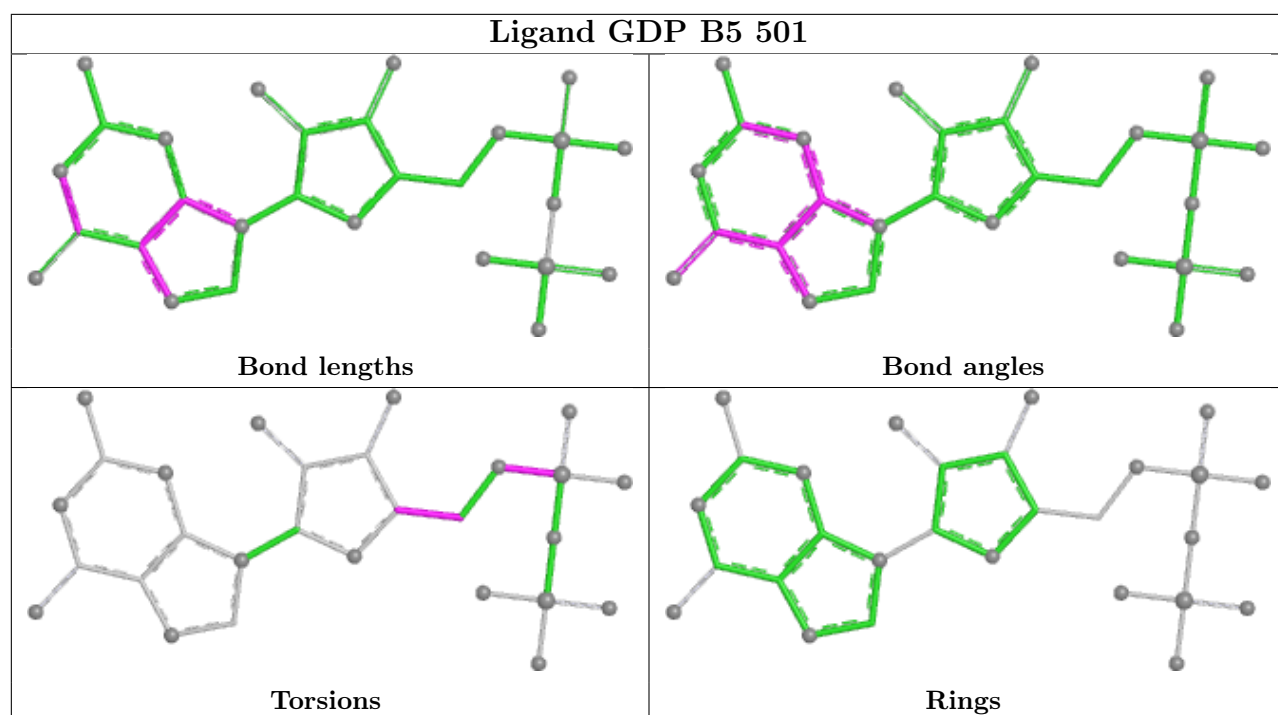




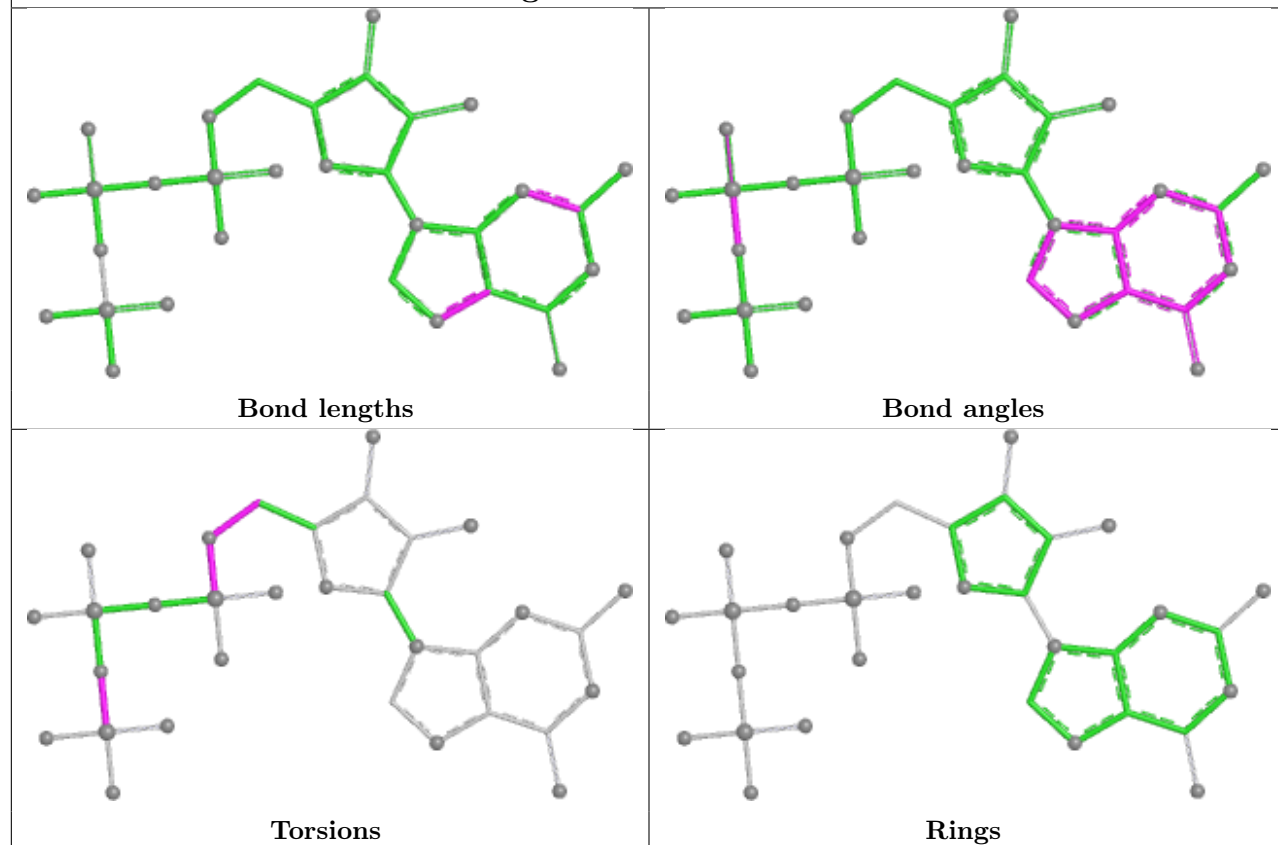




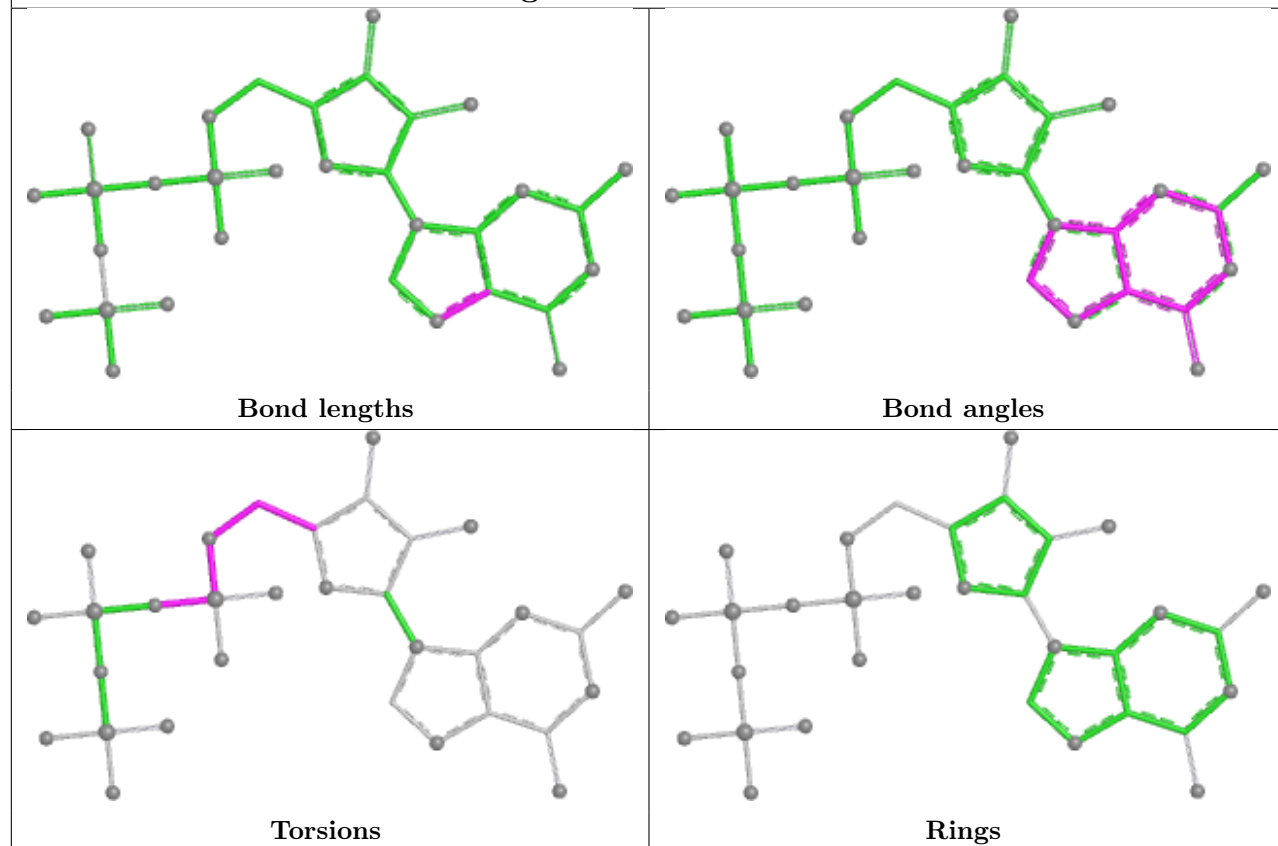


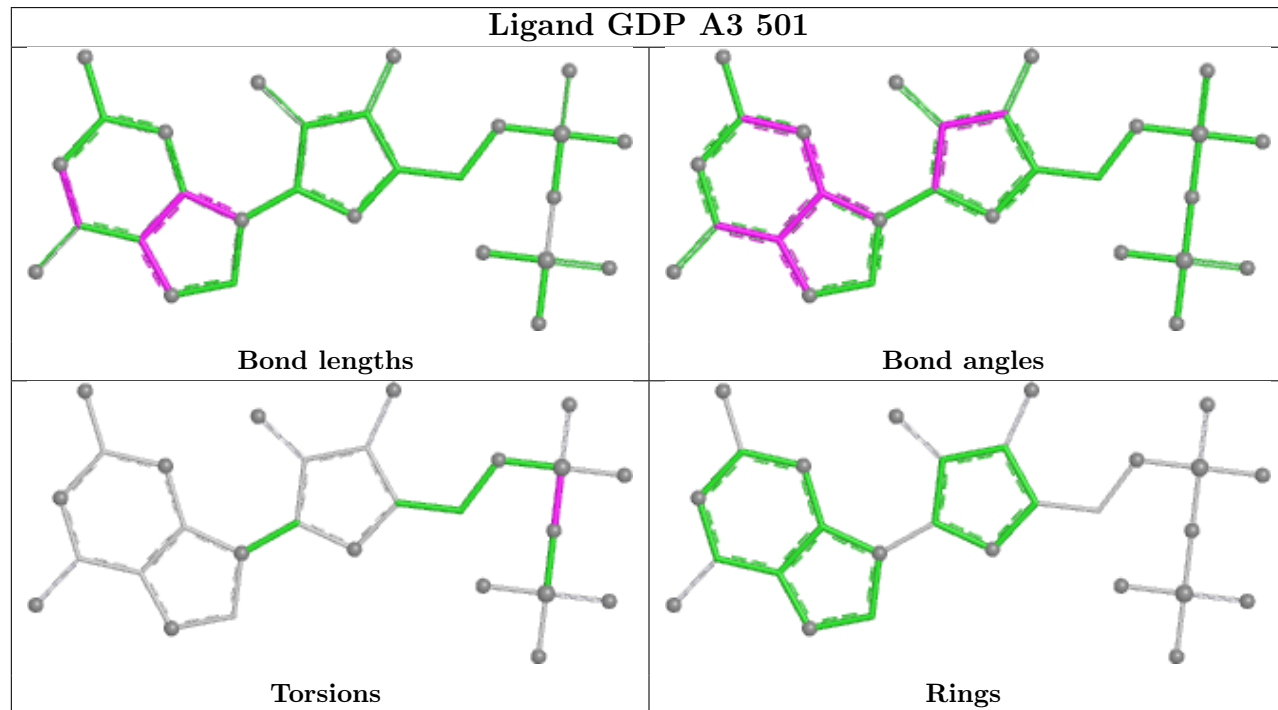
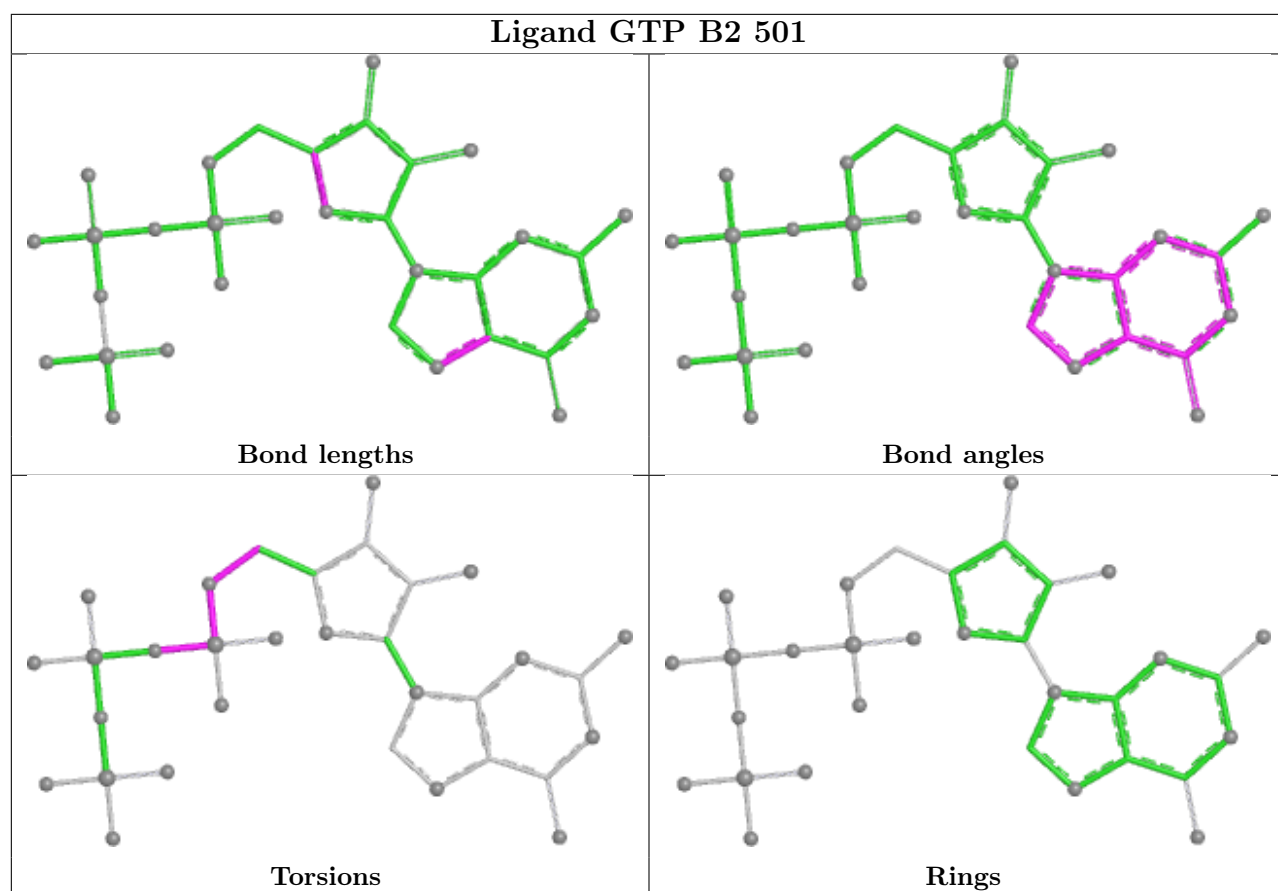


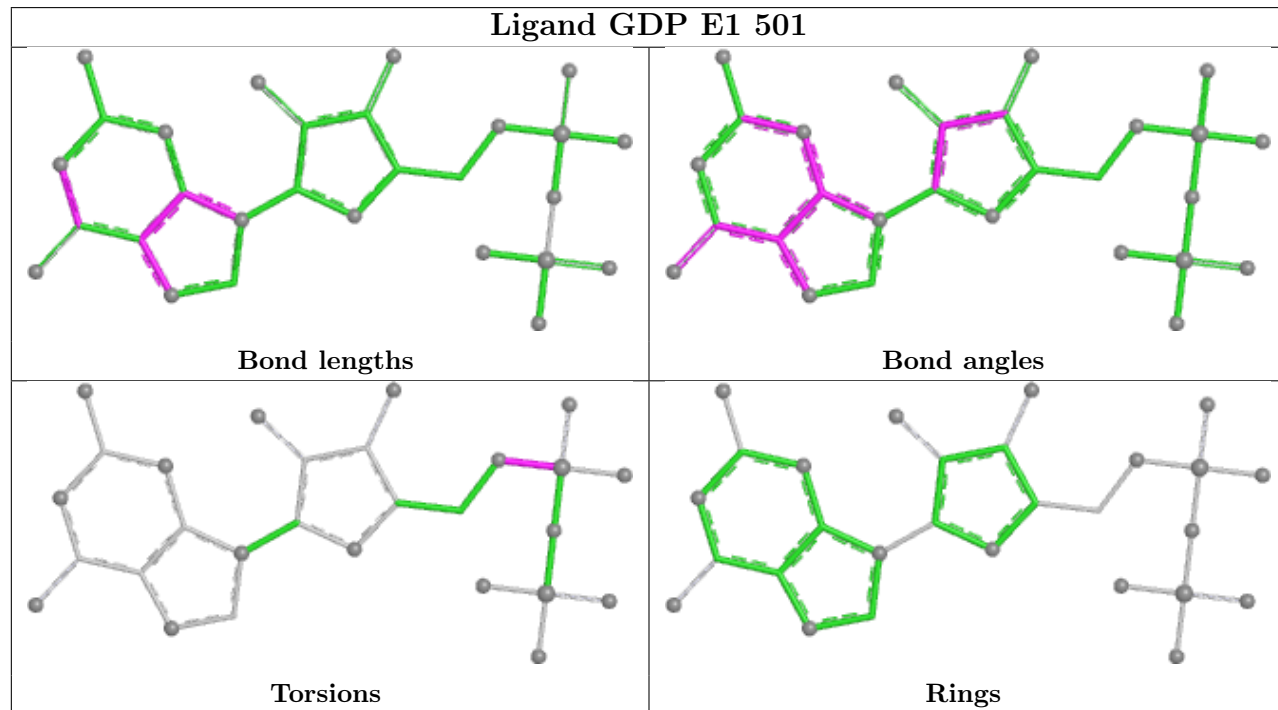
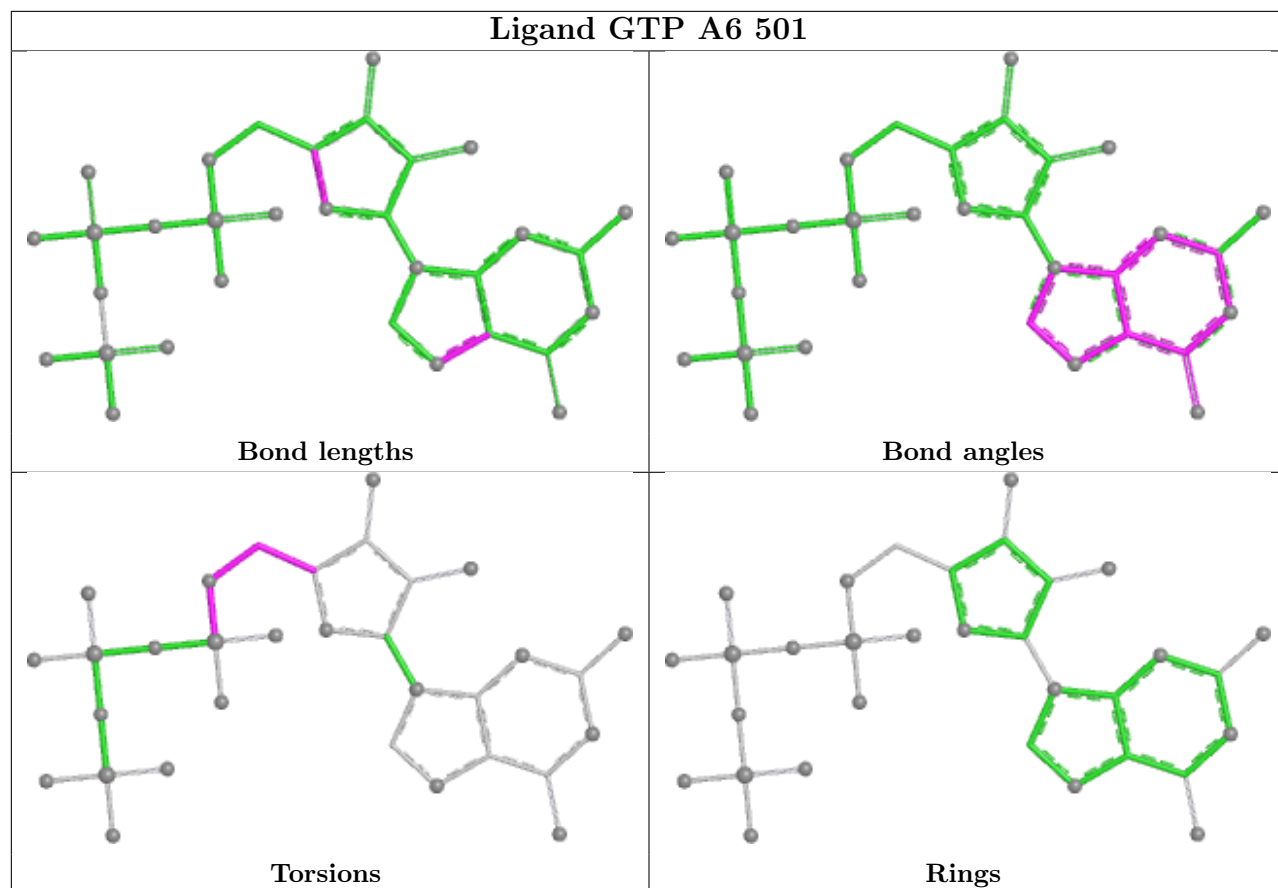
Ligand GTP C4 501



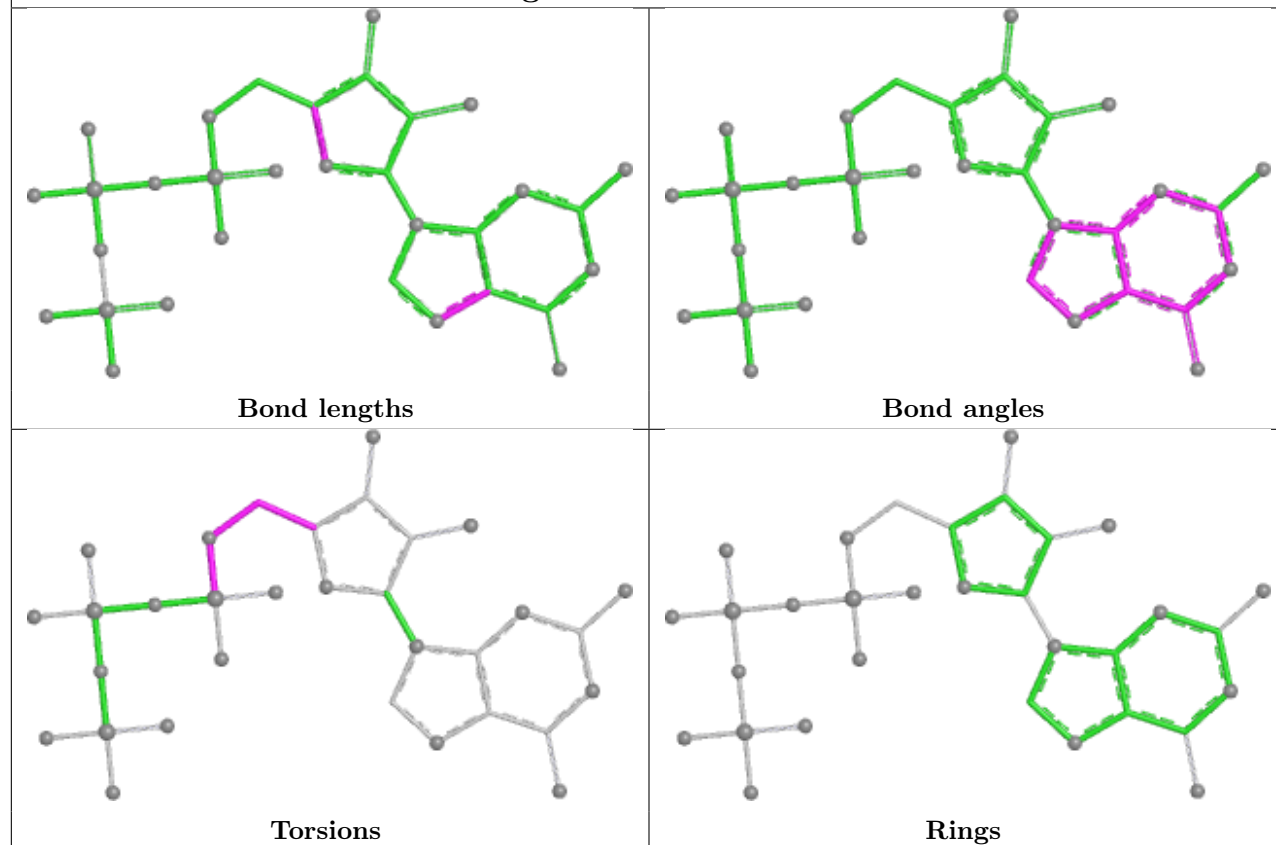
Ligand GTP D6 501



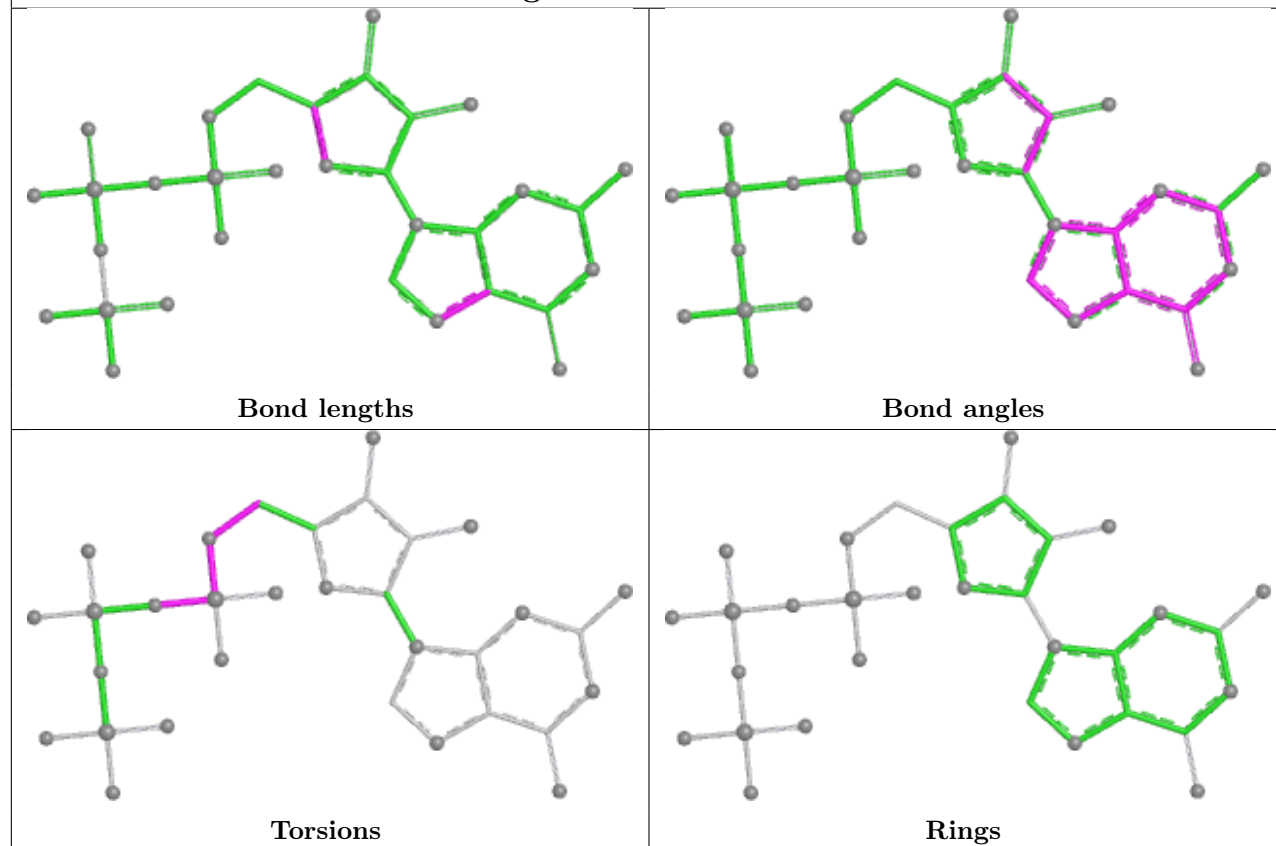


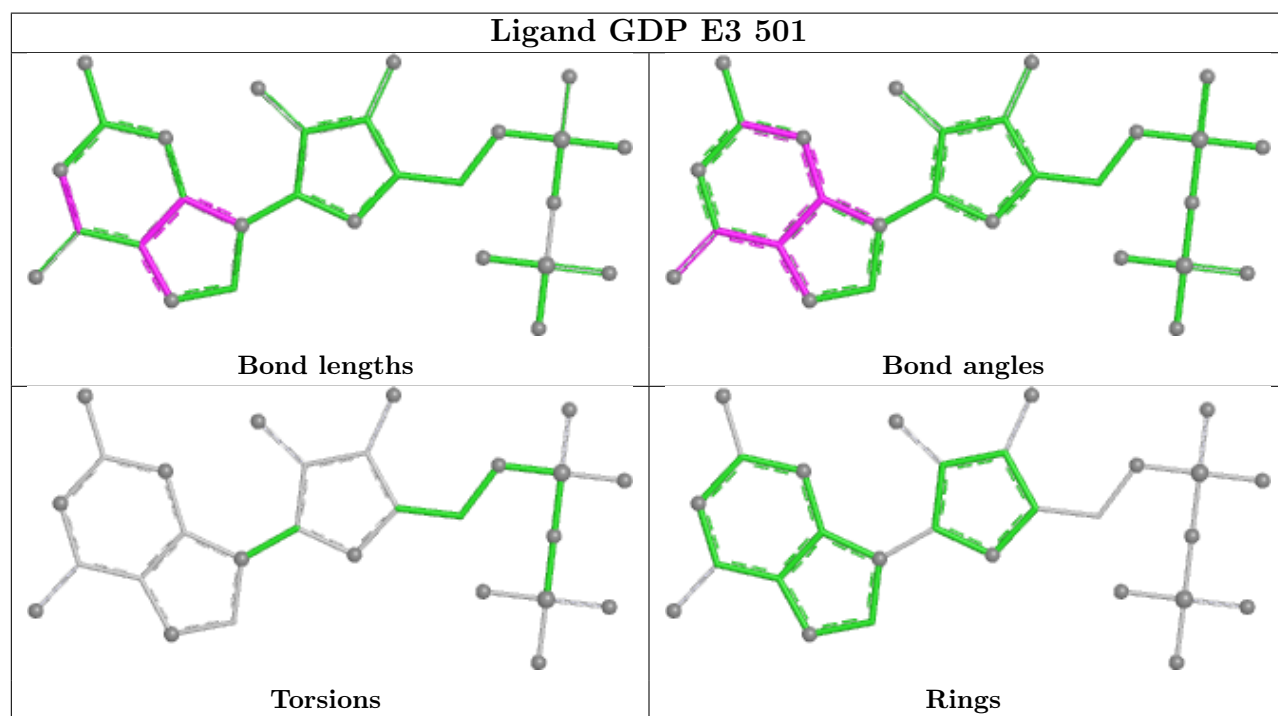
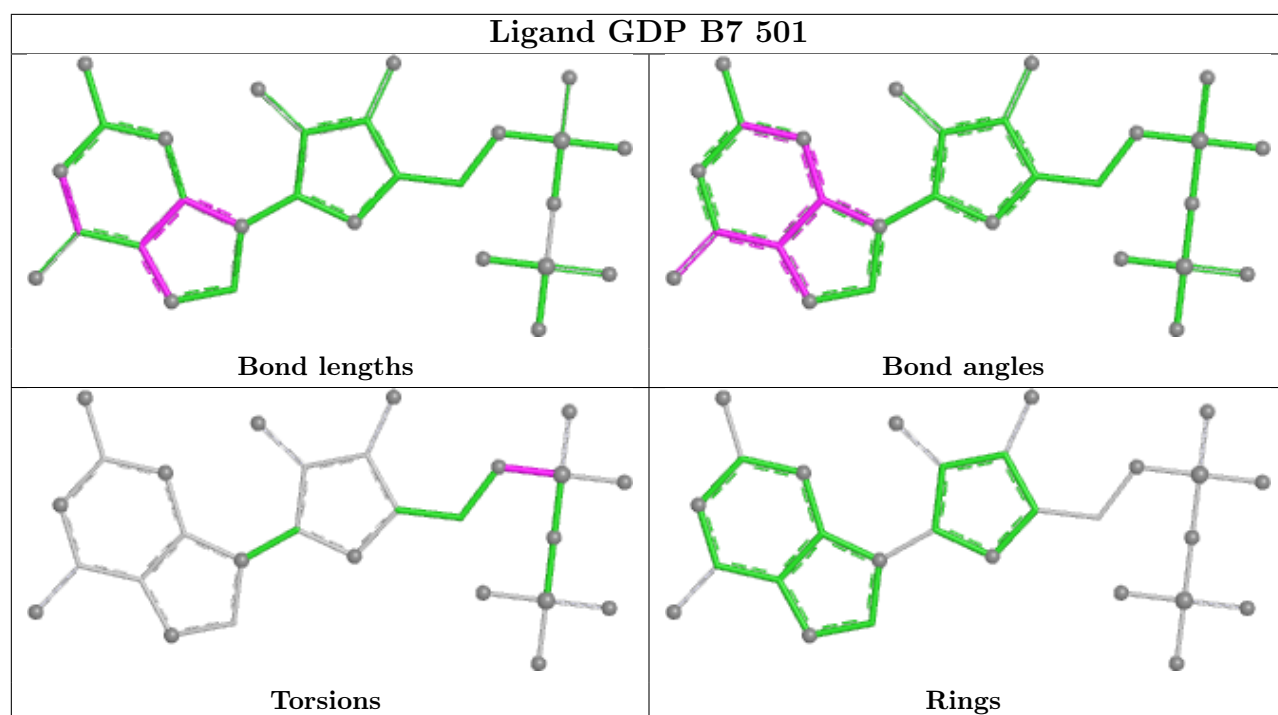


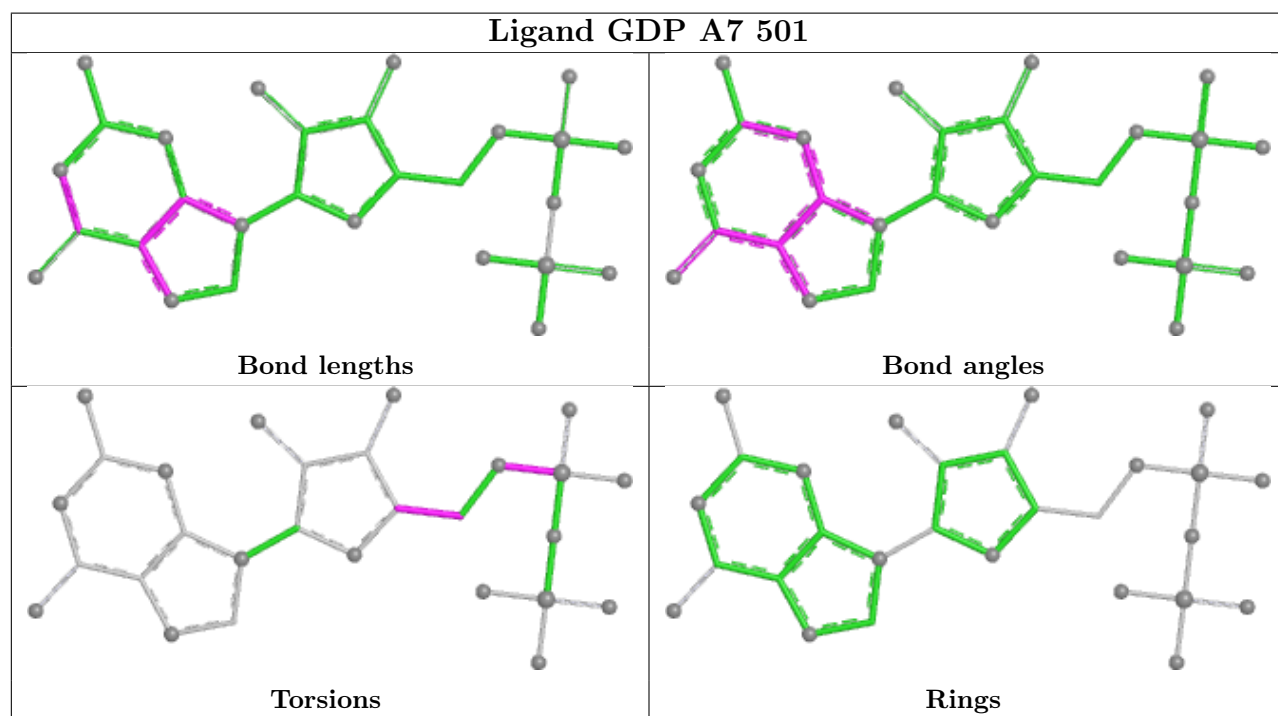
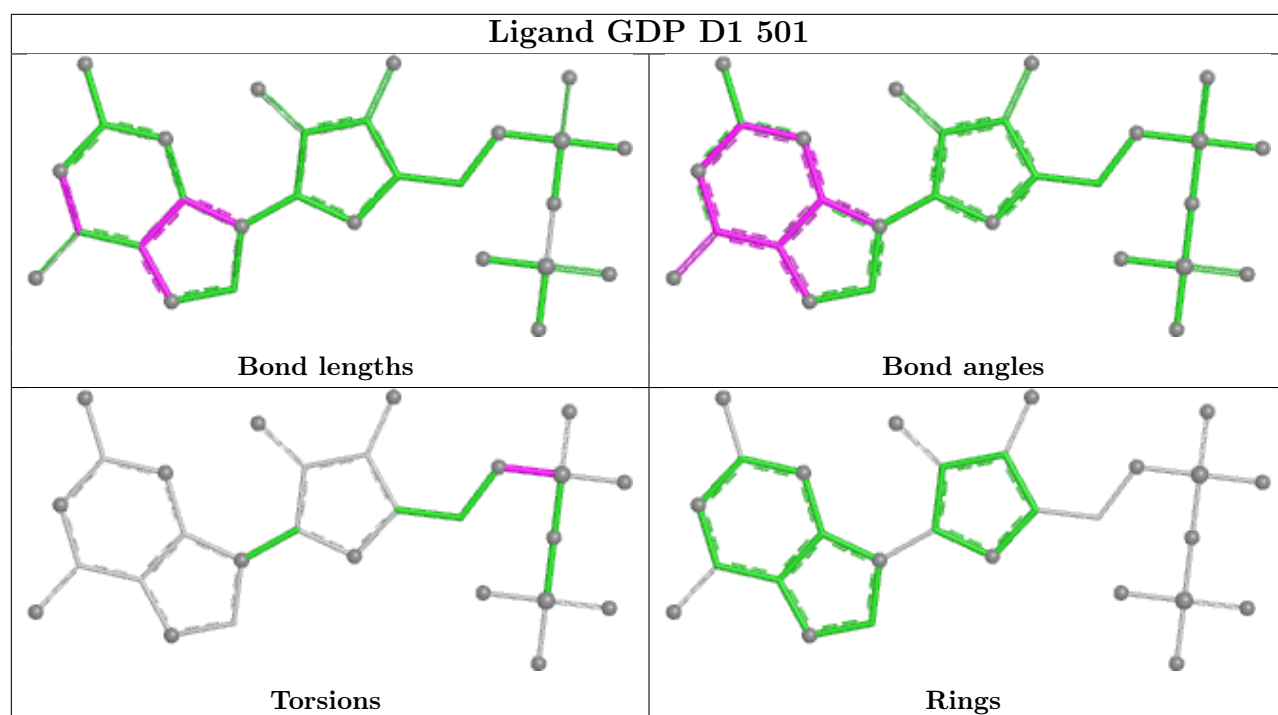
Ligand GTP B8 501

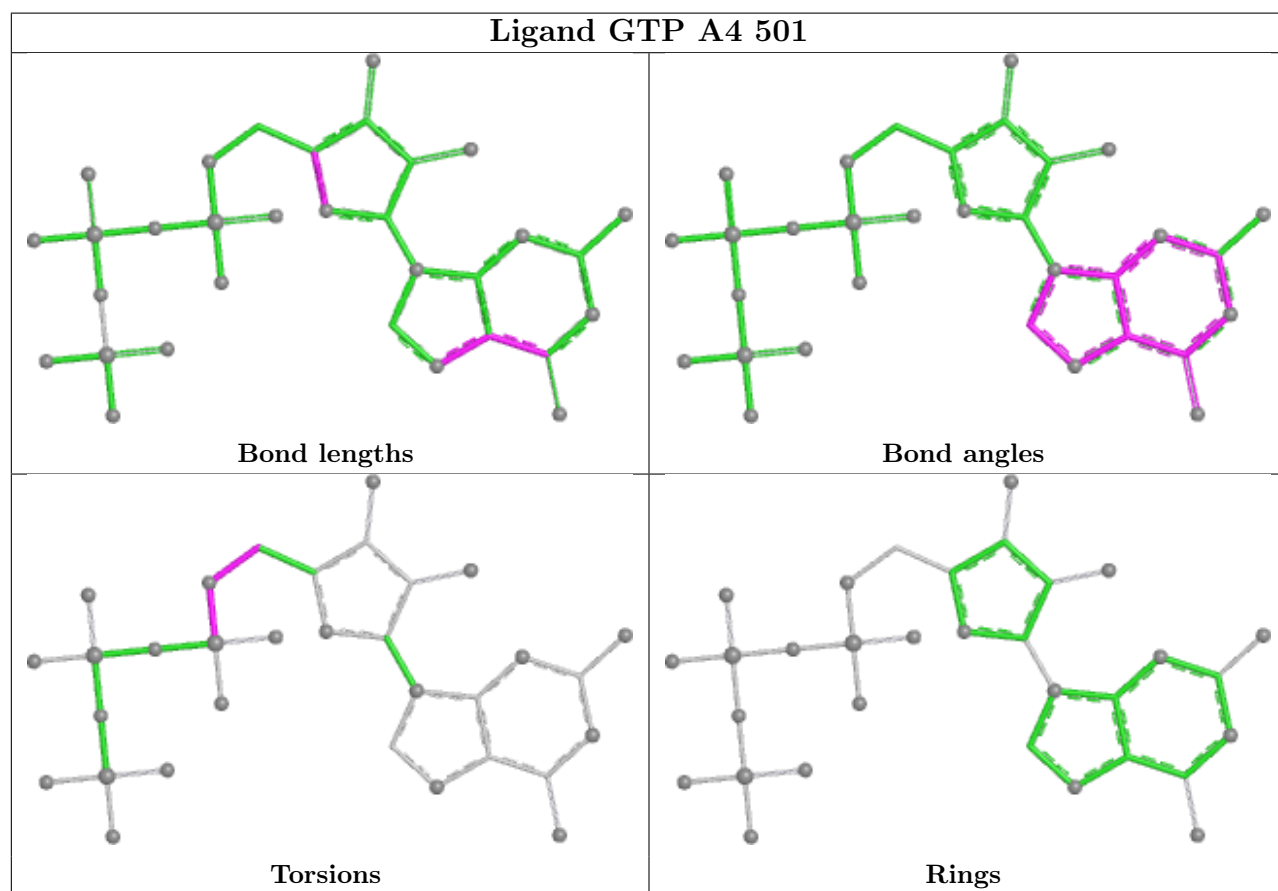
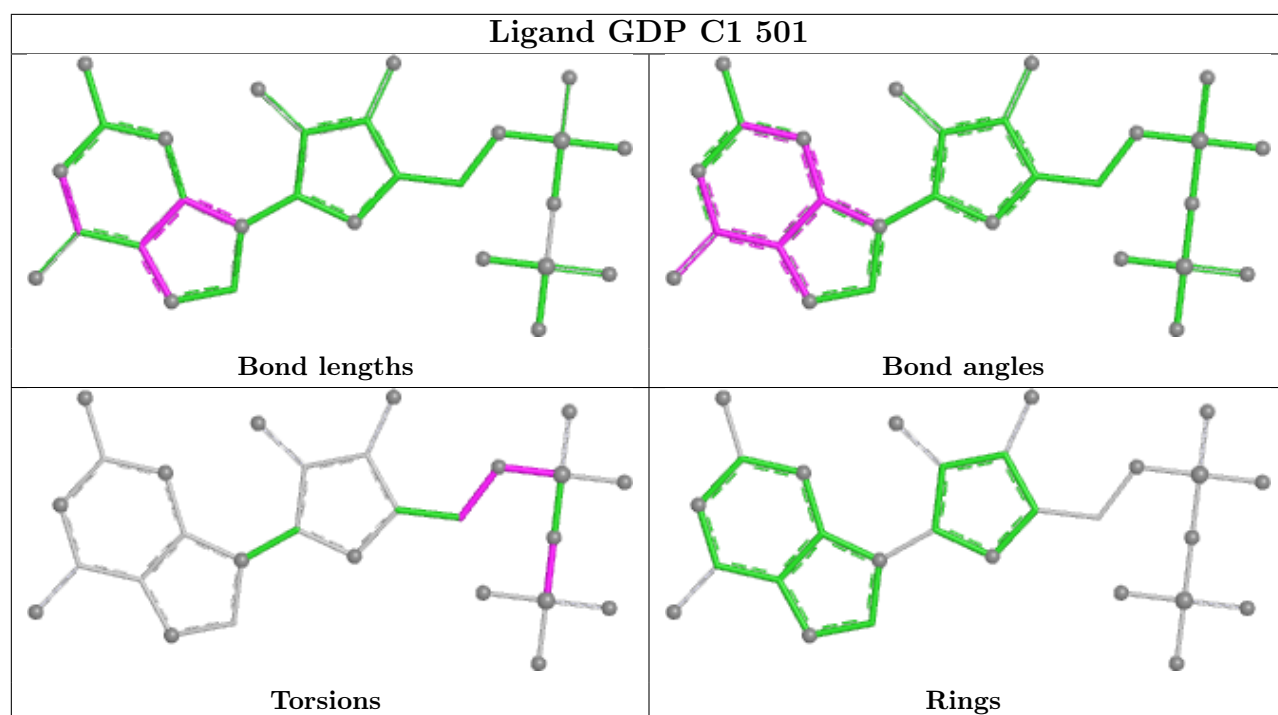


Ligand GTP E6 501

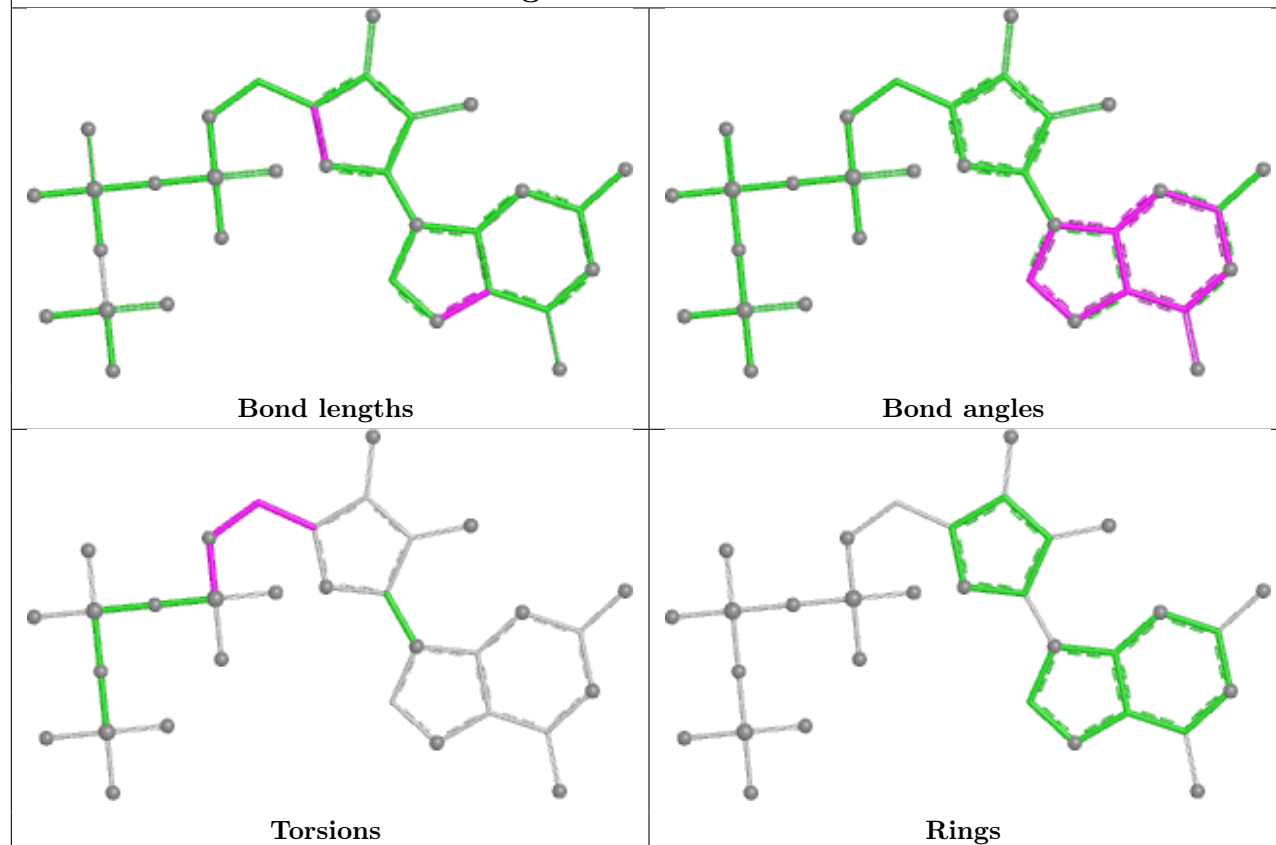




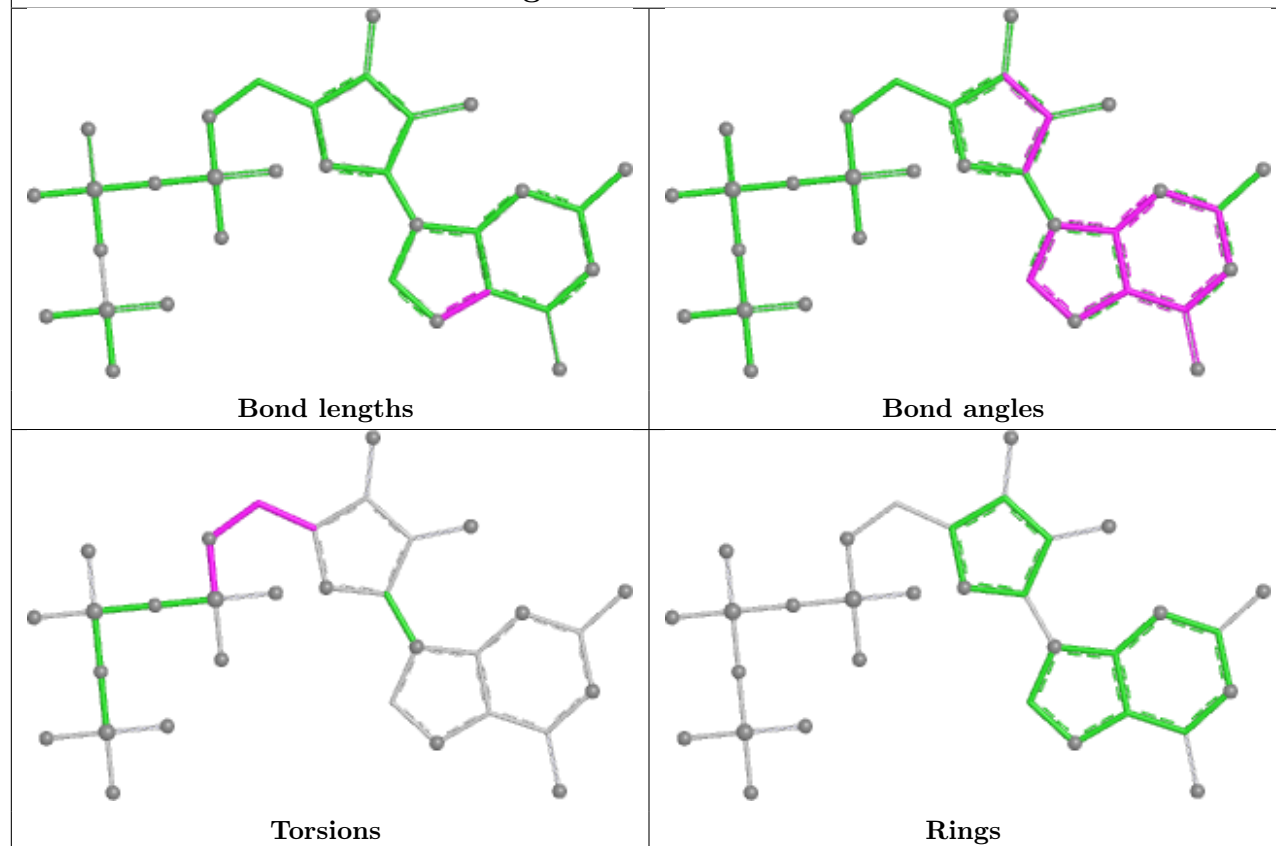


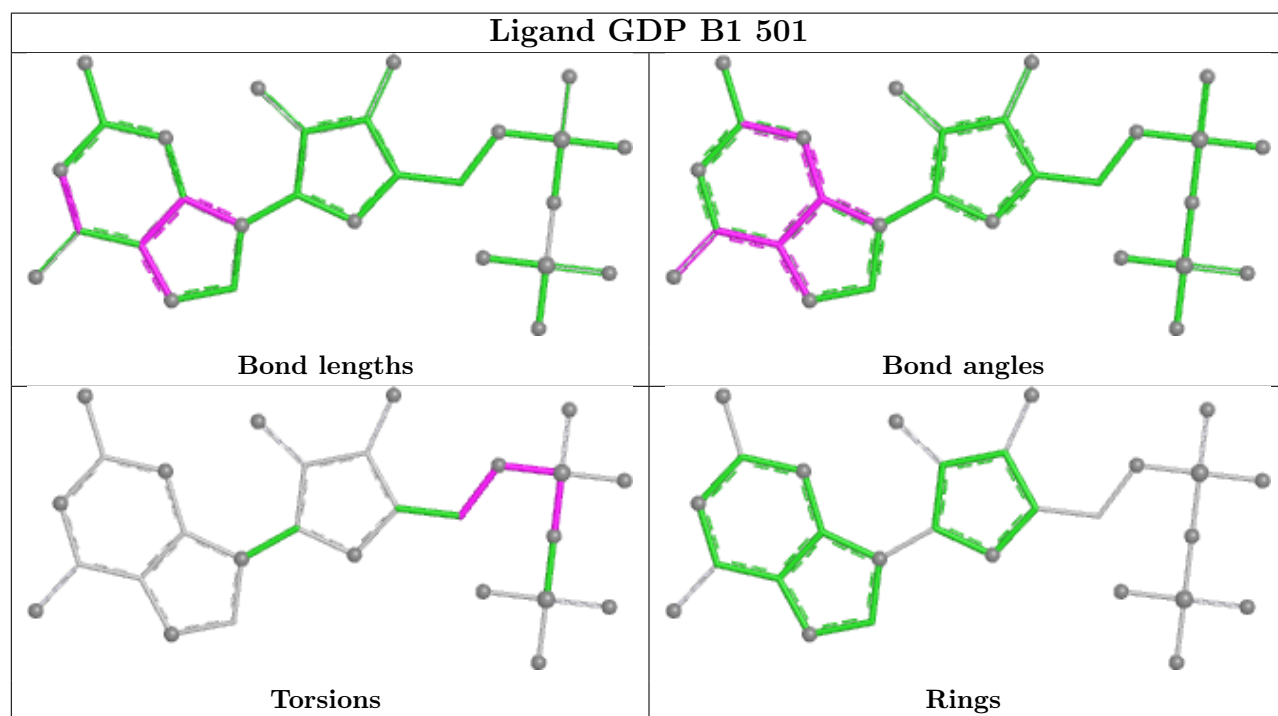
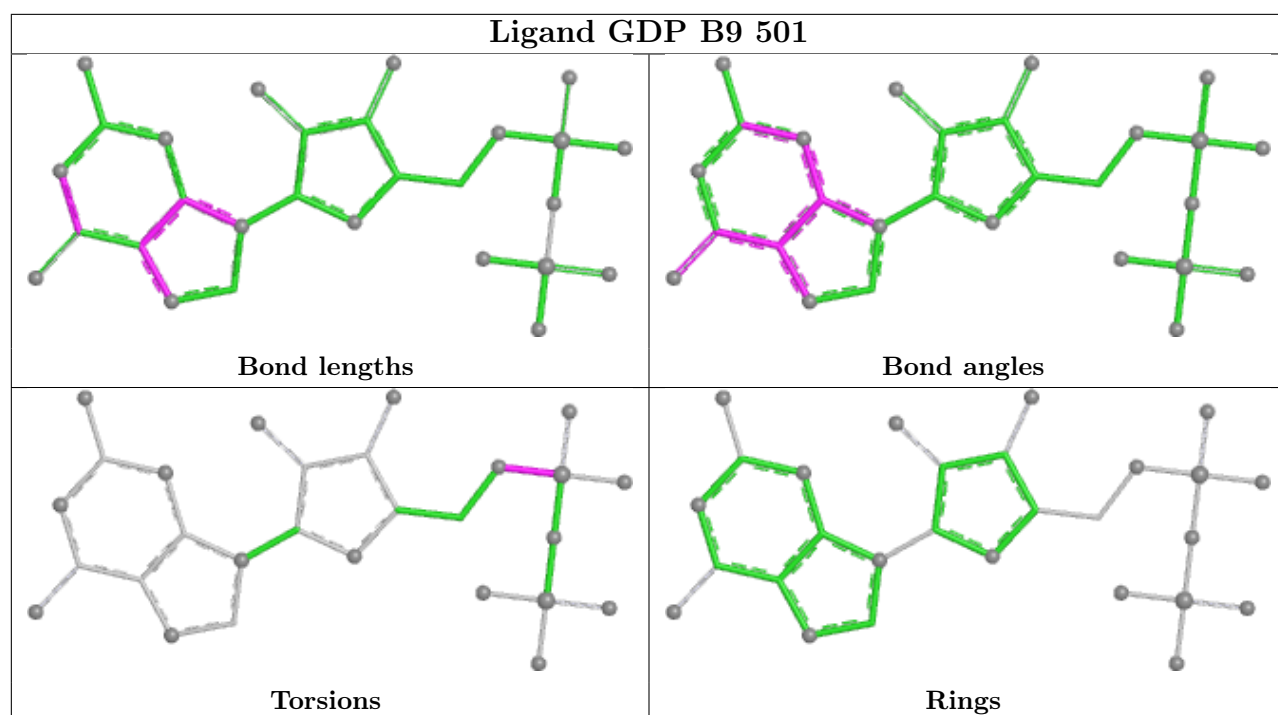


Ligand GTP B6 501

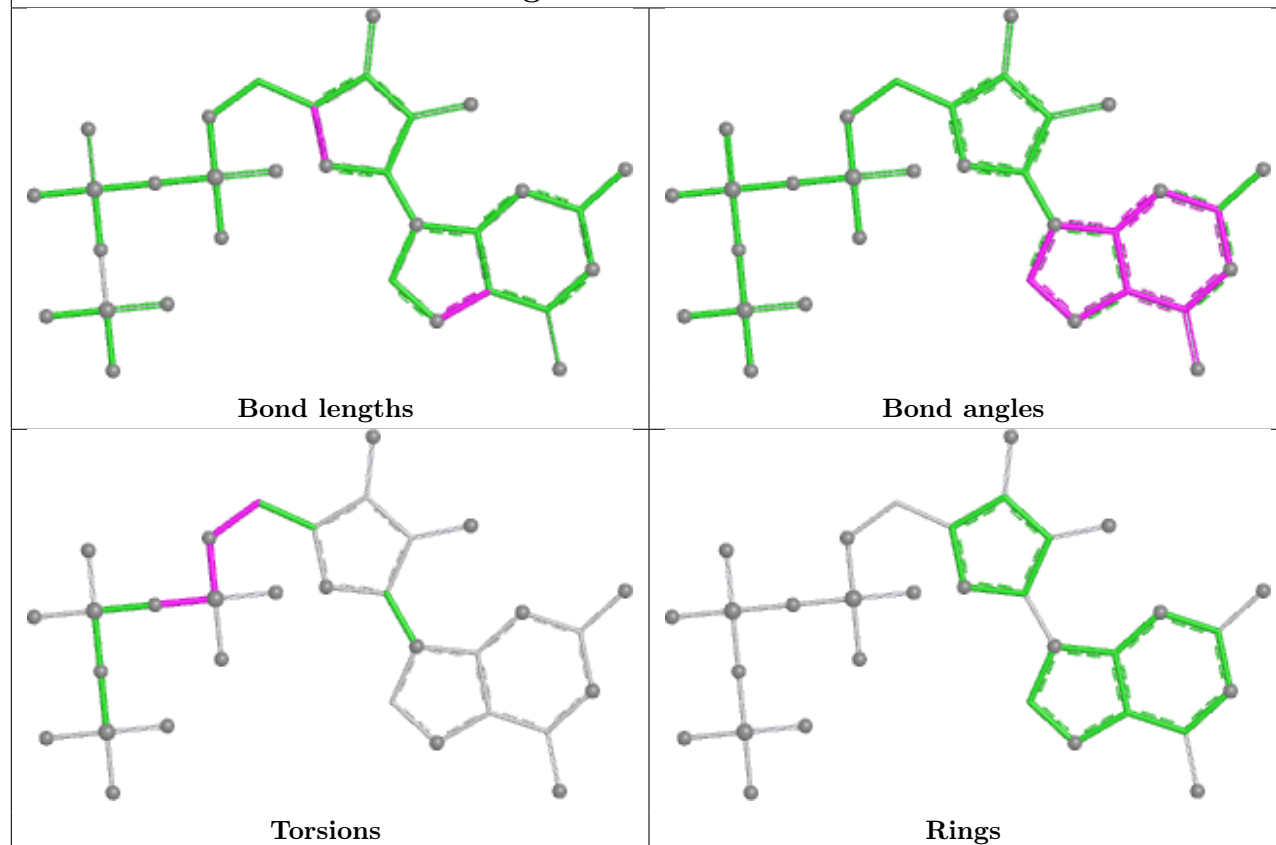


Ligand GTP E4 501

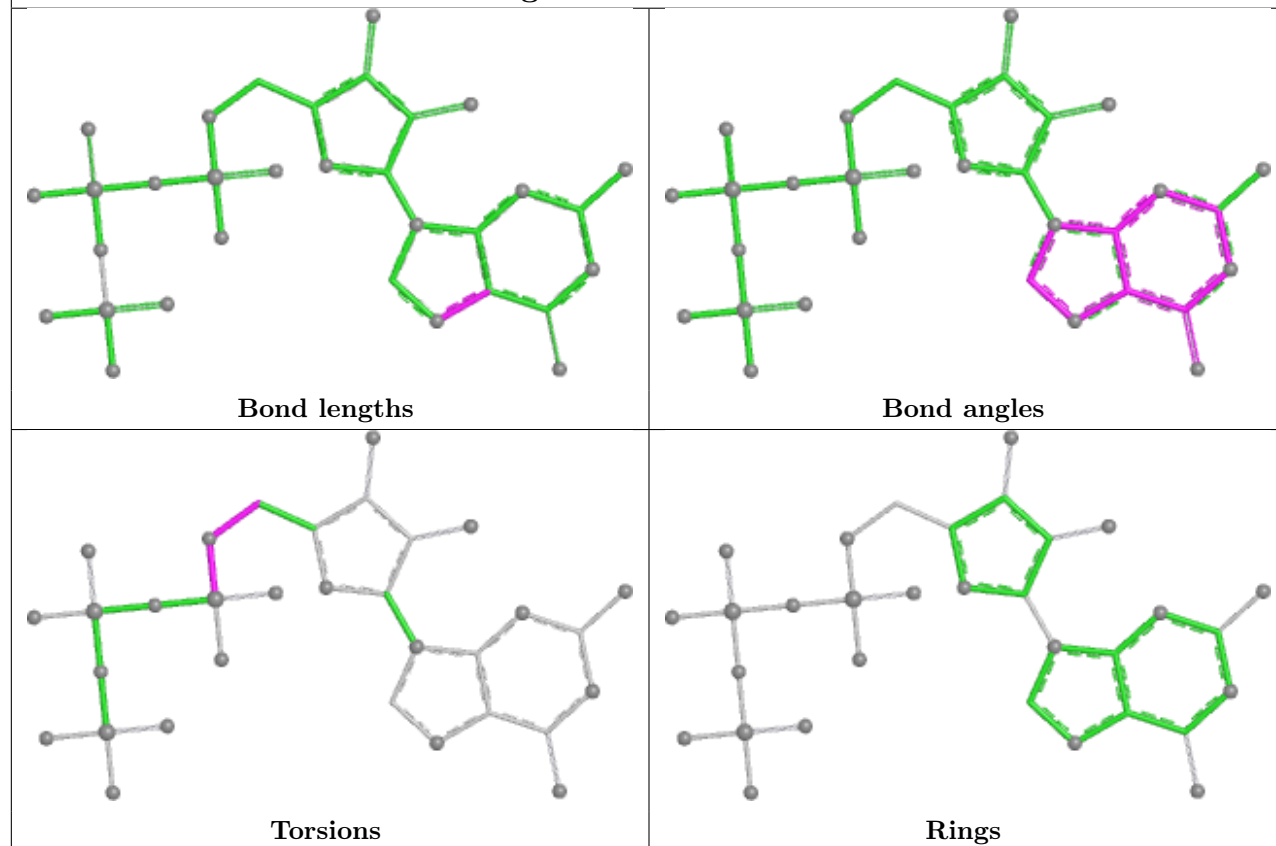


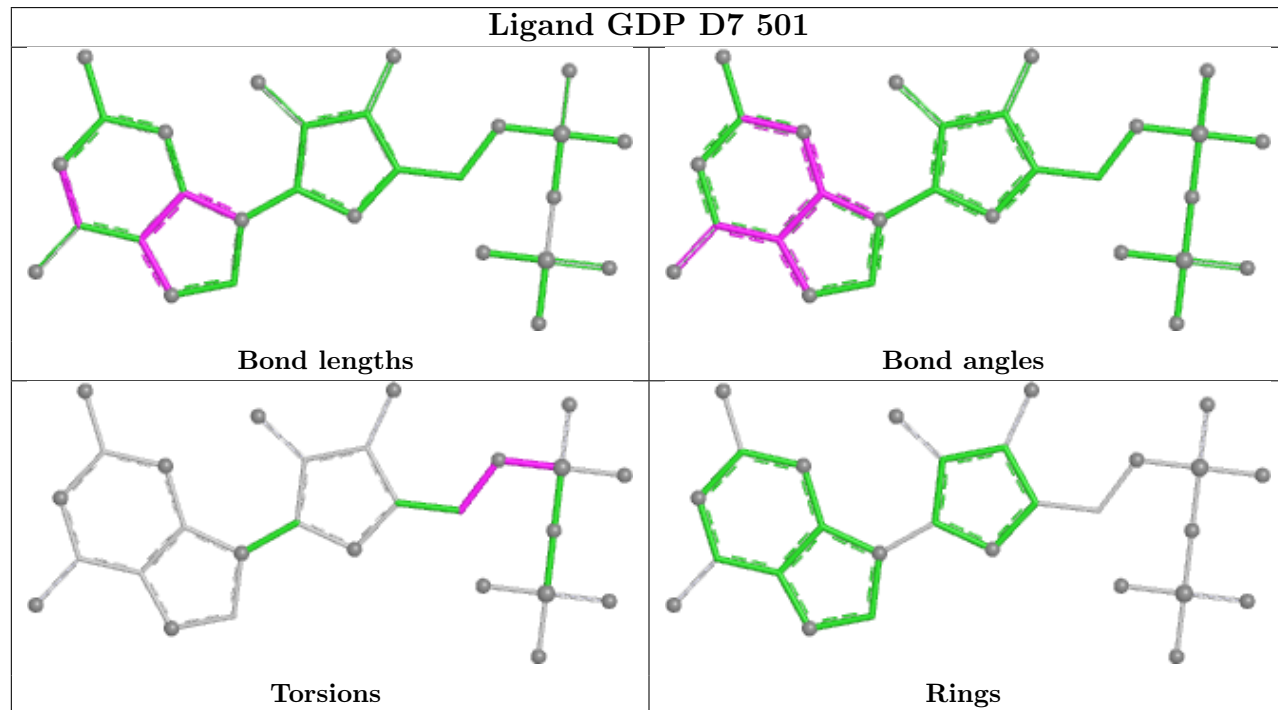
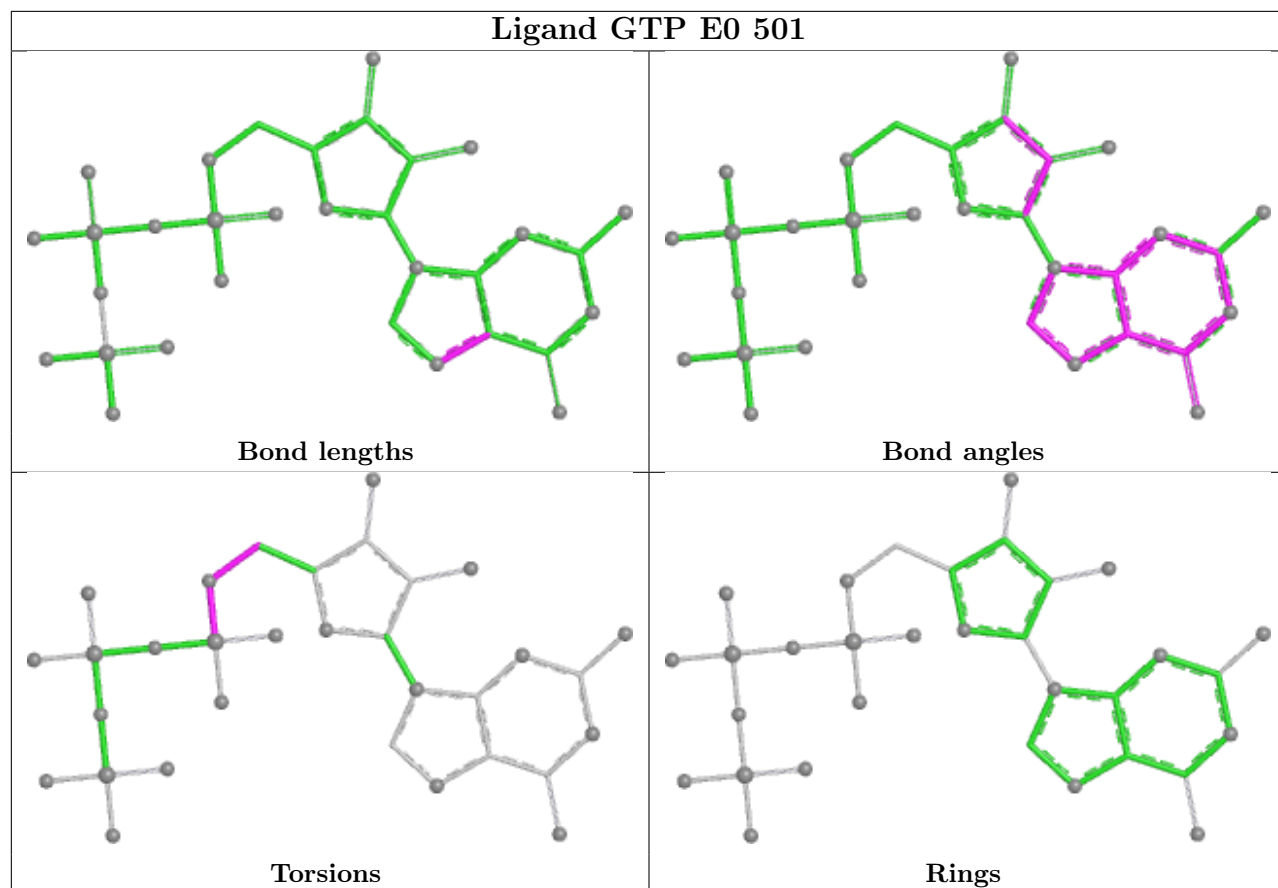


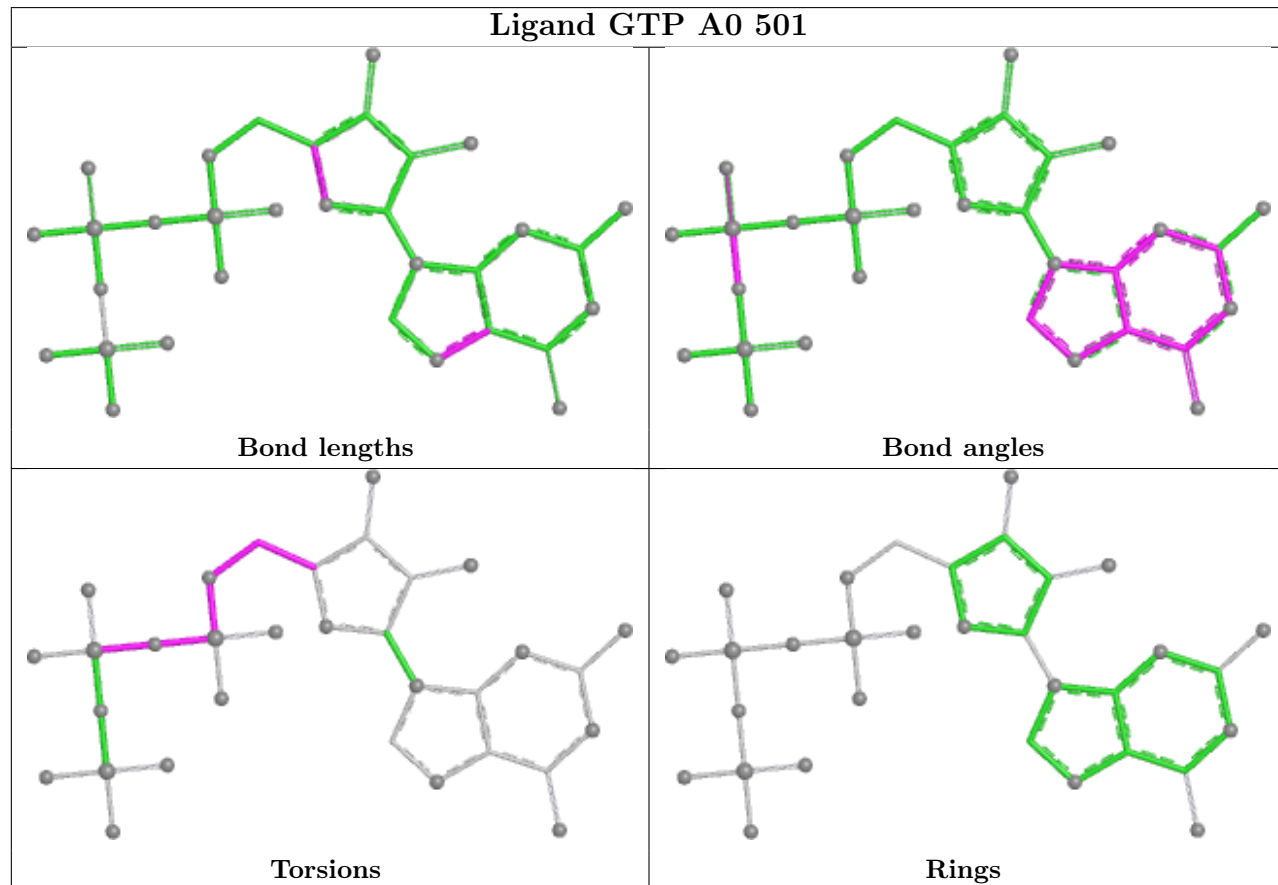
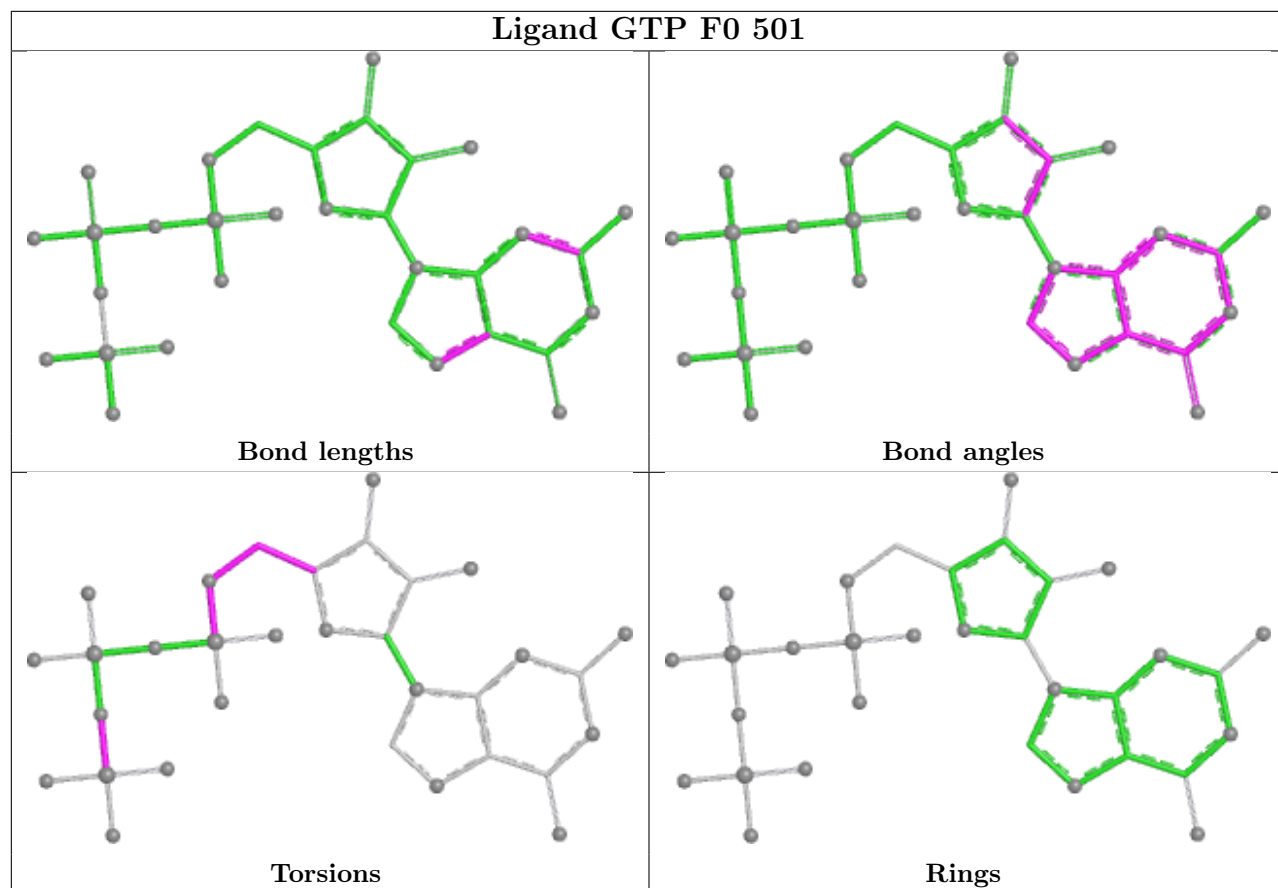
Ligand GTP E2 501



Ligand GTP A8 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.

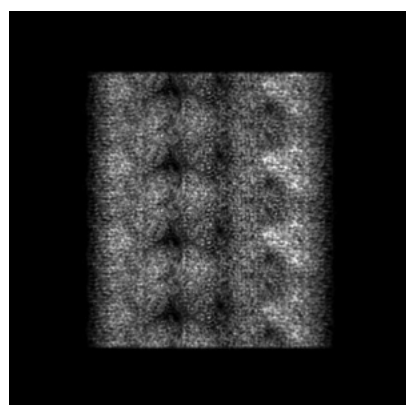
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23869. These allow visual inspection of the internal detail of the map and identification of artifacts.

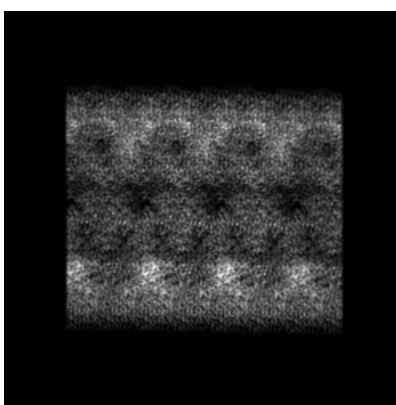
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

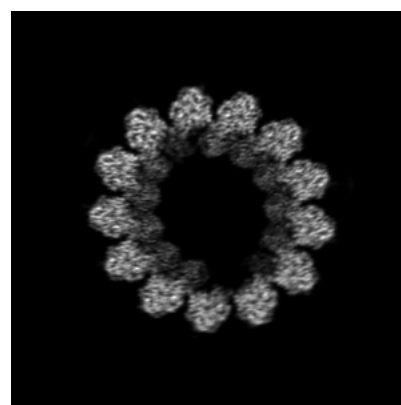
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

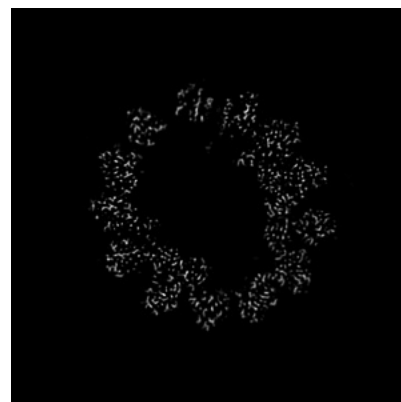
6.2.1 Primary map



X Index: 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](#)

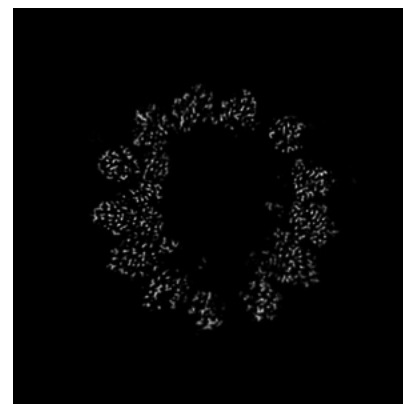
6.3.1 Primary map



X Index: 121



Y Index: 287

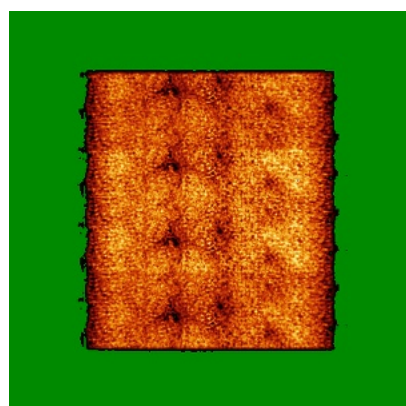


Z Index: 146

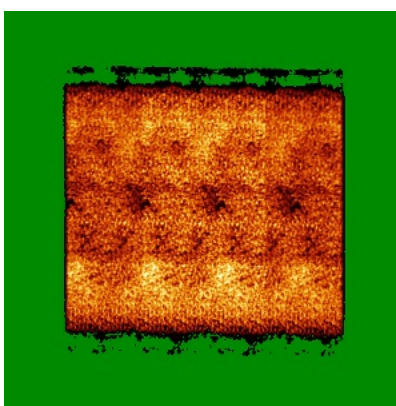
The images above show the largest variance slices of the map in three orthogonal directions.

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

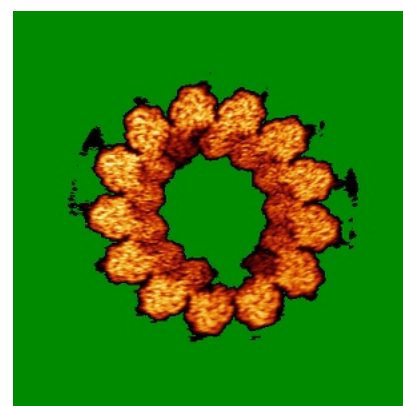
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

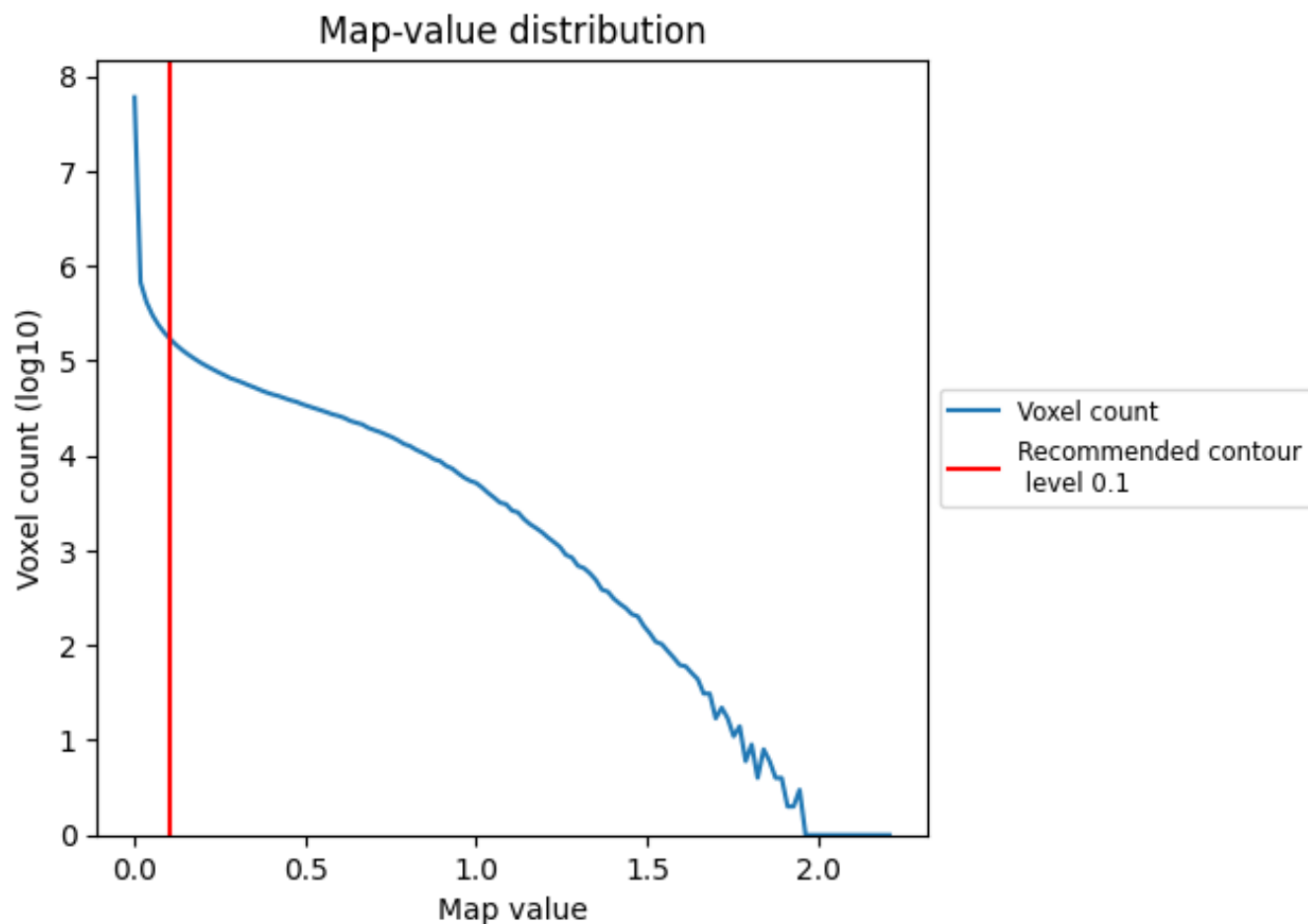
6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

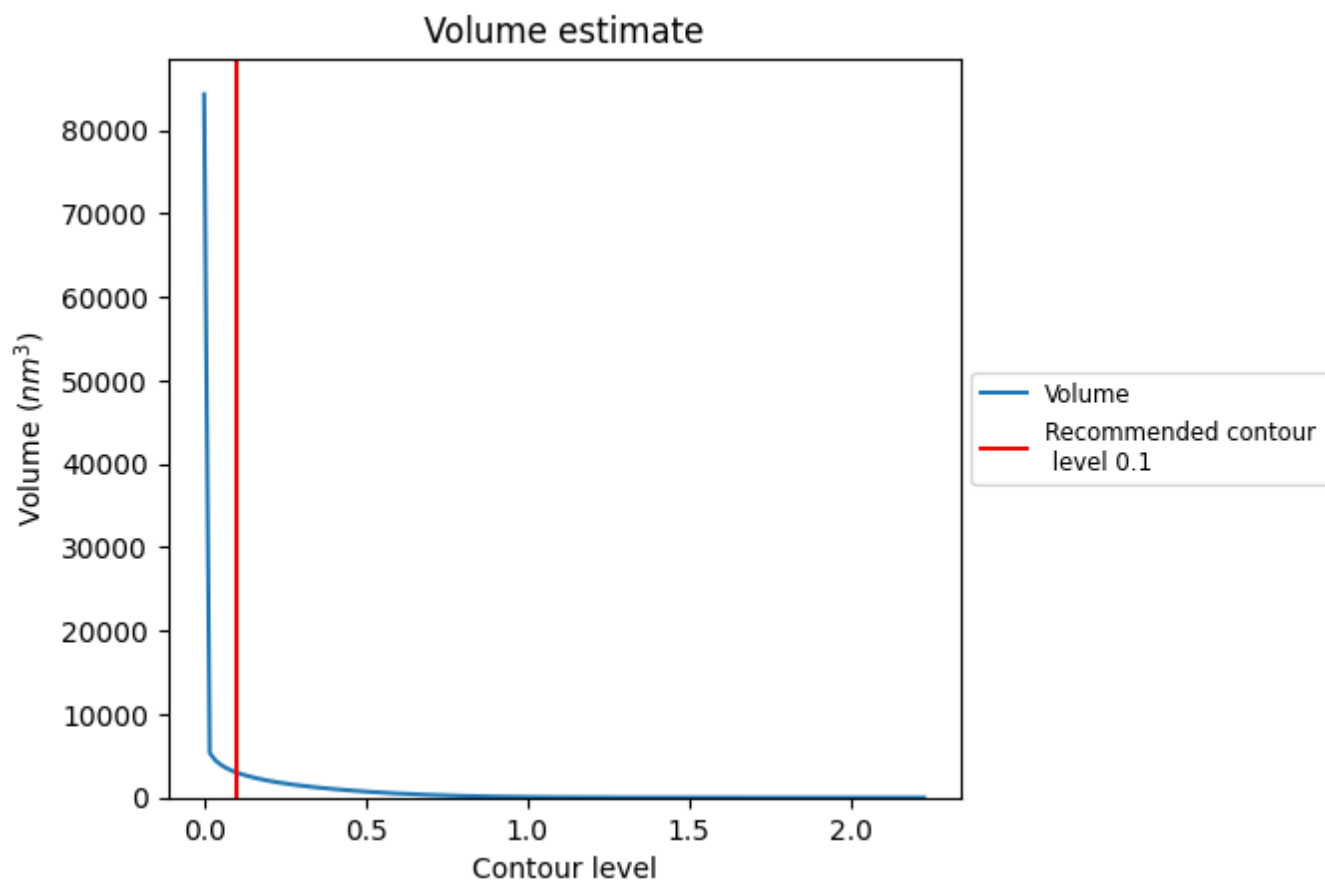
This section contains the results of statistical analysis of the map.

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.

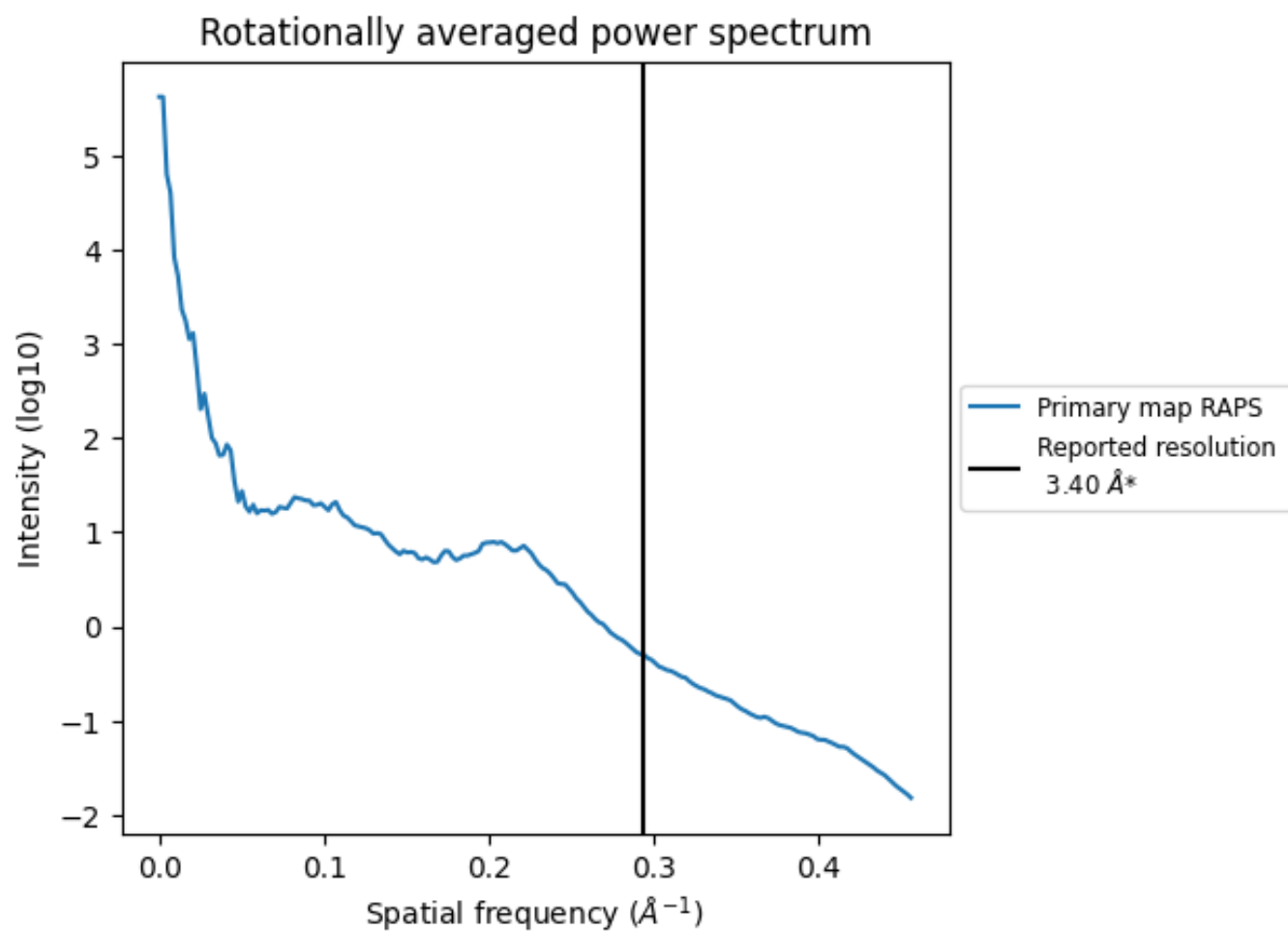
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3014 nm³; this corresponds to an approximate mass of 2723 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

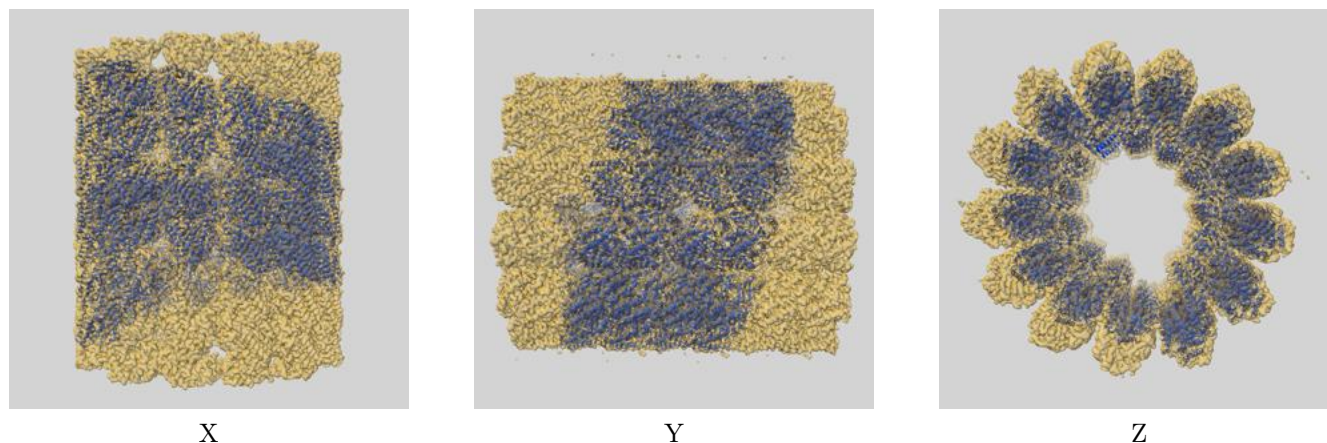
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

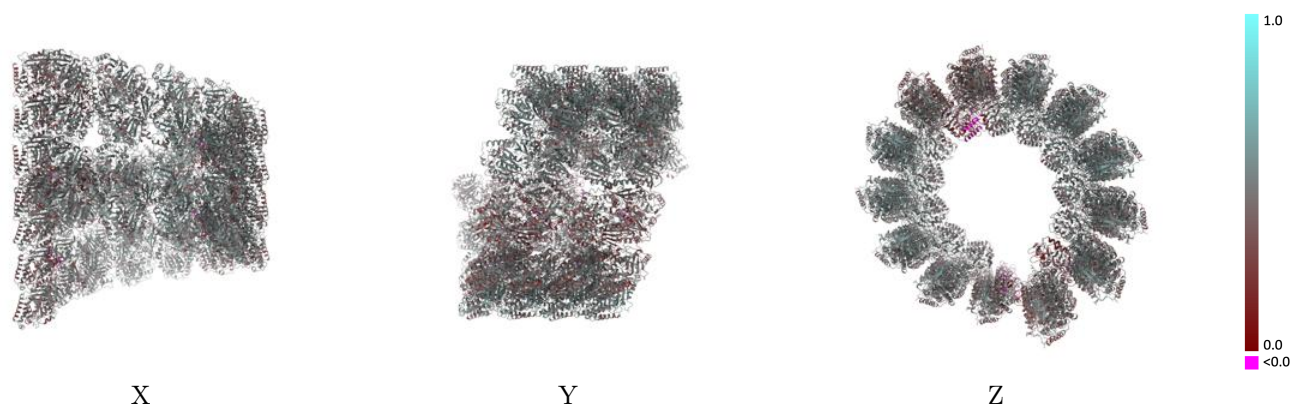
This section contains information regarding the fit between EMDB map EMD-23869 and PDB model 7MIZ. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



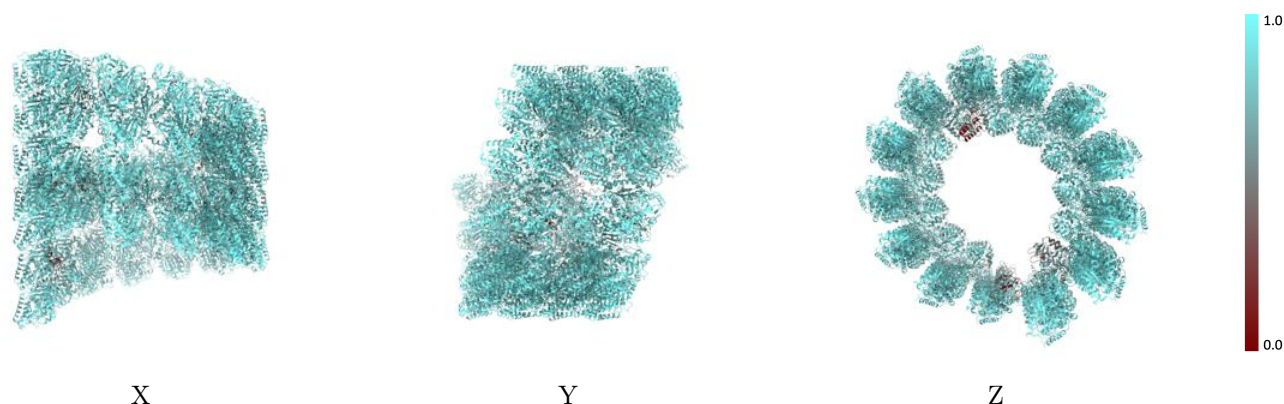
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



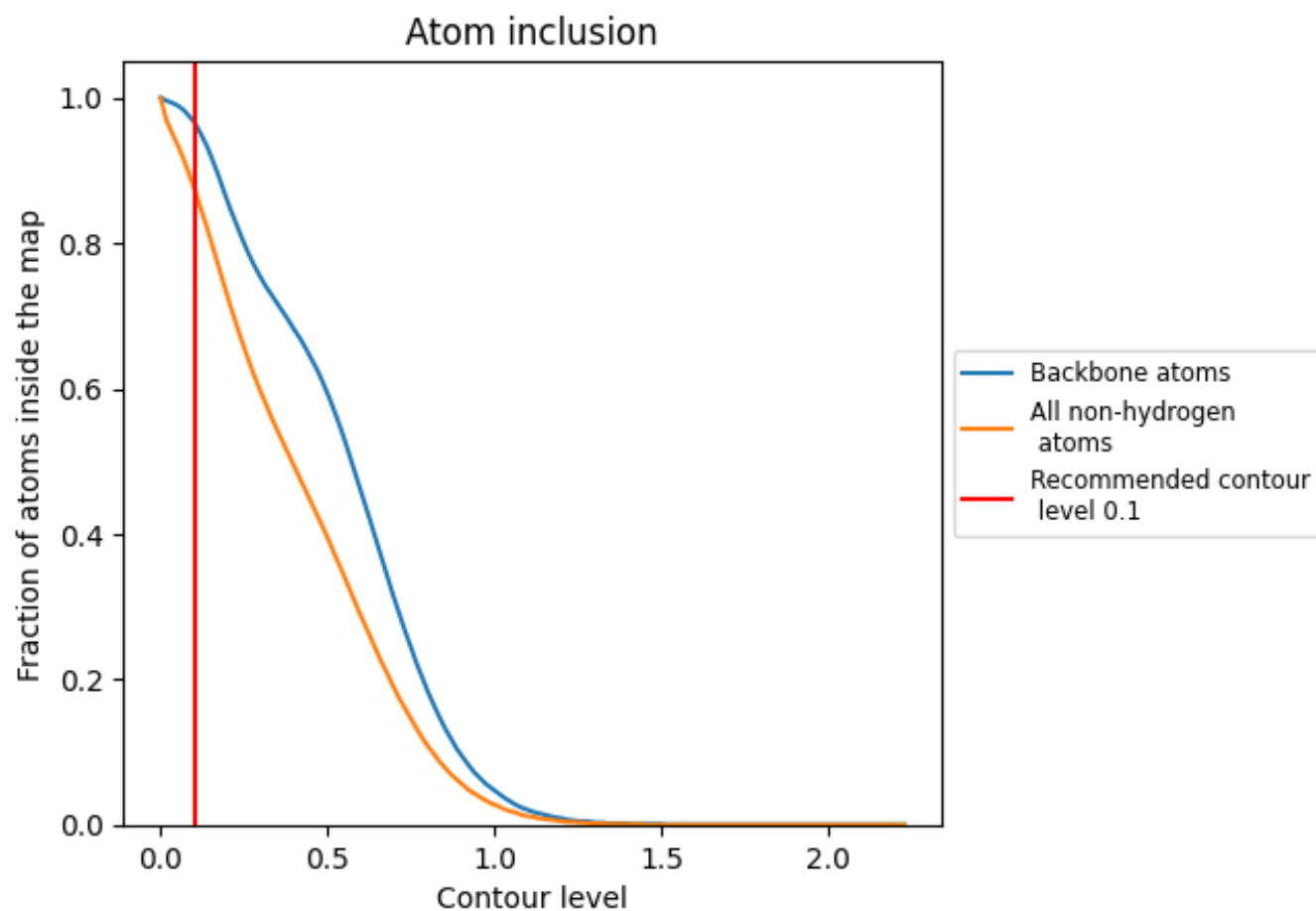
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 88% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.4600
0	 0.8650	 0.4810
1	 0.8350	 0.4680
10	 0.9060	 0.4870
11	 0.9060	 0.4880
12	 0.8820	 0.4790
13	 0.8760	 0.4810
14	 0.8710	 0.4930
15	 0.8530	 0.4860
16	 0.8650	 0.4610
17	 0.8820	 0.4620
18	 0.9350	 0.4860
19	 0.9410	 0.4850
2	 0.8350	 0.4640
20	 0.6940	 0.4110
21	 0.7350	 0.4290
22	 0.5900	 0.3640
23	 0.6150	 0.3760
3	 0.8410	 0.4650
4	 0.8240	 0.4800
5	 0.8410	 0.4860
6	 0.8590	 0.4920
7	 0.8590	 0.4880
8	 0.8240	 0.4230
9	 0.8290	 0.4280
A0	 0.7810	 0.3990
A1	 0.8960	 0.4390
A2	 0.7860	 0.3920
A3	 0.8560	 0.4180
A4	 0.8830	 0.4680
A5	 0.9020	 0.4770
A6	 0.8920	 0.4680
A7	 0.8820	 0.4700
A8	 0.9040	 0.4900
A9	 0.8970	 0.4830



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
B0	 0.8950	 0.4860
B1	 0.8860	 0.4820
B2	 0.9100	 0.5040
B3	 0.8940	 0.5030
B4	 0.9090	 0.5030
B5	 0.8870	 0.4990
B6	 0.9100	 0.4990
B7	 0.8980	 0.5050
B8	 0.9170	 0.5000
B9	 0.9050	 0.4990
C0	 0.8770	 0.4160
C1	 0.8490	 0.4190
C2	 0.8820	 0.4190
C3	 0.8550	 0.4150
C4	 0.8620	 0.4020
C5	 0.8630	 0.4040
C6	 0.8560	 0.4050
C7	 0.8680	 0.4040
C8	 0.8970	 0.4740
C9	 0.9070	 0.4830
D0	 0.8860	 0.4810
D1	 0.9190	 0.4890
D2	 0.8970	 0.4870
D3	 0.9200	 0.5010
D4	 0.8800	 0.4960
D5	 0.9220	 0.5020
D6	 0.9080	 0.4910
D7	 0.9230	 0.4990
D8	 0.8990	 0.5050
D9	 0.9200	 0.5020
E0	 0.8960	 0.4680
E1	 0.9110	 0.4820
E2	 0.9100	 0.4810
E3	 0.9150	 0.4910
E4	 0.9000	 0.4530
E5	 0.9080	 0.4680
E6	 0.9180	 0.4730
E7	 0.9060	 0.4790
E8	 0.8710	 0.4230
E9	 0.8510	 0.4190
F0	 0.8990	 0.4420
F1	 0.8530	 0.4330

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
a	 0.7830	 0.4260
b	 0.7790	 0.4120
c	 0.8410	 0.4650
d	 0.8490	 0.4550
e	 0.8780	 0.4830
f	 0.8900	 0.4800
g	 0.8840	 0.4870
h	 0.8810	 0.4840
i	 0.8820	 0.4470
j	 0.8820	 0.4450
k	 0.6920	 0.2870
l	 0.6830	 0.2870
m	 0.6830	 0.3280
n	 0.6800	 0.3290
o	 0.8890	 0.4830
p	 0.8850	 0.4830
q	 0.8950	 0.4800
r	 0.8940	 0.4950
s	 0.8990	 0.4730
t	 0.8970	 0.4920
u	 0.8750	 0.4490
v	 0.8770	 0.4640
w	 0.5560	 0.2960
x	 0.6150	 0.3200