



wwPDB EM Validation Summary Report ⓘ

Aug 31, 2024 – 08:20 PM EDT

PDB ID : 8SNB
EMDB ID : EMD-40619
Title : atomic model of sea urchin sperm doublet microtubule (48-nm periodicity)
Authors : Zeng, J.; Zhang, R.
Deposited on : 2023-04-26
Resolution : 3.30 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

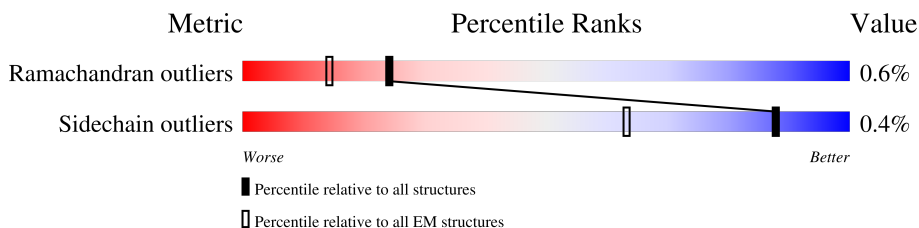
EMDB validation analysis : 0.0.1.dev112
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1A	309	
1	1B	309	
2	1E	448	
2	1F	448	
2	1G	448	
2	1H	448	
3	1K	696	
3	1L	696	
3	1M	696	

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Mol	Chain	Length	Quality of chain
3	1v	696	
3	1w	696	
3	1x	696	
3	1y	696	
3	1z	696	
3	2a	696	
4	1P	204	
4	1Q	204	
5	1T	429	
5	1U	429	
5	1V	429	
5	1W	429	
6	1Y	139	
7	1a	251	
7	1b	251	
7	5E	251	
7	5F	251	
7	5G	251	
7	5H	251	
7	5I	251	
7	5J	251	
7	5K	251	
7	5L	251	
7	5M	251	
7	5N	251	

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Mol	Chain	Length	Quality of chain
7	5O	251	6% 6% 94%
8	1d	359	28% 28% 72%
9	1f	206	12% 17% 83%
9	1g	206	18% 25% 75%
10	1i	188	14% 18% 82%
10	1j	188	15% 15% 84%
10	9M	188	39% 45% 55%
10	9N	188	35% 44% 55%
10	9O	188	22% 20% 78%
11	1l	176	22% 22% 78%
11	1m	176	22% 22% 78%
12	1o	142	15% 19% 80%
12	1p	142	10% 21% 79%
12	1q	142	22% 32% 68%
12	1r	142	11% 18% 81%
13	2A	258	74% 95%
13	2B	258	74% 93%
13	2C	258	72% 95%
13	2D	258	24% 29% 69%
14	2G	235	69% 96%
15	2J	141	73% 76% 24%
15	2K	141	70% 74% 24%
15	2L	141	59% 74% 24%
16	2O	120	81% 99%
17	2R	499	17% 24% 76%

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Mol	Chain	Length	Quality of chain
17	2S	499	62% 75% 25%
18	2V	292	60% 95%
18	2W	292	55% 96%
19	3A	195	28% 95%
19	3B	195	31% 94%
19	3C	195	54% 92% 8%
19	3D	195	47% 89% 10%
19	3E	195	31% 95% 5%
19	3F	195	52% 96%
19	3G	195	32% 95% 5%
20	3J	592	58% 80% 16%
20	3K	592	11% 11% 88%
21	3N	560	26% 45% 54%
21	3O	560	32% 48% 50%
22	3R	172	80% 92%
22	3S	172	61% 71% 26%
22	3T	172	79% 94%
23	3W	541	66% 69% 29%
23	3X	541	49% 58% 42%
23	3Y	541	17% 19% 81%
23	3Z	541	26% 31% 68%
24	4A	635	63% 97%
24	4B	635	52% 96%
24	4C	635	57% 97%
25	4F	516	40% 61% 39%

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Mol	Chain	Length	Quality of chain
25	4G	516	25% 39% 60%
26	4J	380	61% 97%
26	4K	380	73% 98%
27	4N	243	49% 60% 38%
27	4O	243	44% 44% 56%
27	4P	243	59% 61% 38%
27	4Q	243	37% 37% 62%
28	4T	231	62% 60% 38%
28	4U	231	62% 61% 38%
28	4V	231	6% 6% 94%
29	4Y	302	56% 98%
30	5A	277	12% 12% 87%
30	5B	277	58% 74% 23%
30	9Y	277	50% 47% 49%
30	9Z	277	36% 35% 64%
31	6A	236	38% 94% 5%
31	6B	236	92% 92% 7%
31	6C	236	64% 94% 6%
31	6D	236	40% 95% 5%
31	6E	236	39% 94% 5%
31	6F	236	41% 95% 5%
32	6I	123	37% 63% 37%
32	6J	123	28% 43% 57%
33	6M	469	49% 83% 17%
33	6N	469	12% 17% 83%

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Mol	Chain	Length	Quality of chain
34	6Q	310	
34	6R	310	
35	6U	379	
35	6V	379	
35	6W	379	
35	6X	379	
36	7A	744	
36	7B	744	
36	7C	744	
36	7D	744	
37	7G	645	
37	7H	645	
37	7I	645	
38	7M	322	
38	7N	322	
39	7Q	185	
39	7R	185	
40	7U	200	
40	7V	200	
41	7Y	204	
41	7Z	204	
42	8A	268	
43	8D	462	
43	8E	462	
43	8F	462	

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Mol	Chain	Length	Quality of chain
43	8G	462	44% 85% 14%
44	8J	430	36% 93% 6%
44	8K	430	39% 75% 25%
44	8L	430	43% 93% 6%
44	8M	430	13% 30% 70%
44	8N	430	96%
45	8Q	402	5% 95%
45	8R	402	45% 98%
45	8S	402	33% 74% 24%
45	8T	402	37% 99%
45	8U	402	10% 30% 70%
46	8X	119	87% 87% 13%
46	8Y	119	85% 86% 13%
46	8Z	119	87% 83% 13%
47	9A	220	65% 90% 6%
48	9D	171	47% 56% 44%
49	9G	150	57% 97%
50	9J	179	54% 56% 44%
51	9R	153	44% 93% 7%
52	9T	83	64% 90% 10%
53	9V	294	8% 6% 92%
53	9W	294	24% 24% 76%
54	AA	451	35% 96%
54	AB	451	36% 97%
54	AE	451	33% 96%

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Mol	Chain	Length	Quality of chain
54	AG	451	40% 96%
54	AI	451	26% 97%
54	AK	451	56% 96%
54	AM	451	61% 97%
54	BA	451	42% 96%
54	BB	451	49% 96%
54	BE	451	45% 96%
54	BG	451	57% 96%
54	BI	451	48% 96%
54	BK	451	68% 96%
54	BM	451	53% 96%
54	CA	451	34% 96%
54	CB	451	37% 96%
54	CE	451	33% 96%
54	CG	451	61% 96%
54	CI	451	39% 96%
54	CK	451	79% 96%
54	CM	451	54% 96%
54	DA	451	51% 97%
54	DB	451	59% 96%
54	DE	451	44% 96%
54	DG	451	63% 96%
54	DI	451	56% 96%
54	DK	451	93% 96%
54	DM	451	56% 96%

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Mol	Chain	Length	Quality of chain
54	EA	451	51% 87% 10%
54	EC	451	57% 96%
54	EE	451	56% 96%
54	EG	451	62% 96%
54	EI	451	63% 96%
54	EK	451	53% 96%
54	FA	451	38% 86% 10%
54	FB	451	42% 96%
54	FE	451	42% 85% 10%
54	FG	451	43% 96%
54	FI	451	49% 89% 8%
54	FK	451	43% 96%
54	GA	451	42% 96%
54	GB	451	34% 96%
54	GE	451	47% 96%
54	GG	451	39% 96%
54	GI	451	45% 96%
54	GK	451	41% 96%
54	HA	451	43% 96%
54	HB	451	30% 96%
54	HE	451	47% 95%
54	HG	451	34% 95%
54	HI	451	38% 97%
54	HK	451	25% 96%
54	IA	451	51% 96%

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Mol	Chain	Length	Quality of chain
54	IB	451	35% 96%
54	IE	451	70% 97%
54	IG	451	40% 96%
54	II	451	45% 96%
54	IK	451	37% 96%
54	IM	451	90% 96%
54	JA	451	39% 95%
54	JB	451	37% 96%
54	JE	451	42% 96%
54	JG	451	52% 96%
54	JI	451	45% 96%
54	JK	451	45% 97%
54	KA	451	34% 96%
54	KB	451	32% 95%
54	KE	451	40% 96%
54	KG	451	34% 96%
54	KI	451	47% 96%
54	KK	451	32% 97%
54	LA	451	33% 96%
54	LB	451	33% 96%
54	LE	451	41% 96%
54	LG	451	37% 96%
54	LI	451	32% 96%
54	LK	451	34% 97%
54	MA	451	33% 96%

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Mol	Chain	Length	Quality of chain
54	MB	451	37% 96%
54	ME	451	37% 96%
54	MG	451	37% 97%
54	MI	451	21% 96%
54	MK	451	79% 96%
54	ML	451	38% 97%
54	NA	451	46% 96%
54	NB	451	55% 96%
54	NE	451	50% 97%
54	NG	451	74% 96%
54	NI	451	57% 96%
54	NL	451	52% 96%
54	OA	451	20% 96%
54	OB	451	31% 95%
54	OE	451	19% 96%
54	OG	451	27% 96%
54	OI	451	20% 96%
54	OK	451	83% 96%
54	OL	451	22% 97%
54	PA	451	20% 96%
54	PB	451	37% 96%
54	PE	451	19% 96%
54	PG	451	33% 96%
54	PI	451	25% 96%
54	PK	451	67% 96%

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Mol	Chain	Length	Quality of chain
54	PL	451	35% 97%
54	QA	451	20% 96%
54	QB	451	36% 96%
54	QE	451	24% 96%
54	QG	451	29% 96%
54	QI	451	17% 96%
54	QK	451	36% 95%
54	QL	451	54% 96%
54	RA	451	22% 96%
54	RB	451	31% 95%
54	RE	451	23% 95%
54	RG	451	27% 96%
54	RI	451	22% 96%
54	RK	451	28% 96%
54	RL	451	74% 96%
54	SA	451	22% 96%
54	SB	451	28% 96%
54	SE	451	16% 96%
54	SG	451	22% 96%
54	SI	451	17% 96%
54	SK	451	19% 96%
54	TA	451	23% 96%
54	TB	451	23% 96%
54	TE	451	23% 96%
54	TG	451	26% 96%

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Mol	Chain	Length	Quality of chain
54	TI	451	20% 96%
54	TK	451	16% 96%
54	UA	451	50% 96%
54	UB	451	47% 95%
54	UE	451	57% 96%
54	UG	451	59% 96%
54	UI	451	54% 96%
54	UK	451	38% 96%
54	VA	451	51% 96%
54	VB	451	41% 97%
54	VE	451	51% 96%
54	VG	451	45% 96%
54	VI	451	54% 96%
54	VK	451	47% 96%
54	WA	451	44% 96%
54	WB	451	34% 96%
54	WE	451	52% 96%
54	WG	451	39% 96%
54	WI	451	39% 96%
54	WK	451	36% 95%
55	AC	447	40% 95%
55	AD	447	32% 96%
55	AF	447	35% 95%
55	AH	447	30% 95%
55	AJ	447	26% 95%

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Mol	Chain	Length	Quality of chain
55	AL	447	31% 95%
55	BC	447	41% 95%
55	BD	447	42% 95%
55	BF	447	55% 95%
55	BH	447	44% 96%
55	BJ	447	47% 96%
55	BL	447	46% 95%
55	CC	447	37% 95%
55	CD	447	37% 94%
55	CF	447	45% 96%
55	CH	447	36% 95%
55	CJ	447	46% 95%
55	CL	447	37% 95%
55	DC	447	46% 95%
55	DD	447	52% 95%
55	DF	447	53% 95%
55	DH	447	60% 95%
55	DJ	447	50% 95%
55	DL	447	54% 95%
55	EB	447	50% 95%
55	ED	447	62% 94%
55	EF	447	51% 95%
55	EH	447	67% 95%
55	EJ	447	45% 96%
55	EL	447	86% 95%

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Mol	Chain	Length	Quality of chain
55	EM	447	66% 94%
55	FC	447	36% 95%
55	FD	447	51% 95%
55	FF	447	37% 96%
55	FH	447	66% 96%
55	FJ	447	38% 94%
55	FL	447	73% 94%
55	FM	447	63% 95%
55	GC	447	34% 96%
55	GD	447	59% 96%
55	GF	447	33% 95%
55	GH	447	61% 95%
55	GJ	447	44% 96%
55	GL	447	65% 96%
55	GM	447	70% 96%
55	HC	447	37% 95%
55	HD	447	62% 95%
55	HF	447	35% 95%
55	HH	447	49% 95%
55	HJ	447	33% 95%
55	HL	447	62% 95%
55	HM	447	84% 95%
55	IC	447	43% 96%
55	ID	447	47% 95%
55	IF	447	36% 96%

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Mol	Chain	Length	Quality of chain
55	IH	447	59% 96%
55	IJ	447	40% 95%
55	IL	447	68% 95%
55	JC	447	30% 95%
55	JD	447	53% 95%
55	JF	447	37% 94%
55	JH	447	34% 94%
55	JJ	447	32% 95%
55	JL	447	72% 95%
55	JM	447	51% 95%
55	KC	447	34% 95%
55	KD	447	38% 95%
55	KF	447	34% 96%
55	KH	447	35% 95%
55	KJ	447	43% 95%
55	KL	447	54% 96%
55	KM	447	64% 96%
55	LC	447	38% 95%
55	LD	447	32% 96%
55	LF	447	35% 95%
55	LH	447	29% 96%
55	LJ	447	31% 95%
55	LL	447	33% 95%
55	LM	447	81% 95%
55	MC	447	40% 95%

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Mol	Chain	Length	Quality of chain
55	MD	447	30% 95%
55	MF	447	35% 96%
55	MH	447	29% 95%
55	MJ	447	32% 95%
55	MM	447	36% 95%
55	NC	447	58% 95%
55	ND	447	48% 95%
55	NF	447	48% 95%
55	NH	447	51% 95%
55	NJ	447	70% 94%
55	NK	447	84% 95%
55	NM	447	49% 95%
55	OC	447	30% 95%
55	OD	447	26% 96%
55	OF	447	17% 95%
55	OH	447	19% 95%
55	OJ	447	34% 95%
55	OM	447	26% 95%
55	PC	447	34% 94%
55	PD	447	22% 95%
55	PF	447	22% 95%
55	PH	447	26% 95%
55	PJ	447	42% 95%
55	PM	447	28% 95%
55	QC	447	27% 94%

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Mol	Chain	Length	Quality of chain
55	QD	447	24% 96%
55	QF	447	27% 95%
55	QH	447	27% 95%
55	QJ	447	24% 95%
55	QM	447	17% 95%
55	RC	447	23% 95%
55	RD	447	26% 95%
55	RF	447	21% 95%
55	RH	447	23% 96%
55	RJ	447	17% 95%
55	RM	447	24% 95%
55	SC	447	21% 95%
55	SD	447	18% 95%
55	SF	447	21% 95%
55	SH	447	24% 96%
55	SJ	447	17% 95%
55	SL	447	83% 95%
55	SM	447	28% 95%
55	TC	447	23% 95%
55	TD	447	24% 95%
55	TF	447	20% 96%
55	TH	447	30% 95%
55	TJ	447	16% 95%
55	TL	447	70% 96%
55	TM	447	36% 95%

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Mol	Chain	Length	Quality of chain
55	UC	447	54% 94%
55	UD	447	57% 95%
55	UF	447	54% 95%
55	UH	447	66% 94%
55	UJ	447	53% 95%
55	UL	447	75% 95%
55	UM	447	71% 95%
55	VC	447	41% 95%
55	VD	447	49% 95%
55	VF	447	45% 96%
55	VH	447	64% 94%
55	VJ	447	57% 95%
55	VL	447	57% 94%
55	VM	447	69% 95%
55	WC	447	34% 95%
55	WD	447	42% 95%
55	WF	447	35% 94%
55	WH	447	51% 96%
55	WJ	447	30% 96%
55	WL	447	36% 95%

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 1270897 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 CFAP96(C4orf47).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1A	42	Total 324	C 205	N 55	O 61	S 3	0	0
1	1B	267	Total 2033	C 1284	N 371	O 373	S 5	0	0

- Molecule 2 is a protein called Coiled-coil domain-containing protein 105.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1E	419	Total 3281	C 2005	N 647	O 619	S 10	0	0
2	1F	170	Total 1281	C 781	N 237	O 257	S 6	0	0
2	1G	294	Total 2355	C 1440	N 478	O 432	S 5	0	0
2	1H	420	Total 3294	C 2012	N 649	O 623	S 10	0	0

- Molecule 3 is a protein called Coiled-coil domain-containing protein 81.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1K	175	Total 1406	C 897	N 246	O 257	S 6	0	0
3	1L	175	Total 1406	C 897	N 246	O 257	S 6	0	0
3	1M	175	Total 1393	C 889	N 244	O 254	S 6	0	0
3	1v	207	Total 1719	C 1051	N 329	O 333	S 6	0	0
3	1w	87	Total 727	C 441	N 145	O 138	S 3	0	0
3	1x	250	Total 2088	C 1276	N 406	O 401	S 5	0	0
3	1y	198	Total 1639	C 999	N 315	O 319	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	1z	87	Total	C	N	O	S	0	0
			727	441	145	138	3		
3	2a	54	Total	C	N	O	S	0	0
			452	276	83	90	3		

- Molecule 4 is a protein called FAM166C.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1P	203	Total	C	N	O	S	0	0
			1628	993	310	317	8		
4	1Q	138	Total	C	N	O	S	0	0
			1130	686	223	217	4		

- Molecule 5 is a protein called Protein FAM166B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1T	228	Total	C	N	O	S	0	0
			1845	1171	328	337	9		
5	1U	111	Total	C	N	O	S	0	0
			898	575	158	161	4		
5	1V	229	Total	C	N	O	S	0	0
			1857	1180	329	339	9		
5	1W	107	Total	C	N	O	S	0	0
			871	549	156	162	4		

- Molecule 6 is a protein called CFAP144(FAM183A).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1Y	119	Total	C	N	O	S	0	0
			1009	638	176	191	4		

- Molecule 7 is a protein called Outer dense fiber protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1a	134	Total	C	N	O	S	0	0
			1030	647	184	193	6		
7	1b	122	Total	C	N	O	S	0	0
			922	578	169	171	4		
7	5E	154	Total	C	N	O	S	0	0
			1158	727	211	215	5		
7	5F	112	Total	C	N	O	S	0	0
			861	542	153	160	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	5G	142	Total	C	N	O	S	0	0
			1074	675	194	201	4		
7	5H	117	Total	C	N	O	S	0	0
			896	563	160	167	6		
7	5I	27	Total	C	N	O	S	0	0
			198	126	35	36	1		
7	5J	233	Total	C	N	O	S	0	0
			1776	1115	321	330	10		
7	5K	134	Total	C	N	O	S	0	0
			1011	635	184	188	4		
7	5L	125	Total	C	N	O	S	0	0
			958	603	170	179	6		
7	5M	14	Total	C	N	O		0	0
			112	71	18	23			
7	5N	244	Total	C	N	O	S	0	0
			1856	1166	335	345	10		
7	5O	15	Total	C	N	O		0	0
			117	78	20	19			

- Molecule 8 is a protein called Tex33.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1d	101	Total	C	N	O	S	0	0
			808	521	136	148	3		

- Molecule 9 is a protein called C20Orf85.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1f	36	Total	C	N	O		0	0
			339	216	70	53			
9	1g	51	Total	C	N	O	S	0	0
			473	300	91	81	1		

- Molecule 10 is a protein called ATP6V1FNB.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1i	34	Total	C	N	O		0	0
			304	197	52	55			
10	1j	31	Total	C	N	O		0	0
			275	177	48	50			
10	9M	84	Total	C	N	O	S	0	0
			705	453	125	124	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	9N	84	Total	C	N	O	S	0	0
			705	453	125	124	3		
10	9O	41	Total	C	N	O		0	0
			344	222	62	60			

- Molecule 11 is a protein called Tex26(LOC100888047).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1l	39	Total	C	N	O	S	0	0
			300	193	50	55	2		
11	1m	39	Total	C	N	O	S	0	0
			300	193	50	55	2		

- Molecule 12 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1o	29	Total	C	N	O	S	0	0
			252	155	51	44	2		
12	1p	30	Total	C	N	O	S	0	0
			261	160	52	47	2		
12	1q	46	Total	C	N	O	S	0	0
			382	240	69	72	1		
12	1r	27	Total	C	N	O	S	0	0
			235	146	49	38	2		

- Molecule 13 is a protein called Enkurin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	2A	250	Total	C	N	O	S	0	0
			2045	1285	363	388	9		
13	2B	251	Total	C	N	O	S	0	0
			2051	1289	366	387	9		
13	2C	251	Total	C	N	O	S	0	0
			2054	1290	365	390	9		
13	2D	79	Total	C	N	O	S	0	0
			637	402	110	123	2		

- Molecule 14 is a protein called CFAP107.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2G	227	Total	C	N	O	S	0	0
			1874	1159	364	346	5		

- Molecule 15 is a protein called Cilia- and flagella-associated protein 126.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	2J	107	Total	C	N	O	S	0	0
			862	534	161	164	3		
15	2K	107	Total	C	N	O	S	0	0
			862	534	161	164	3		
15	2L	107	Total	C	N	O	S	0	0
			862	534	161	164	3		

- Molecule 16 is a protein called Flagellar FliJ protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2O	119	Total	C	N	O	S	0	0
			978	611	184	182	1		

- Molecule 17 is a protein called Meiosis-specific nuclear structural protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	2R	120	Total	C	N	O	S	0	0
			1035	628	200	202	5		
17	2S	376	Total	C	N	O	S	0	0
			3254	1957	631	647	19		

- Molecule 18 is a protein called Cilia- and flagella-associated protein 161.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	2V	284	Total	C	N	O	S	0	0
			2215	1382	392	427	14		
18	2W	284	Total	C	N	O	S	0	0
			2215	1382	392	427	14		

- Molecule 19 is a protein called CFA20 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3A	187	Total	C	N	O	S	0	0
			1550	996	273	274	7		
19	3B	187	Total	C	N	O	S	0	0
			1550	996	273	274	7		
19	3C	180	Total	C	N	O	S	0	0
			1496	963	265	261	7		
19	3D	176	Total	C	N	O	S	0	0
			1463	942	259	255	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	3E	186	Total	C	N	O	S	0	0
			1542	990	272	273	7		
19	3F	187	Total	C	N	O	S	0	0
			1550	996	273	274	7		
19	3G	186	Total	C	N	O	S	0	0
			1542	990	272	273	7		

- Molecule 20 is a protein called EF-hand domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3J	495	Total	C	N	O	S	0	0
			3933	2460	699	763	11		
20	3K	70	Total	C	N	O	S	0	0
			550	340	103	103	4		

- Molecule 21 is a protein called Trichohyalin-plectin-homology domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	3N	258	Total	C	N	O	S	0	0
			2126	1306	406	405	9		
21	3O	278	Total	C	N	O	S	0	0
			2329	1429	444	450	6		

- Molecule 22 is a protein called CFAP276.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	3R	165	Total	C	N	O	S	0	0
			1317	820	242	252	3		
22	3S	127	Total	C	N	O	S	0	0
			1006	625	191	188	2		
22	3T	165	Total	C	N	O	S	0	0
			1317	820	242	252	3		

- Molecule 23 is a protein called Cilia- and flagella-associated protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	3W	384	Total	C	N	O	S	0	0
			3224	1971	601	640	12		
23	3X	315	Total	C	N	O	S	0	0
			2661	1623	506	523	9		
23	3Y	104	Total	C	N	O	S	0	0
			862	523	168	168	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	3Z	172	1415	865	259	284	7	0	0

- Molecule 24 is a protein called Cilia- and flagella-associated protein 52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	4A	617	4804	3030	841	902	31	0	0
24	4B	615	4792	3022	839	901	30	0	0
24	4C	617	4804	3030	841	902	31	0	0

- Molecule 25 is a protein called Trichohyalin-plectin-homology domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	4F	313	2613	1593	502	502	16	0	0
25	4G	206	1753	1065	343	333	12	0	0

- Molecule 26 is a protein called Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	4J	378	2987	1875	520	569	23	0	0
26	4K	376	2976	1869	518	566	23	0	0

- Molecule 27 is a protein called Cilia- and flagella-associated protein 77.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	4N	151	1237	772	235	224	6	0	0
27	4O	108	878	553	162	159	4	0	0
27	4P	150	1220	761	230	223	6	0	0
27	4Q	93	744	462	146	133	3	0	0

- Molecule 28 is a protein called Cilia- and flagella-associated protein 97.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	4T	143	Total	C	N	O	S	0	0
			1221	767	234	211	9		
28	4U	143	Total	C	N	O	S	0	0
			1221	767	234	211	9		
28	4V	14	Total	C	N	O	S	0	0
			116	77	19	19	1		

- Molecule 29 is a protein called HeLo_like_N(LOC577943).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4Y	300	Total	C	N	O	S	0	0
			2422	1513	448	453	8		

- Molecule 30 is a protein called Outer dense fiber protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5A	35	Total	C	N	O	S	0	0
			265	168	50	46	1		
30	5B	213	Total	C	N	O	S	0	0
			1650	1038	306	299	7		
30	9Y	140	Total	C	N	O	S	0	0
			1083	677	208	193	5		
30	9Z	101	Total	C	N	O	S	0	0
			783	495	145	140	3		

- Molecule 31 is a protein called PACRG.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6A	225	Total	C	N	O	S	0	0
			1792	1151	310	323	8		
31	6B	219	Total	C	N	O	S	0	0
			1737	1116	299	314	8		
31	6C	223	Total	C	N	O	S	0	0
			1769	1139	304	318	8		
31	6D	224	Total	C	N	O	S	0	0
			1784	1147	308	321	8		
31	6E	224	Total	C	N	O	S	0	0
			1784	1147	308	321	8		
31	6F	224	Total	C	N	O	S	0	0
			1784	1147	308	321	8		

- Molecule 32 is a protein called Pierce1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6I	78	Total	C	N	O	S	0	0
			632	397	112	119	4		
32	6J	53	Total	C	N	O	S	0	0
			410	258	69	78	5		

- Molecule 33 is a protein called Protein phosphatase 1 regulatory subunit 32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6M	391	Total	C	N	O	S	0	0
			3107	1936	567	593	11		
33	6N	80	Total	C	N	O	S	0	0
			648	406	121	119	2		

- Molecule 34 is a protein called RIB35.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	6Q	201	Total	C	N	O	S	0	0
			1634	1028	292	306	8		
34	6R	72	Total	C	N	O	S	0	0
			598	384	107	104	3		

- Molecule 35 is a protein called RIB43A-like with coiled-coils protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	6U	149	Total	C	N	O	S	0	0
			1242	750	239	249	4		
35	6V	274	Total	C	N	O	S	0	0
			2273	1370	435	458	10		
35	6W	243	Total	C	N	O	S	0	0
			2035	1227	391	408	9		
35	6X	121	Total	C	N	O	S	0	0
			1030	627	200	200	3		

- Molecule 36 is a protein called EF-hand domain-containing family member C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	7A	725	Total	C	N	O	S	0	0
			5901	3763	1025	1093	20		
36	7B	455	Total	C	N	O	S	0	0
			3734	2386	641	694	13		
36	7C	543	Total	C	N	O	S	0	0
			4414	2816	773	810	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	7D	724	5894	3758	1024	1092	20	0	0

- Molecule 37 is a protein called Flagellar protofilament ribbon protein rib74.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	7G	529	4301	2746	733	805	17	0	0
37	7H	529	4301	2746	733	805	17	0	0
37	7I	616	4996	3177	856	942	21	0	0

- Molecule 38 is a protein called SAXO3(LOC115918676).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	7M	263	2153	1350	401	391	11	0	0
38	7N	68	527	339	82	101	5	0	0

- Molecule 39 is a protein called TEPP protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	7Q	145	1199	760	220	215	4	0	0
39	7R	142	1140	713	213	210	4	0	0

- Molecule 40 is a protein called SPATA48.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	7U	93	755	476	136	134	9	0	0
40	7V	53	456	289	89	78		0	0

- Molecule 41 is a protein called Sperm-associated antigen 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	7Y	200	1593	991	270	327	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
41	7Z	64	Total	C	N	O	S	0	0
			491	297	89	103	2		

- Molecule 42 is a protein called Testicular haploid expressed gene protein-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	8A	243	Total	C	N	O	S	0	0
			1931	1213	359	354	5		

- Molecule 43 is a protein called Tektin.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	8D	397	Total	C	N	O	S	0	0
			3244	1990	594	640	20		
43	8E	178	Total	C	N	O	S	0	0
			1476	906	268	295	7		
43	8F	265	Total	C	N	O	S	0	0
			2142	1309	397	421	15		
43	8G	397	Total	C	N	O	S	0	0
			3244	1990	594	640	20		

- Molecule 44 is a protein called Tektin.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	8J	403	Total	C	N	O	S	0	0
			3272	1986	606	668	12		
44	8K	322	Total	C	N	O	S	0	0
			2623	1594	485	534	10		
44	8L	403	Total	C	N	O	S	0	0
			3272	1986	606	668	12		
44	8M	128	Total	C	N	O	S	0	0
			1041	632	190	216	3		
44	8N	17	Total	C	N	O	S	0	0
			144	84	30	29	1		

- Molecule 45 is a protein called Tektin.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	8Q	21	Total	C	N	O		0	0
			176	112	34	30			
45	8R	400	Total	C	N	O	S	0	0
			3241	1979	597	650	15		

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Mol	Chain	Residues	Atoms					AltConf	Trace
45	8S	304	Total	C	N	O	S	0	0
			2476	1513	453	499	11		
45	8T	400	Total	C	N	O	S	0	0
			3241	1979	597	650	15		
45	8U	120	Total	C	N	O	S	0	0
			958	584	180	189	5		

- Molecule 46 is a protein called Tex43.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	8X	104	Total	C	N	O	S	0	0
			879	553	164	157	5		
46	8Y	104	Total	C	N	O	S	0	0
			879	553	164	157	5		
46	8Z	104	Total	C	N	O	S	0	0
			879	553	164	157	5		

- Molecule 47 is a protein called Tex36(CFAP95, C9orf135).

Mol	Chain	Residues	Atoms					AltConf	Trace
47	9A	207	Total	C	N	O	S	0	0
			1704	1053	314	334	3		

- Molecule 48 is a protein called CFAP90(C5orf49).

Mol	Chain	Residues	Atoms					AltConf	Trace
48	9D	96	Total	C	N	O	S	0	0
			808	504	157	145	2		

- Molecule 49 is a protein called Tex49.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	9G	150	Total	C	N	O	S	0	0
			1229	787	216	221	5		

- Molecule 50 is a protein called Tex49_homologue(LOC580808).

Mol	Chain	Residues	Atoms					AltConf	Trace
50	9J	101	Total	C	N	O	S	0	0
			822	513	157	147	5		

- Molecule 51 is a protein called CFAP68(UPF0686, C11orf1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	9R	142	1166	736	208	220	2	0	0

- Molecule 52 is a protein called SPATA45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	9T	75	629	388	119	117	5	0	0

- Molecule 53 is a protein called C4orf45.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	9V	24	190	117	39	34	0	0
53	9W	70	602	391	107	104	0	0

- Molecule 54 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	AA	437	3414	2164	581	647	22	0	0
54	AB	437	3414	2164	581	647	22	0	0
54	AE	437	3414	2164	581	647	22	0	0
54	AG	437	3414	2164	581	647	22	0	0
54	AI	437	3414	2164	581	647	22	0	0
54	AK	437	3414	2164	581	647	22	0	0
54	AM	437	3414	2164	581	647	22	0	0
54	BA	437	3414	2164	581	647	22	0	0
54	BB	437	3414	2164	581	647	22	0	0
54	BE	437	3414	2164	581	647	22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	BG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	BI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	BK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	BM	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	CA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	CB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	CE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	CG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	CI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	CK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	CM	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	DA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	DB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	DE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	DG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	DI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	DK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	DM	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	EA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	EC	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	EE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	EG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	EI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	EK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	FA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	FB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	FE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	FG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	FI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	FK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	GA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	GB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	GE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	GG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	GI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	GK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	HA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	HB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	HE	432	Total	C	N	O	S	0	0
			3382	2144	575	641	22		
54	HG	435	Total	C	N	O	S	0	0
			3406	2160	579	645	22		
54	HI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	HK	435	Total	C	N	O	S	0	0
			3406	2160	579	645	22		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	IA	437	3414	2164	581	647	22	0	0
54	IB	434	3398	2154	578	644	22	0	0
54	IE	437	3414	2164	581	647	22	0	0
54	IG	437	3414	2164	581	647	22	0	0
54	II	435	3402	2156	579	645	22	0	0
54	IK	437	3414	2164	581	647	22	0	0
54	IM	437	3414	2164	581	647	22	0	0
54	JA	432	3387	2148	576	641	22	0	0
54	JB	437	3414	2164	581	647	22	0	0
54	JE	437	3414	2164	581	647	22	0	0
54	JG	437	3414	2164	581	647	22	0	0
54	JI	437	3414	2164	581	647	22	0	0
54	JK	437	3414	2164	581	647	22	0	0
54	KA	437	3414	2164	581	647	22	0	0
54	KB	434	3398	2154	578	644	22	0	0
54	KE	437	3414	2164	581	647	22	0	0
54	KG	437	3414	2164	581	647	22	0	0
54	KI	437	3414	2164	581	647	22	0	0
54	KK	437	3414	2164	581	647	22	0	0
54	LA	437	3414	2164	581	647	22	0	0
54	LB	437	3414	2164	581	647	22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	LE	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	LG	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	LI	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	LK	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	MA	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	MB	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	ME	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	MG	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	MI	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	MK	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	ML	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	NA	435	Total 3406	C 2160	N 579	O 645	S 22	0	0
54	NB	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	NE	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	NG	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	NI	434	Total 3398	C 2154	N 578	O 644	S 22	0	0
54	NL	433	Total 3391	C 2150	N 577	O 642	S 22	0	0
54	OA	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	OB	434	Total 3398	C 2154	N 578	O 644	S 22	0	0
54	OE	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	OG	437	Total 3414	C 2164	N 581	O 647	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	OI	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	OK	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	OL	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	PA	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	PB	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	PE	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	PG	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	PI	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	PK	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	PL	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	QA	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	QB	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	QE	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	QG	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	QI	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	QK	433	Total 3391	C 2150	N 577	O 642	S 22	0	0
54	QL	436	Total 3410	C 2162	N 580	O 646	S 22	0	0
54	RA	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	RB	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	RE	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	RG	437	Total 3414	C 2164	N 581	O 647	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	RI	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	RK	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	RL	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	SA	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	SB	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	SE	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	SG	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	SI	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	SK	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	TA	436	Total 3410	C 2162	N 580	O 646	S 22	0	0
54	TB	436	Total 3410	C 2162	N 580	O 646	S 22	0	0
54	TE	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	TG	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	TI	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	TK	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	UA	436	Total 3410	C 2162	N 580	O 646	S 22	0	0
54	UB	434	Total 3395	C 2152	N 578	O 643	S 22	0	0
54	UE	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	UG	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	UI	437	Total 3414	C 2164	N 581	O 647	S 22	0	0
54	UK	437	Total 3414	C 2164	N 581	O 647	S 22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
54	VA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	VB	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	VE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	VG	435	Total	C	N	O	S	0	0
			3406	2160	579	645	22		
54	VI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	VK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	WA	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	WB	436	Total	C	N	O	S	0	0
			3410	2162	580	646	22		
54	WE	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	WG	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	WI	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		
54	WK	437	Total	C	N	O	S	0	0
			3414	2164	581	647	22		

- Molecule 55 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AC	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	AD	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	AF	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	AH	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	AJ	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	AL	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	BC	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	BD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	BF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	BH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	BJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	BL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	CC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	CD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	CF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	CH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	CJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	CL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	DC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	DD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	DF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	DH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	DJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	DL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	EB	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	ED	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	EF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	EH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	EJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	EL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	EM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	FC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	FD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	FF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	FH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	FJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	FL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	FM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	GC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	GD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	GF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	GH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	GJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	GL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	GM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	HC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	HD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	HF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	HH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	HJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	HL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	HM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	IC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	ID	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	IF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	IH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	IJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	IL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	JC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	JD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	JF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	JH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	JJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	JL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	JM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	KC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	KD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	KF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	KH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	KJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	KL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	KM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	LC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	LD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	LF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	LH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	LJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	LL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	LM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	MC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	MD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	MF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	MH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	MJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	MM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	NC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	ND	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	NF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	NH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	NJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	NK	431	Total 3383	C 2124	N 579	O 653	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	NM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	OC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	OD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	OF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	OH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	OJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	OM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	PC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	PD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	PF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	PH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	PJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	PM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	QC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	QD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	QF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	QH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	QJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	QM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	RC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	RD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	RF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	RH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	RJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	RM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	TC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	TD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	TF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	TH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	TJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	TL	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	TM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	UC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	UD	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	UF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
55	UH	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	UJ	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	UL	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	UM	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	VC	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	VD	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	VF	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	VH	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	VJ	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	VL	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	VM	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	WC	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	WD	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	WF	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	WH	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	WJ	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		
55	WL	431	Total	C	N	O	S	0	0
			3383	2124	579	653	27		

- Molecule 56 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	AA	1	Total 32	C 10	N 5	O 14	P 3	0
56	AB	1	Total 32	C 10	N 5	O 14	P 3	0
56	AE	1	Total 32	C 10	N 5	O 14	P 3	0
56	AG	1	Total 32	C 10	N 5	O 14	P 3	0
56	AI	1	Total 32	C 10	N 5	O 14	P 3	0
56	AK	1	Total 32	C 10	N 5	O 14	P 3	0
56	AM	1	Total 32	C 10	N 5	O 14	P 3	0
56	BA	1	Total 32	C 10	N 5	O 14	P 3	0
56	BB	1	Total 32	C 10	N 5	O 14	P 3	0
56	BE	1	Total 32	C 10	N 5	O 14	P 3	0
56	BG	1	Total 32	C 10	N 5	O 14	P 3	0
56	BI	1	Total 32	C 10	N 5	O 14	P 3	0
56	BK	1	Total 32	C 10	N 5	O 14	P 3	0
56	BM	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	CA	1	Total 32	C 10	N 5	O 14	P 3	0
56	CB	1	Total 32	C 10	N 5	O 14	P 3	0
56	CE	1	Total 32	C 10	N 5	O 14	P 3	0
56	CG	1	Total 32	C 10	N 5	O 14	P 3	0
56	CI	1	Total 32	C 10	N 5	O 14	P 3	0
56	CK	1	Total 32	C 10	N 5	O 14	P 3	0
56	CM	1	Total 32	C 10	N 5	O 14	P 3	0
56	DA	1	Total 32	C 10	N 5	O 14	P 3	0
56	DB	1	Total 32	C 10	N 5	O 14	P 3	0
56	DE	1	Total 32	C 10	N 5	O 14	P 3	0
56	DG	1	Total 32	C 10	N 5	O 14	P 3	0
56	DI	1	Total 32	C 10	N 5	O 14	P 3	0
56	DK	1	Total 32	C 10	N 5	O 14	P 3	0
56	DM	1	Total 32	C 10	N 5	O 14	P 3	0
56	EA	1	Total 32	C 10	N 5	O 14	P 3	0
56	EC	1	Total 32	C 10	N 5	O 14	P 3	0
56	EE	1	Total 32	C 10	N 5	O 14	P 3	0
56	EG	1	Total 32	C 10	N 5	O 14	P 3	0
56	EI	1	Total 32	C 10	N 5	O 14	P 3	0
56	EK	1	Total 32	C 10	N 5	O 14	P 3	0
56	FA	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	FB	1	Total 32	C 10	N 5	O 14	P 3	0
56	FE	1	Total 32	C 10	N 5	O 14	P 3	0
56	FG	1	Total 32	C 10	N 5	O 14	P 3	0
56	FI	1	Total 32	C 10	N 5	O 14	P 3	0
56	FK	1	Total 32	C 10	N 5	O 14	P 3	0
56	GA	1	Total 32	C 10	N 5	O 14	P 3	0
56	GB	1	Total 32	C 10	N 5	O 14	P 3	0
56	GE	1	Total 32	C 10	N 5	O 14	P 3	0
56	GG	1	Total 32	C 10	N 5	O 14	P 3	0
56	GI	1	Total 32	C 10	N 5	O 14	P 3	0
56	GK	1	Total 32	C 10	N 5	O 14	P 3	0
56	HA	1	Total 32	C 10	N 5	O 14	P 3	0
56	HB	1	Total 32	C 10	N 5	O 14	P 3	0
56	HE	1	Total 32	C 10	N 5	O 14	P 3	0
56	HG	1	Total 32	C 10	N 5	O 14	P 3	0
56	HI	1	Total 32	C 10	N 5	O 14	P 3	0
56	HK	1	Total 32	C 10	N 5	O 14	P 3	0
56	IA	1	Total 32	C 10	N 5	O 14	P 3	0
56	IB	1	Total 32	C 10	N 5	O 14	P 3	0
56	IE	1	Total 32	C 10	N 5	O 14	P 3	0
56	IG	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	II	1	Total 32	C 10	N 5	O 14	P 3	0
56	IK	1	Total 32	C 10	N 5	O 14	P 3	0
56	IM	1	Total 32	C 10	N 5	O 14	P 3	0
56	JA	1	Total 32	C 10	N 5	O 14	P 3	0
56	JB	1	Total 32	C 10	N 5	O 14	P 3	0
56	JE	1	Total 32	C 10	N 5	O 14	P 3	0
56	JG	1	Total 32	C 10	N 5	O 14	P 3	0
56	JI	1	Total 32	C 10	N 5	O 14	P 3	0
56	JK	1	Total 32	C 10	N 5	O 14	P 3	0
56	KA	1	Total 32	C 10	N 5	O 14	P 3	0
56	KB	1	Total 32	C 10	N 5	O 14	P 3	0
56	KE	1	Total 32	C 10	N 5	O 14	P 3	0
56	KG	1	Total 32	C 10	N 5	O 14	P 3	0
56	KI	1	Total 32	C 10	N 5	O 14	P 3	0
56	KK	1	Total 32	C 10	N 5	O 14	P 3	0
56	LA	1	Total 32	C 10	N 5	O 14	P 3	0
56	LB	1	Total 32	C 10	N 5	O 14	P 3	0
56	LE	1	Total 32	C 10	N 5	O 14	P 3	0
56	LG	1	Total 32	C 10	N 5	O 14	P 3	0
56	LI	1	Total 32	C 10	N 5	O 14	P 3	0
56	LK	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	MA	1	Total 32	C 10	N 5	O 14	P 3	0
56	MB	1	Total 32	C 10	N 5	O 14	P 3	0
56	ME	1	Total 32	C 10	N 5	O 14	P 3	0
56	MG	1	Total 32	C 10	N 5	O 14	P 3	0
56	MI	1	Total 32	C 10	N 5	O 14	P 3	0
56	MK	1	Total 32	C 10	N 5	O 14	P 3	0
56	ML	1	Total 32	C 10	N 5	O 14	P 3	0
56	NA	1	Total 32	C 10	N 5	O 14	P 3	0
56	NB	1	Total 32	C 10	N 5	O 14	P 3	0
56	NE	1	Total 32	C 10	N 5	O 14	P 3	0
56	NG	1	Total 32	C 10	N 5	O 14	P 3	0
56	NI	1	Total 32	C 10	N 5	O 14	P 3	0
56	NL	1	Total 32	C 10	N 5	O 14	P 3	0
56	OA	1	Total 32	C 10	N 5	O 14	P 3	0
56	OB	1	Total 32	C 10	N 5	O 14	P 3	0
56	OE	1	Total 32	C 10	N 5	O 14	P 3	0
56	OG	1	Total 32	C 10	N 5	O 14	P 3	0
56	OI	1	Total 32	C 10	N 5	O 14	P 3	0
56	OK	1	Total 32	C 10	N 5	O 14	P 3	0
56	OL	1	Total 32	C 10	N 5	O 14	P 3	0
56	PA	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	PB	1	Total 32	C 10	N 5	O 14	P 3	0
56	PE	1	Total 32	C 10	N 5	O 14	P 3	0
56	PG	1	Total 32	C 10	N 5	O 14	P 3	0
56	PI	1	Total 32	C 10	N 5	O 14	P 3	0
56	PK	1	Total 32	C 10	N 5	O 14	P 3	0
56	PL	1	Total 32	C 10	N 5	O 14	P 3	0
56	QA	1	Total 32	C 10	N 5	O 14	P 3	0
56	QB	1	Total 32	C 10	N 5	O 14	P 3	0
56	QE	1	Total 32	C 10	N 5	O 14	P 3	0
56	QG	1	Total 32	C 10	N 5	O 14	P 3	0
56	QI	1	Total 32	C 10	N 5	O 14	P 3	0
56	QK	1	Total 32	C 10	N 5	O 14	P 3	0
56	QL	1	Total 32	C 10	N 5	O 14	P 3	0
56	RA	1	Total 32	C 10	N 5	O 14	P 3	0
56	RB	1	Total 32	C 10	N 5	O 14	P 3	0
56	RE	1	Total 32	C 10	N 5	O 14	P 3	0
56	RG	1	Total 32	C 10	N 5	O 14	P 3	0
56	RI	1	Total 32	C 10	N 5	O 14	P 3	0
56	RK	1	Total 32	C 10	N 5	O 14	P 3	0
56	RL	1	Total 32	C 10	N 5	O 14	P 3	0
56	SA	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	SB	1	Total 32	C 10	N 5	O 14	P 3	0
56	SE	1	Total 32	C 10	N 5	O 14	P 3	0
56	SG	1	Total 32	C 10	N 5	O 14	P 3	0
56	SI	1	Total 32	C 10	N 5	O 14	P 3	0
56	SK	1	Total 32	C 10	N 5	O 14	P 3	0
56	TA	1	Total 32	C 10	N 5	O 14	P 3	0
56	TB	1	Total 32	C 10	N 5	O 14	P 3	0
56	TE	1	Total 32	C 10	N 5	O 14	P 3	0
56	TG	1	Total 32	C 10	N 5	O 14	P 3	0
56	TI	1	Total 32	C 10	N 5	O 14	P 3	0
56	TK	1	Total 32	C 10	N 5	O 14	P 3	0
56	UA	1	Total 32	C 10	N 5	O 14	P 3	0
56	UB	1	Total 32	C 10	N 5	O 14	P 3	0
56	UE	1	Total 32	C 10	N 5	O 14	P 3	0
56	UG	1	Total 32	C 10	N 5	O 14	P 3	0
56	UI	1	Total 32	C 10	N 5	O 14	P 3	0
56	UK	1	Total 32	C 10	N 5	O 14	P 3	0
56	VA	1	Total 32	C 10	N 5	O 14	P 3	0
56	VB	1	Total 32	C 10	N 5	O 14	P 3	0
56	VE	1	Total 32	C 10	N 5	O 14	P 3	0
56	VG	1	Total 32	C 10	N 5	O 14	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
56	VI	1	32	10	5	14	3	0
56	VK	1	32	10	5	14	3	0
56	WA	1	32	10	5	14	3	0
56	WB	1	32	10	5	14	3	0
56	WE	1	32	10	5	14	3	0
56	WG	1	32	10	5	14	3	0
56	WI	1	32	10	5	14	3	0
56	WK	1	32	10	5	14	3	0

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	AA	1	1	1	0
57	AB	1	1	1	0
57	AE	1	1	1	0
57	AG	1	1	1	0
57	AI	1	1	1	0
57	AK	1	1	1	0
57	AM	1	1	1	0
57	BA	1	1	1	0
57	BB	1	1	1	0
57	BE	1	1	1	0
57	BG	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	BI	1	1	1	0
57	BK	1	1	1	0
57	BM	1	1	1	0
57	CA	1	1	1	0
57	CB	1	1	1	0
57	CE	1	1	1	0
57	CG	1	1	1	0
57	CI	1	1	1	0
57	CK	1	1	1	0
57	CM	1	1	1	0
57	DA	1	1	1	0
57	DB	1	1	1	0
57	DE	1	1	1	0
57	DG	1	1	1	0
57	DI	1	1	1	0
57	DK	1	1	1	0
57	DM	1	1	1	0
57	EA	1	1	1	0
57	EC	1	1	1	0
57	EE	1	1	1	0
57	EG	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	EI	1	1	1	0
57	EK	1	1	1	0
57	FA	1	1	1	0
57	FB	1	1	1	0
57	FE	1	1	1	0
57	FG	1	1	1	0
57	FI	1	1	1	0
57	FK	1	1	1	0
57	GA	1	1	1	0
57	GB	1	1	1	0
57	GE	1	1	1	0
57	GG	1	1	1	0
57	GI	1	1	1	0
57	GK	1	1	1	0
57	HA	1	1	1	0
57	HB	1	1	1	0
57	HE	1	1	1	0
57	HG	1	1	1	0
57	HI	1	1	1	0
57	HK	1	1	1	0
57	IA	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	IB	1	1	1	0
57	IE	1	1	1	0
57	IG	1	1	1	0
57	II	1	1	1	0
57	IK	1	1	1	0
57	IM	1	1	1	0
57	JA	1	1	1	0
57	JB	1	1	1	0
57	JE	1	1	1	0
57	JG	1	1	1	0
57	JI	1	1	1	0
57	JK	1	1	1	0
57	KA	1	1	1	0
57	KB	1	1	1	0
57	KE	1	1	1	0
57	KG	1	1	1	0
57	KI	1	1	1	0
57	KK	1	1	1	0
57	LA	1	1	1	0
57	LB	1	1	1	0
57	LE	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	LG	1	1	1	0
57	LI	1	1	1	0
57	LK	1	1	1	0
57	MA	1	1	1	0
57	MB	1	1	1	0
57	ME	1	1	1	0
57	MG	1	1	1	0
57	MI	1	1	1	0
57	MK	1	1	1	0
57	ML	1	1	1	0
57	NA	1	1	1	0
57	NB	1	1	1	0
57	NE	1	1	1	0
57	NG	1	1	1	0
57	NI	1	1	1	0
57	NL	1	1	1	0
57	OA	1	1	1	0
57	OB	1	1	1	0
57	OE	1	1	1	0
57	OG	1	1	1	0
57	OI	1	1	1	0

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Mol	Chain	Residues	Atoms		AltConf
57	OK	1	Total 1	Mg 1	0
57	OL	1	Total 1	Mg 1	0
57	PA	1	Total 1	Mg 1	0
57	PB	1	Total 1	Mg 1	0
57	PE	1	Total 1	Mg 1	0
57	PG	1	Total 1	Mg 1	0
57	PI	1	Total 1	Mg 1	0
57	PK	1	Total 1	Mg 1	0
57	PL	1	Total 1	Mg 1	0
57	QA	1	Total 1	Mg 1	0
57	QB	1	Total 1	Mg 1	0
57	QE	1	Total 1	Mg 1	0
57	QG	1	Total 1	Mg 1	0
57	QI	1	Total 1	Mg 1	0
57	QK	1	Total 1	Mg 1	0
57	QL	1	Total 1	Mg 1	0
57	RA	1	Total 1	Mg 1	0
57	RB	1	Total 1	Mg 1	0
57	RE	1	Total 1	Mg 1	0
57	RG	1	Total 1	Mg 1	0
57	RI	1	Total 1	Mg 1	0

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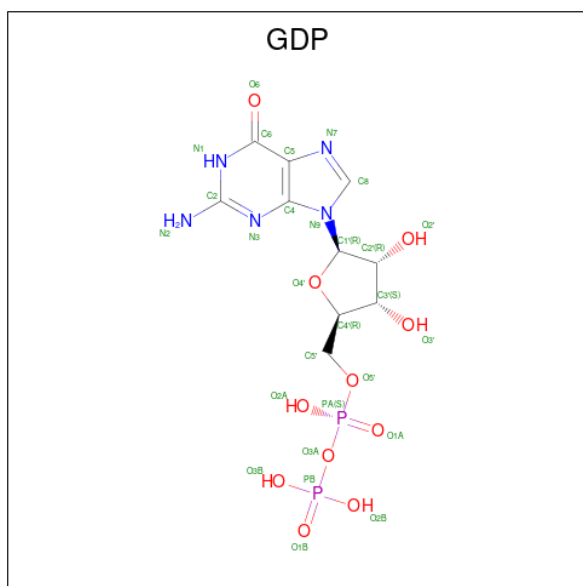
Mol	Chain	Residues	Atoms		AltConf
57	RK	1	Total 1	Mg 1	0
57	RL	1	Total 1	Mg 1	0
57	SA	1	Total 1	Mg 1	0
57	SB	1	Total 1	Mg 1	0
57	SE	1	Total 1	Mg 1	0
57	SG	1	Total 1	Mg 1	0
57	SI	1	Total 1	Mg 1	0
57	SK	1	Total 1	Mg 1	0
57	TA	1	Total 1	Mg 1	0
57	TB	1	Total 1	Mg 1	0
57	TE	1	Total 1	Mg 1	0
57	TG	1	Total 1	Mg 1	0
57	TI	1	Total 1	Mg 1	0
57	TK	1	Total 1	Mg 1	0
57	UA	1	Total 1	Mg 1	0
57	UB	1	Total 1	Mg 1	0
57	UE	1	Total 1	Mg 1	0
57	UG	1	Total 1	Mg 1	0
57	UI	1	Total 1	Mg 1	0
57	UK	1	Total 1	Mg 1	0
57	VA	1	Total 1	Mg 1	0

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Mol	Chain	Residues	Atoms		AltConf
57	VB	1	Total 1	Mg 1	0
57	VE	1	Total 1	Mg 1	0
57	VG	1	Total 1	Mg 1	0
57	VI	1	Total 1	Mg 1	0
57	VK	1	Total 1	Mg 1	0
57	WA	1	Total 1	Mg 1	0
57	WB	1	Total 1	Mg 1	0
57	WE	1	Total 1	Mg 1	0
57	WG	1	Total 1	Mg 1	0
57	WI	1	Total 1	Mg 1	0
57	WK	1	Total 1	Mg 1	0

- Molecule 58 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	AC	1	28	10	5	11	2	0
58	AD	1	28	10	5	11	2	0
58	AF	1	28	10	5	11	2	0
58	AH	1	28	10	5	11	2	0
58	AJ	1	28	10	5	11	2	0
58	AL	1	28	10	5	11	2	0
58	BC	1	28	10	5	11	2	0
58	BD	1	28	10	5	11	2	0
58	BF	1	28	10	5	11	2	0
58	BH	1	28	10	5	11	2	0
58	BJ	1	28	10	5	11	2	0
58	BL	1	28	10	5	11	2	0
58	CC	1	28	10	5	11	2	0
58	CD	1	28	10	5	11	2	0
58	CF	1	28	10	5	11	2	0
58	CH	1	28	10	5	11	2	0
58	CJ	1	28	10	5	11	2	0
58	CL	1	28	10	5	11	2	0
58	DC	1	28	10	5	11	2	0
58	DD	1	28	10	5	11	2	0
58	DF	1	28	10	5	11	2	0
58	DH	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	DJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	DL	1	Total 28	C 10	N 5	O 11	P 2	0
58	EB	1	Total 28	C 10	N 5	O 11	P 2	0
58	ED	1	Total 28	C 10	N 5	O 11	P 2	0
58	EF	1	Total 28	C 10	N 5	O 11	P 2	0
58	EH	1	Total 28	C 10	N 5	O 11	P 2	0
58	EJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	EL	1	Total 28	C 10	N 5	O 11	P 2	0
58	EM	1	Total 28	C 10	N 5	O 11	P 2	0
58	FC	1	Total 28	C 10	N 5	O 11	P 2	0
58	FD	1	Total 28	C 10	N 5	O 11	P 2	0
58	FF	1	Total 28	C 10	N 5	O 11	P 2	0
58	FH	1	Total 28	C 10	N 5	O 11	P 2	0
58	FJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	FL	1	Total 28	C 10	N 5	O 11	P 2	0
58	FM	1	Total 28	C 10	N 5	O 11	P 2	0
58	GC	1	Total 28	C 10	N 5	O 11	P 2	0
58	GD	1	Total 28	C 10	N 5	O 11	P 2	0
58	GF	1	Total 28	C 10	N 5	O 11	P 2	0
58	GH	1	Total 28	C 10	N 5	O 11	P 2	0
58	GJ	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	GL	1	Total 28	C 10	N 5	O 11	P 2	0
58	GM	1	Total 28	C 10	N 5	O 11	P 2	0
58	HC	1	Total 28	C 10	N 5	O 11	P 2	0
58	HD	1	Total 28	C 10	N 5	O 11	P 2	0
58	HF	1	Total 28	C 10	N 5	O 11	P 2	0
58	HH	1	Total 28	C 10	N 5	O 11	P 2	0
58	HJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	HL	1	Total 28	C 10	N 5	O 11	P 2	0
58	HM	1	Total 28	C 10	N 5	O 11	P 2	0
58	IC	1	Total 28	C 10	N 5	O 11	P 2	0
58	ID	1	Total 28	C 10	N 5	O 11	P 2	0
58	IF	1	Total 28	C 10	N 5	O 11	P 2	0
58	IH	1	Total 28	C 10	N 5	O 11	P 2	0
58	IJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	IL	1	Total 28	C 10	N 5	O 11	P 2	0
58	JC	1	Total 28	C 10	N 5	O 11	P 2	0
58	JD	1	Total 28	C 10	N 5	O 11	P 2	0
58	JF	1	Total 28	C 10	N 5	O 11	P 2	0
58	JH	1	Total 28	C 10	N 5	O 11	P 2	0
58	JJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	JL	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	JM	1	Total 28	C 10	N 5	O 11	P 2	0
58	KC	1	Total 28	C 10	N 5	O 11	P 2	0
58	KD	1	Total 28	C 10	N 5	O 11	P 2	0
58	KF	1	Total 28	C 10	N 5	O 11	P 2	0
58	KH	1	Total 28	C 10	N 5	O 11	P 2	0
58	KJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	KL	1	Total 28	C 10	N 5	O 11	P 2	0
58	KM	1	Total 28	C 10	N 5	O 11	P 2	0
58	LC	1	Total 28	C 10	N 5	O 11	P 2	0
58	LD	1	Total 28	C 10	N 5	O 11	P 2	0
58	LF	1	Total 28	C 10	N 5	O 11	P 2	0
58	LH	1	Total 28	C 10	N 5	O 11	P 2	0
58	LJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	LL	1	Total 28	C 10	N 5	O 11	P 2	0
58	LM	1	Total 28	C 10	N 5	O 11	P 2	0
58	MC	1	Total 28	C 10	N 5	O 11	P 2	0
58	MD	1	Total 28	C 10	N 5	O 11	P 2	0
58	MF	1	Total 28	C 10	N 5	O 11	P 2	0
58	MH	1	Total 28	C 10	N 5	O 11	P 2	0
58	MJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	MM	1	Total 28	C 10	N 5	O 11	P 2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	NC	1	28	10	5	11	2	0
58	ND	1	28	10	5	11	2	0
58	NF	1	28	10	5	11	2	0
58	NH	1	28	10	5	11	2	0
58	NJ	1	28	10	5	11	2	0
58	NK	1	28	10	5	11	2	0
58	NM	1	28	10	5	11	2	0
58	OC	1	28	10	5	11	2	0
58	OD	1	28	10	5	11	2	0
58	OF	1	28	10	5	11	2	0
58	OH	1	28	10	5	11	2	0
58	OJ	1	28	10	5	11	2	0
58	OM	1	28	10	5	11	2	0
58	PC	1	28	10	5	11	2	0
58	PD	1	28	10	5	11	2	0
58	PF	1	28	10	5	11	2	0
58	PH	1	28	10	5	11	2	0
58	PJ	1	28	10	5	11	2	0
58	PM	1	28	10	5	11	2	0
58	QC	1	28	10	5	11	2	0
58	QD	1	28	10	5	11	2	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	QF	1	Total 28	C 10	N 5	O 11	P 2	0
58	QH	1	Total 28	C 10	N 5	O 11	P 2	0
58	QJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	QM	1	Total 28	C 10	N 5	O 11	P 2	0
58	RC	1	Total 28	C 10	N 5	O 11	P 2	0
58	RD	1	Total 28	C 10	N 5	O 11	P 2	0
58	RF	1	Total 28	C 10	N 5	O 11	P 2	0
58	RH	1	Total 28	C 10	N 5	O 11	P 2	0
58	RJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	RM	1	Total 28	C 10	N 5	O 11	P 2	0
58	SC	1	Total 28	C 10	N 5	O 11	P 2	0
58	SD	1	Total 28	C 10	N 5	O 11	P 2	0
58	SF	1	Total 28	C 10	N 5	O 11	P 2	0
58	SH	1	Total 28	C 10	N 5	O 11	P 2	0
58	SJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	SL	1	Total 28	C 10	N 5	O 11	P 2	0
58	SM	1	Total 28	C 10	N 5	O 11	P 2	0
58	TC	1	Total 28	C 10	N 5	O 11	P 2	0
58	TD	1	Total 28	C 10	N 5	O 11	P 2	0
58	TF	1	Total 28	C 10	N 5	O 11	P 2	0
58	TH	1	Total 28	C 10	N 5	O 11	P 2	0

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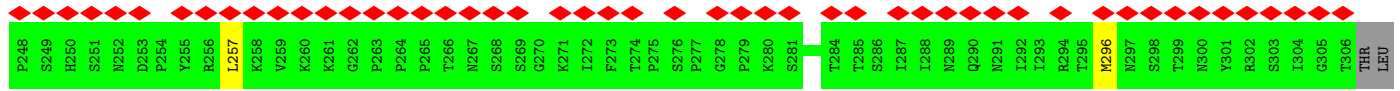
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	TJ	1	28	10	5	11	2	0
58	TL	1	28	10	5	11	2	0
58	TM	1	28	10	5	11	2	0
58	UC	1	28	10	5	11	2	0
58	UD	1	28	10	5	11	2	0
58	UF	1	28	10	5	11	2	0
58	UH	1	28	10	5	11	2	0
58	UJ	1	28	10	5	11	2	0
58	UL	1	28	10	5	11	2	0
58	UM	1	28	10	5	11	2	0
58	VC	1	28	10	5	11	2	0
58	VD	1	28	10	5	11	2	0
58	VF	1	28	10	5	11	2	0
58	VH	1	28	10	5	11	2	0
58	VJ	1	28	10	5	11	2	0
58	VL	1	28	10	5	11	2	0
58	VM	1	28	10	5	11	2	0
58	WC	1	28	10	5	11	2	0
58	WD	1	28	10	5	11	2	0
58	WF	1	28	10	5	11	2	0
58	WH	1	28	10	5	11	2	0

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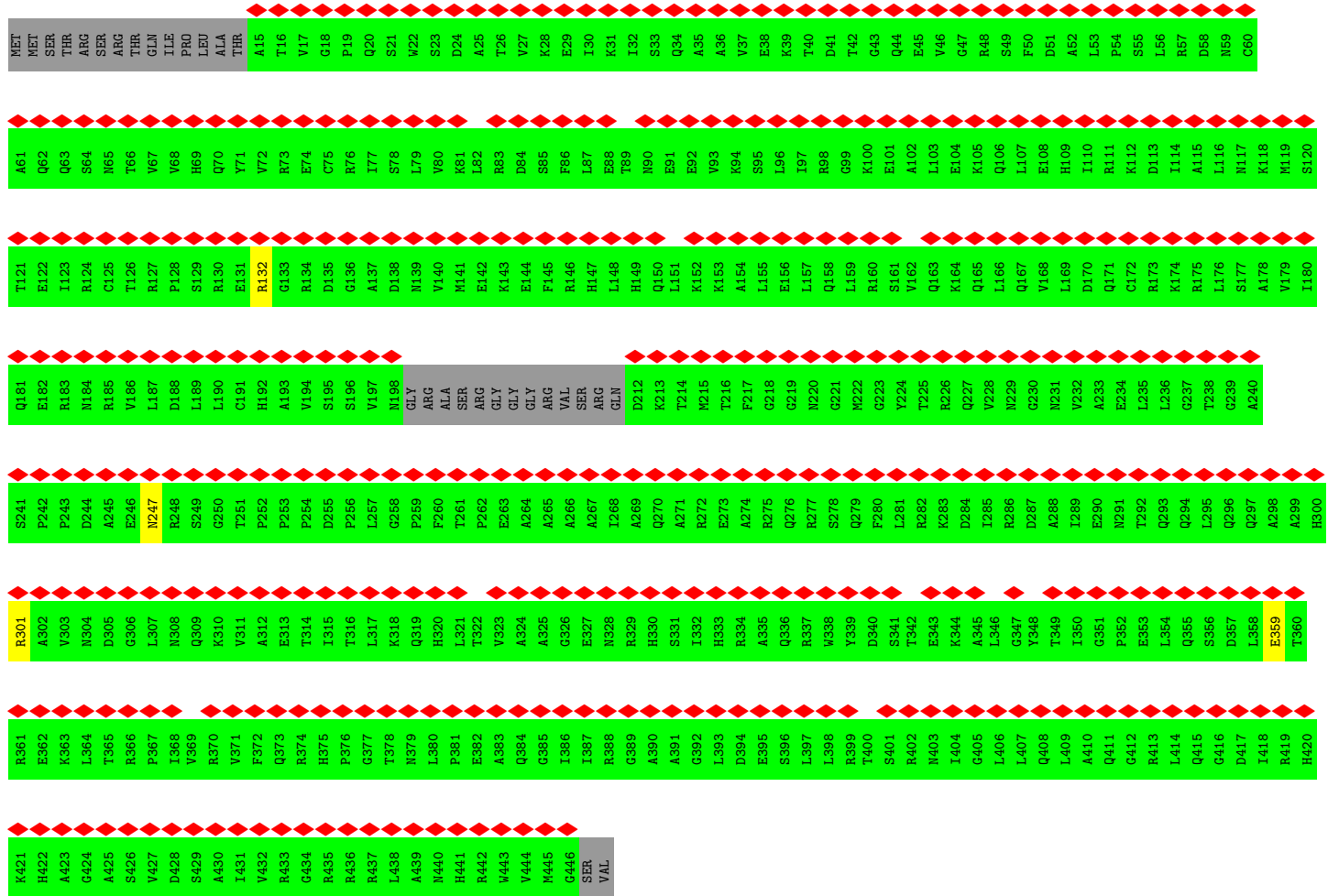
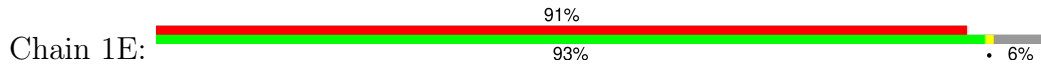
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	WJ	1	28	10	5	11	2	0
58	WL	1	28	10	5	11	2	0

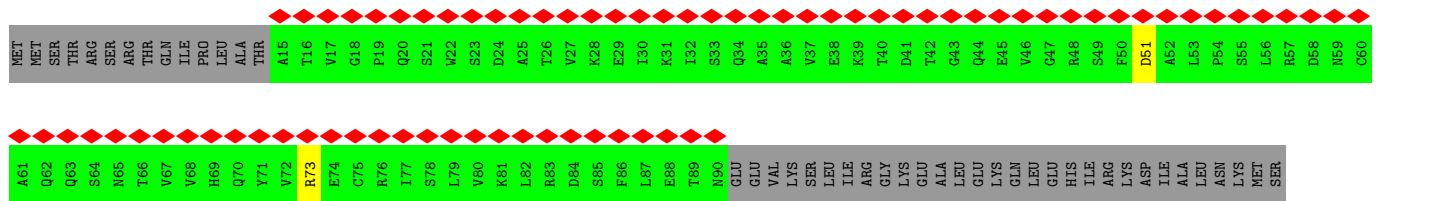


ALA

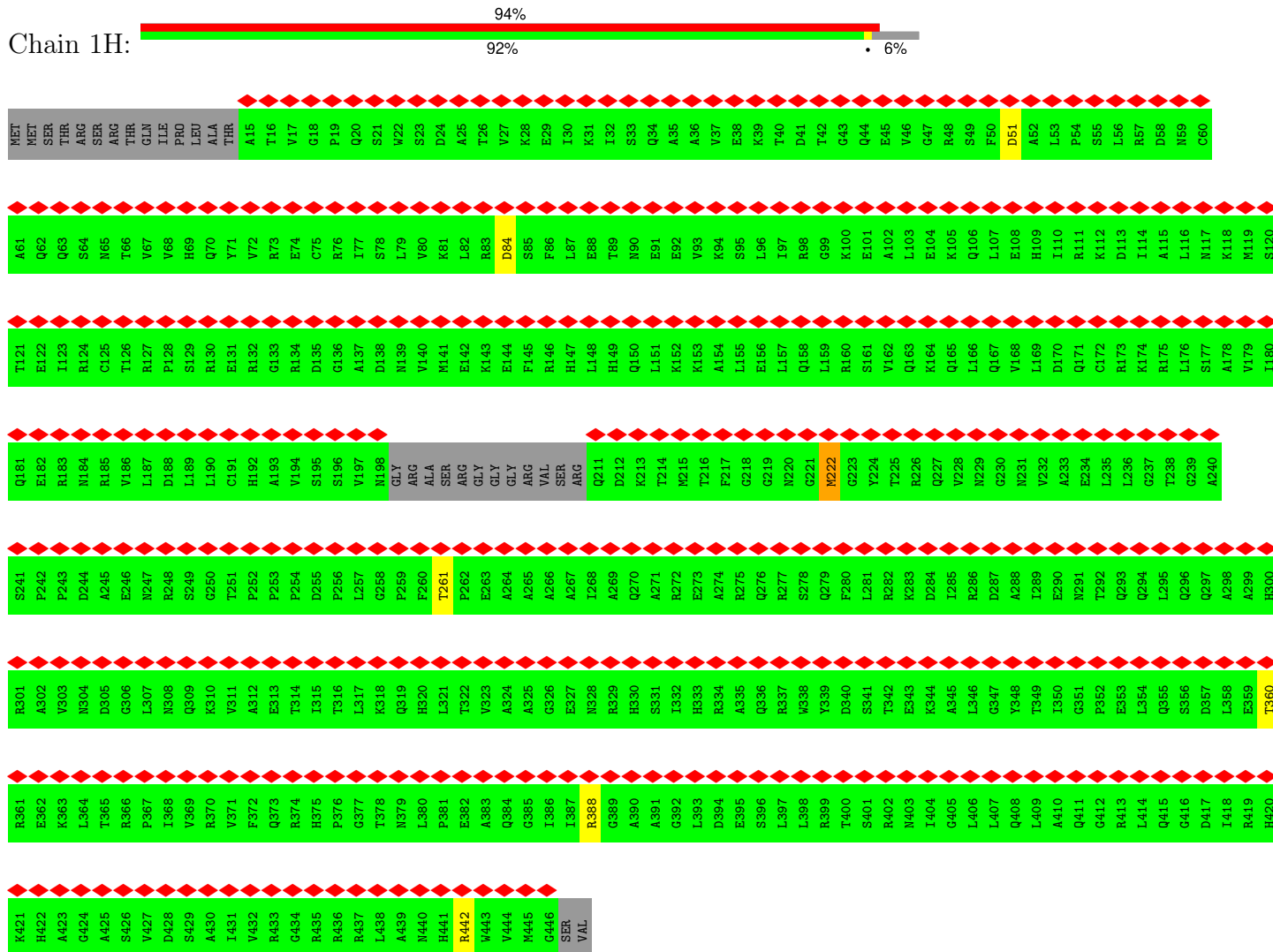
• Molecule 2: Coiled-coil domain-containing protein 105



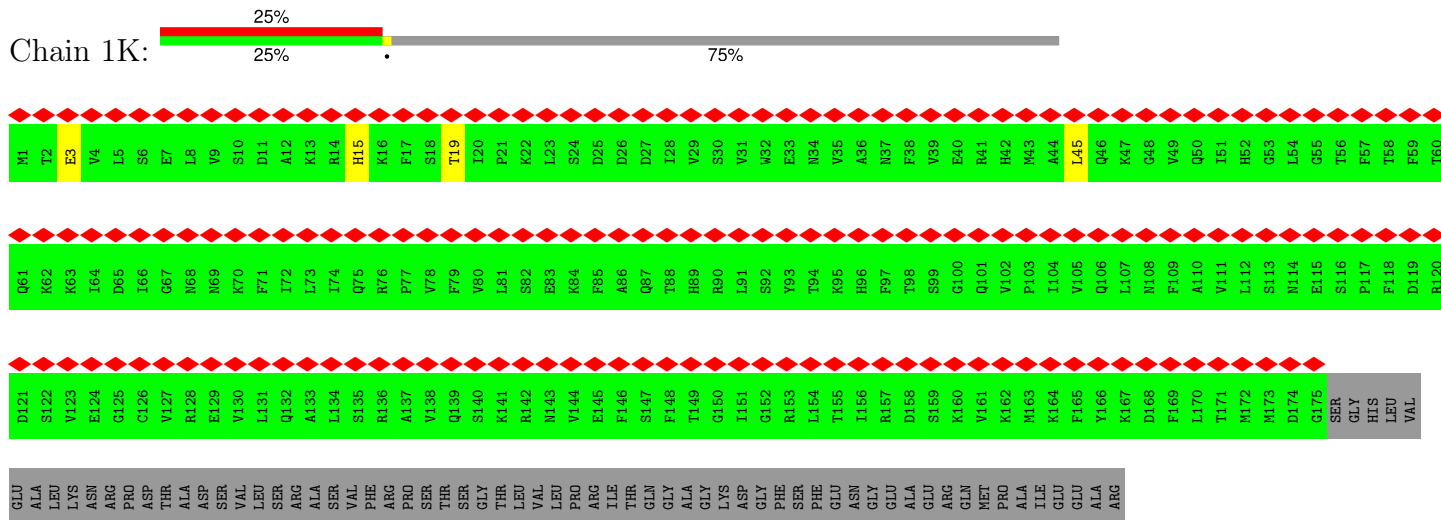
• Molecule 2: Coiled-coil domain-containing protein 105

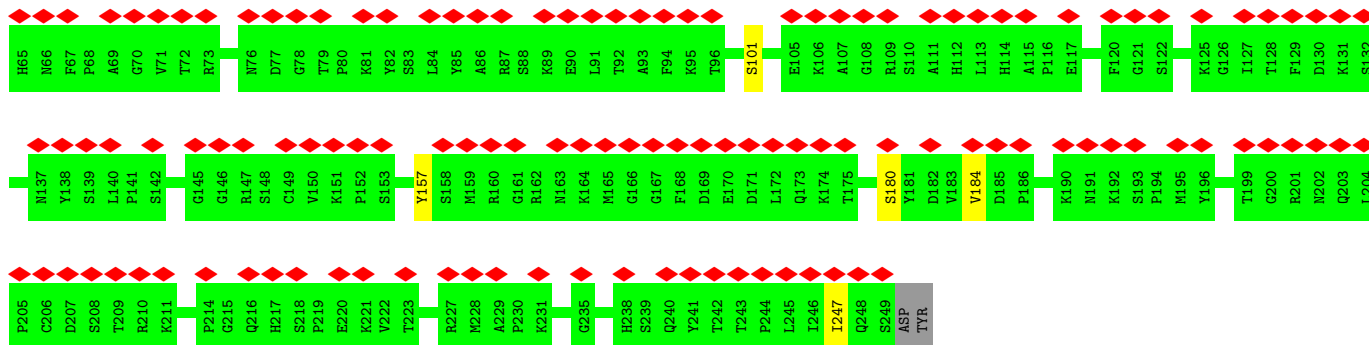


• Molecule 2: Coiled-coil domain-containing protein 105

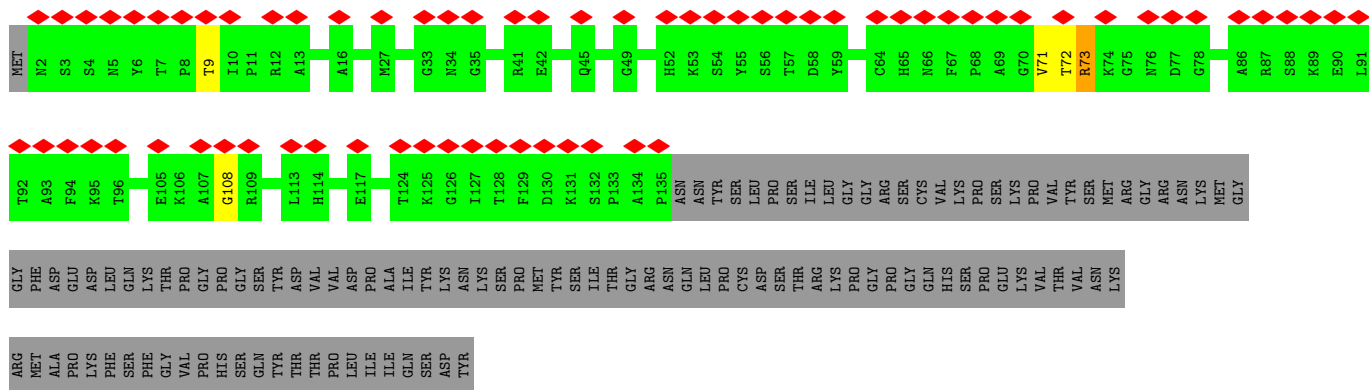


• Molecule 3: Coiled-coil domain-containing protein 81

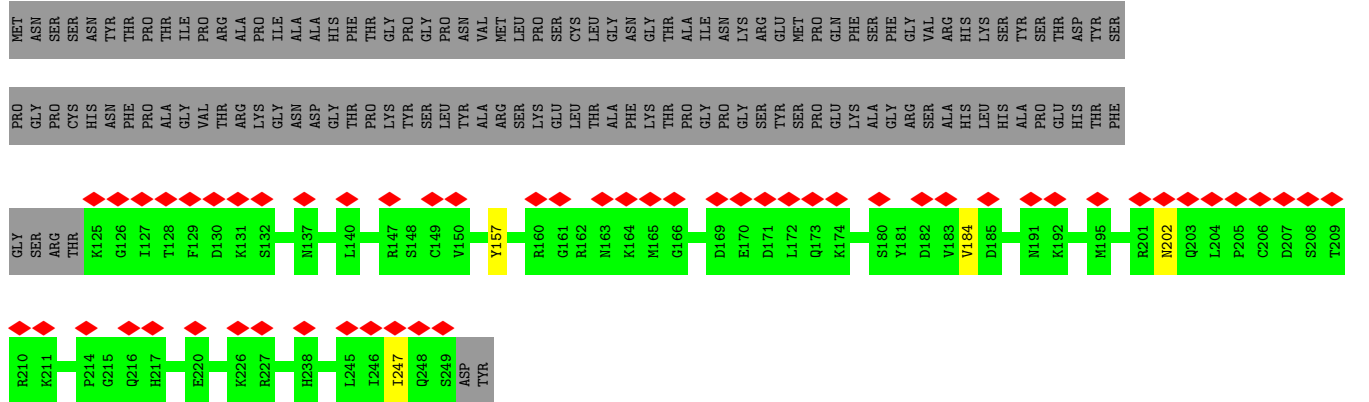




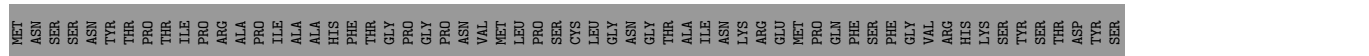
• Molecule 7: Outer dense fiber protein 3

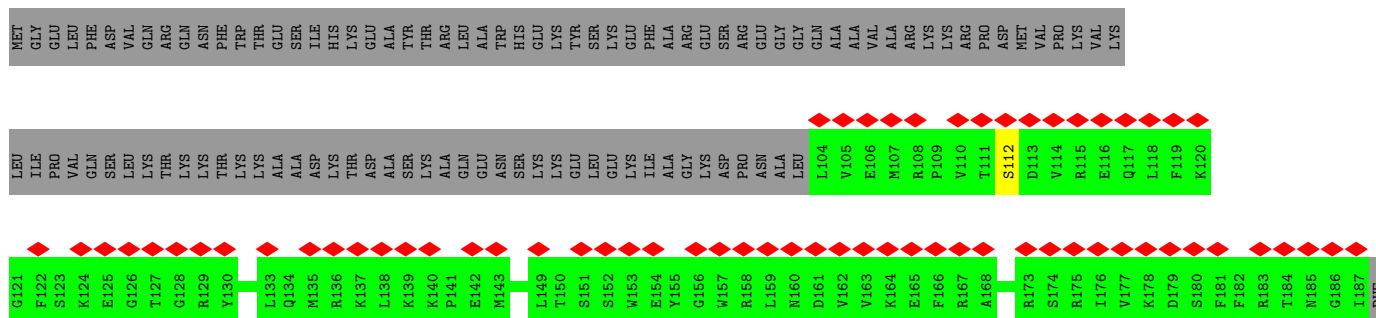


• Molecule 7: Outer dense fiber protein 3

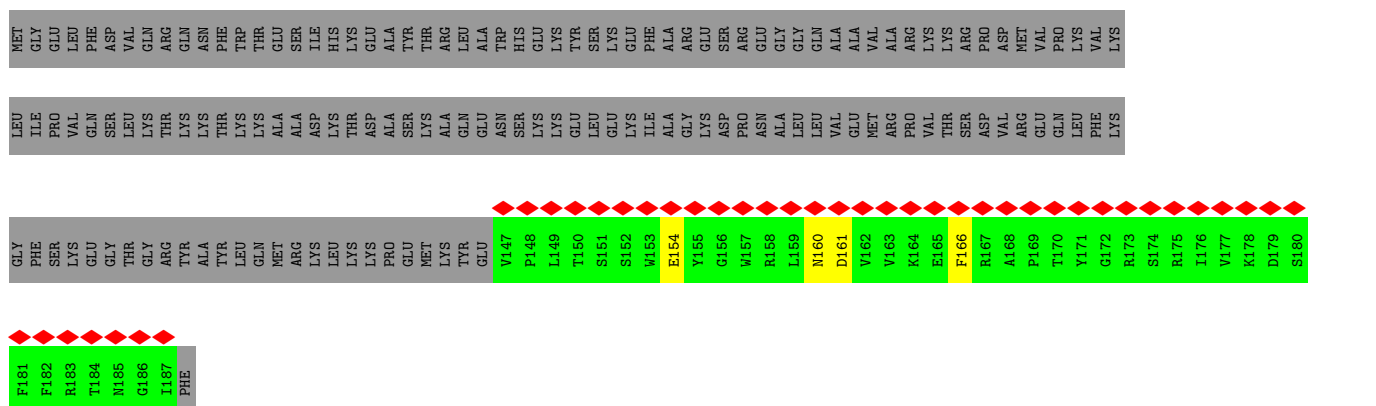


• Molecule 7: Outer dense fiber protein 3

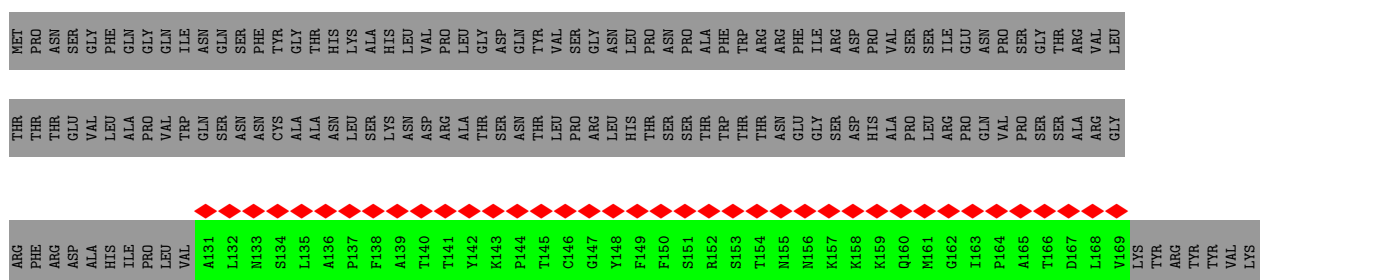




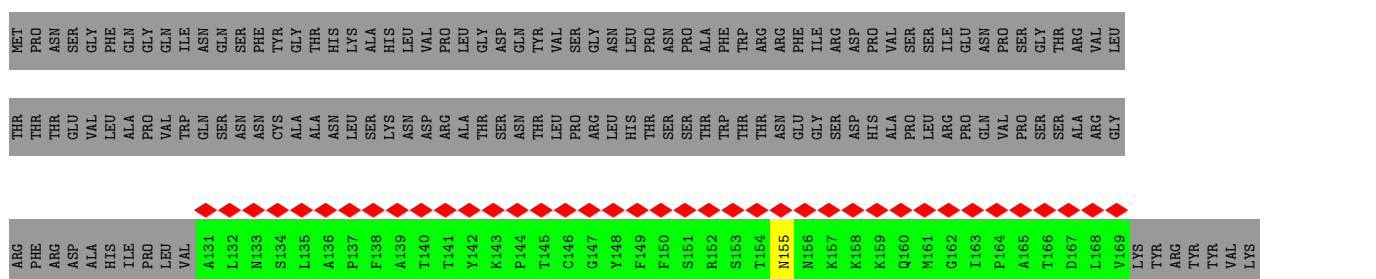
• Molecule 10: ATP6V1FNB



• Molecule 11: Tex26(LOC100888047)

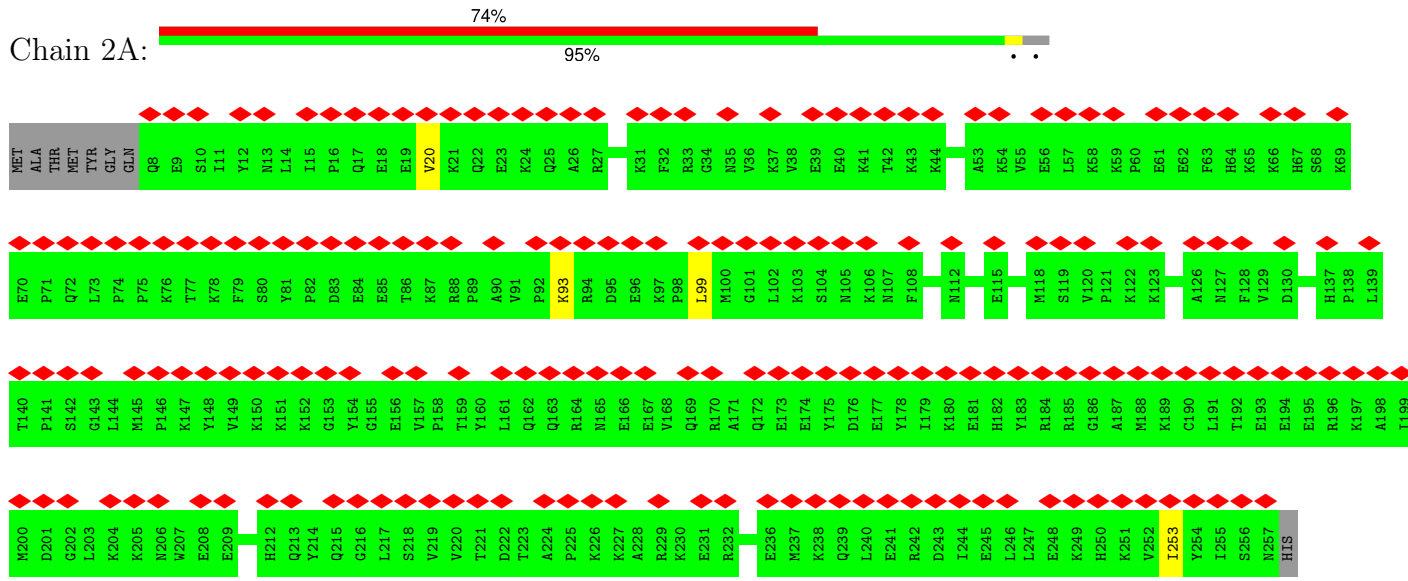


• Molecule 11: Tex26(LOC100888047)



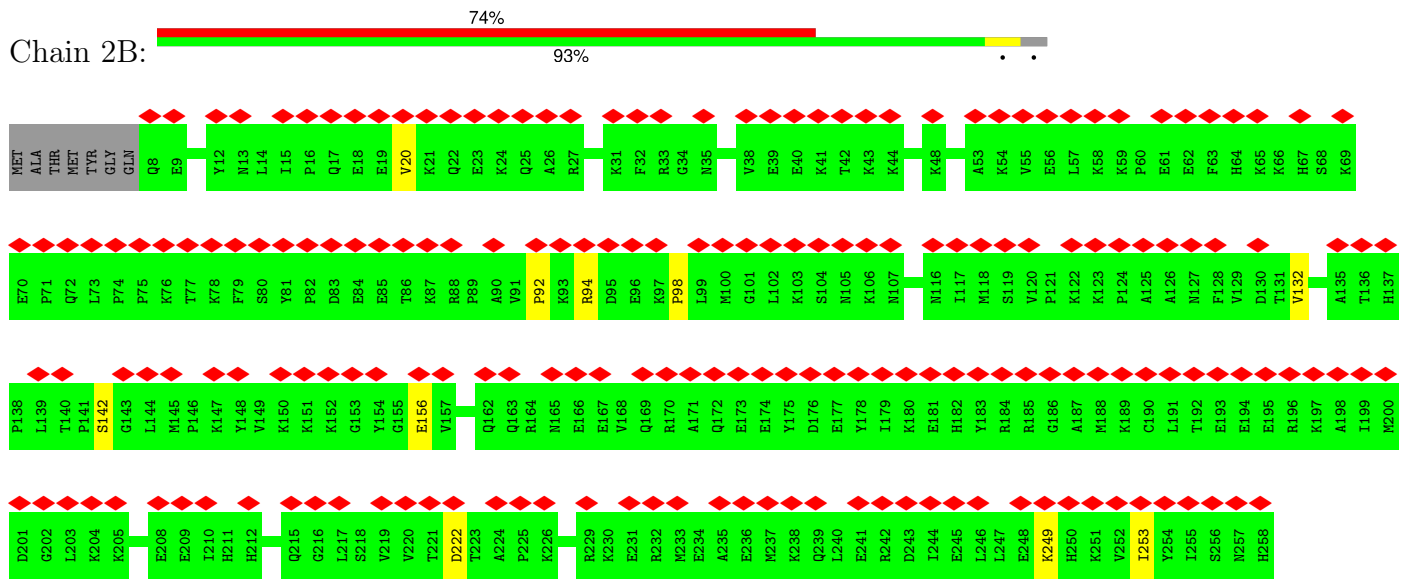
• Molecule 13: Enkurin domain-containing protein

Chain 2A:



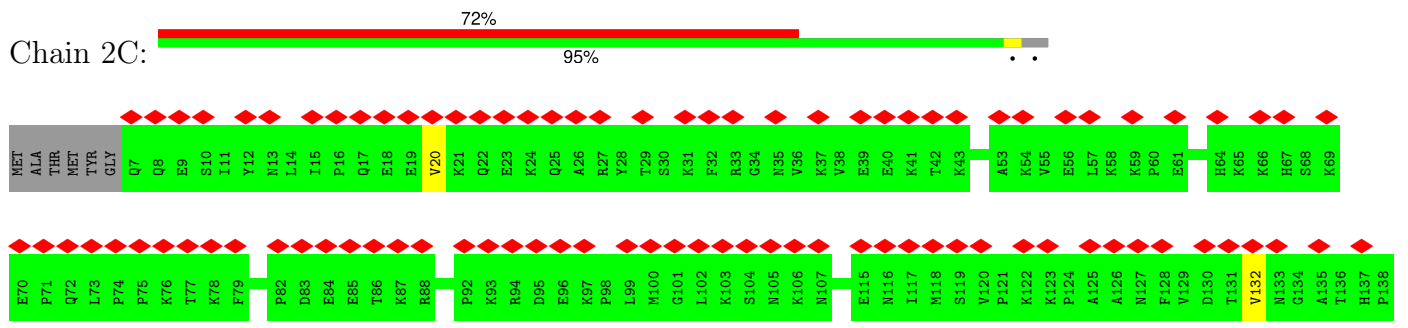
• Molecule 13: Enkurin domain-containing protein

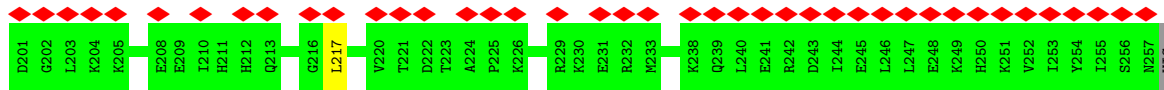
Chain 2B:



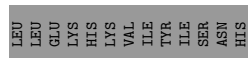
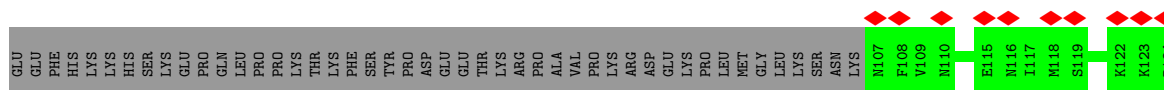
• Molecule 13: Enkurin domain-containing protein

Chain 2C:

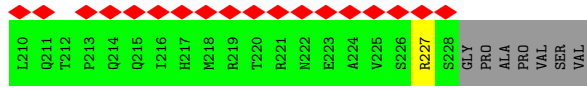
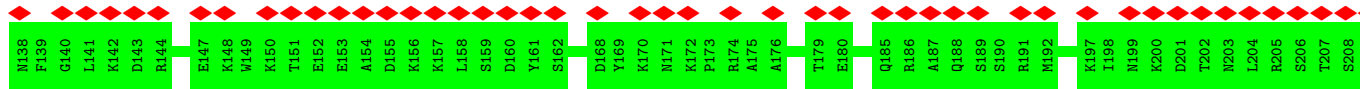
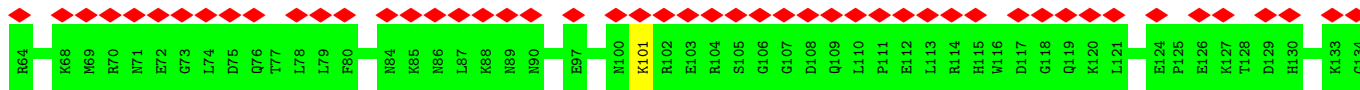




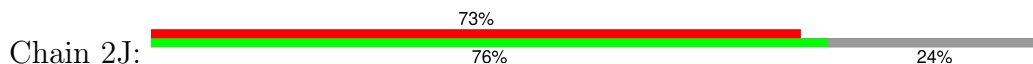
• Molecule 13: Enkurin domain-containing protein

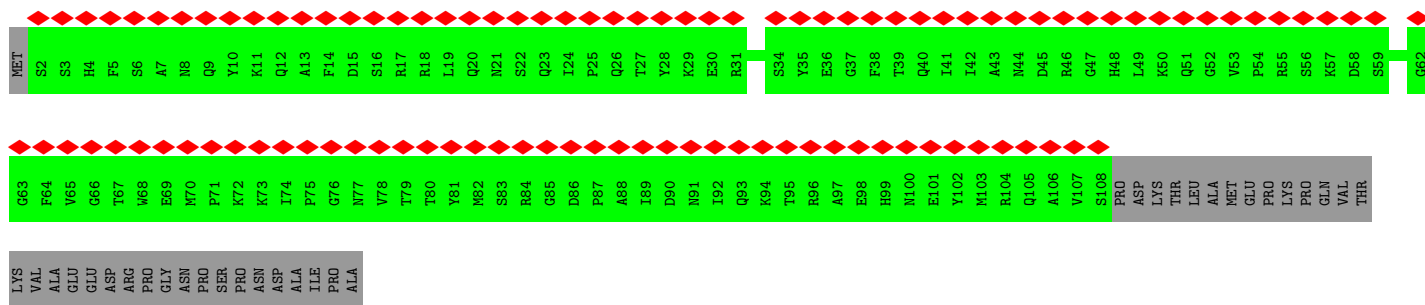


• Molecule 14: CFAP107

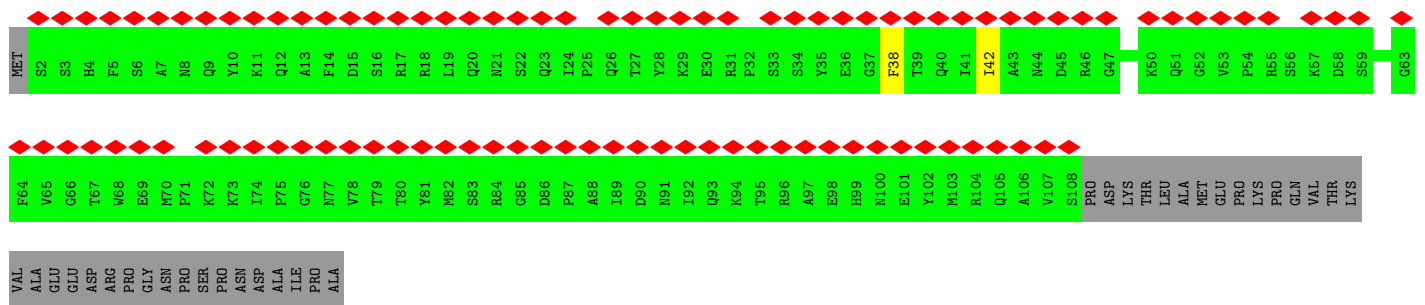
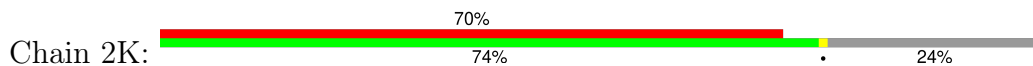


• Molecule 15: Cilia- and flagella-associated protein 126

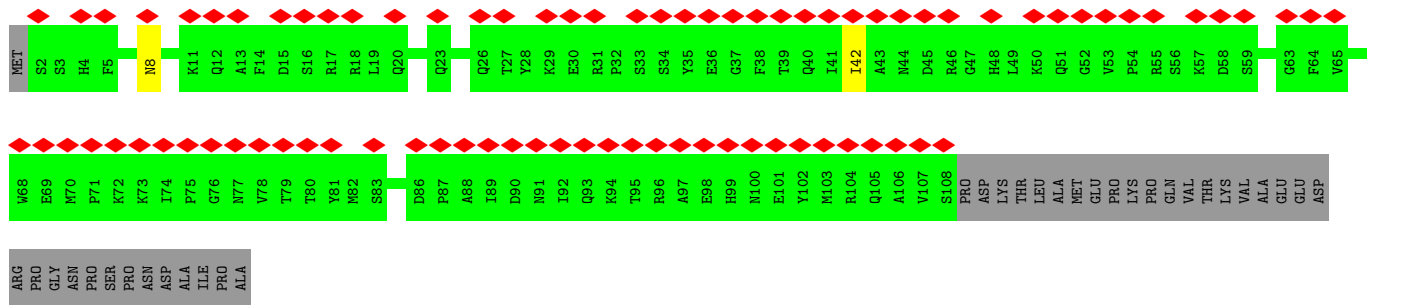
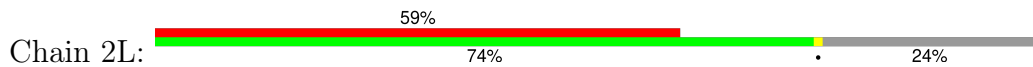




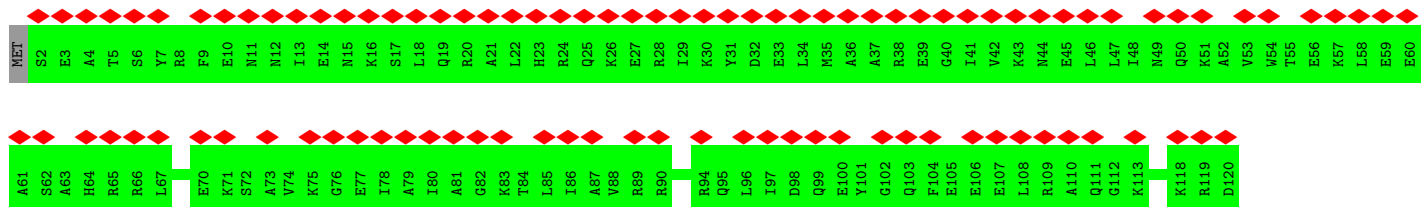
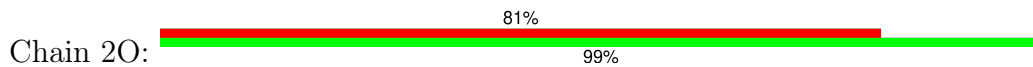
• Molecule 15: Cilia- and flagella-associated protein 126



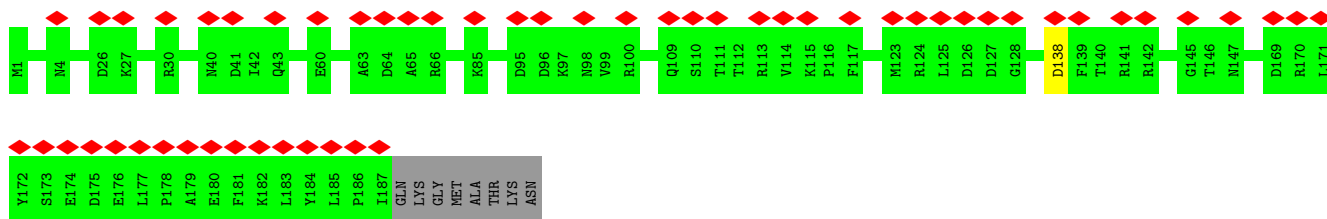
• Molecule 15: Cilia- and flagella-associated protein 126



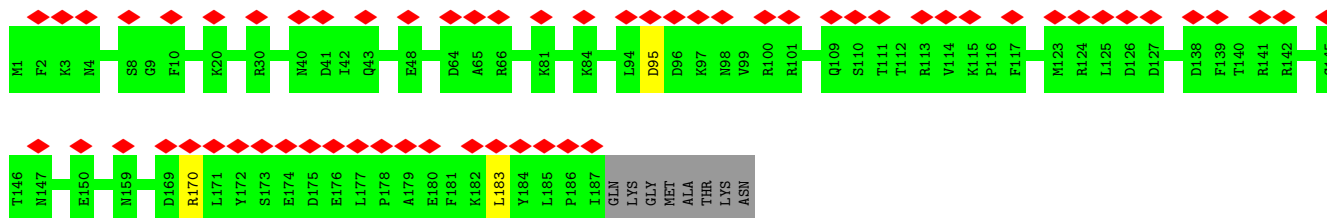
• Molecule 16: Flagellar FliJ protein



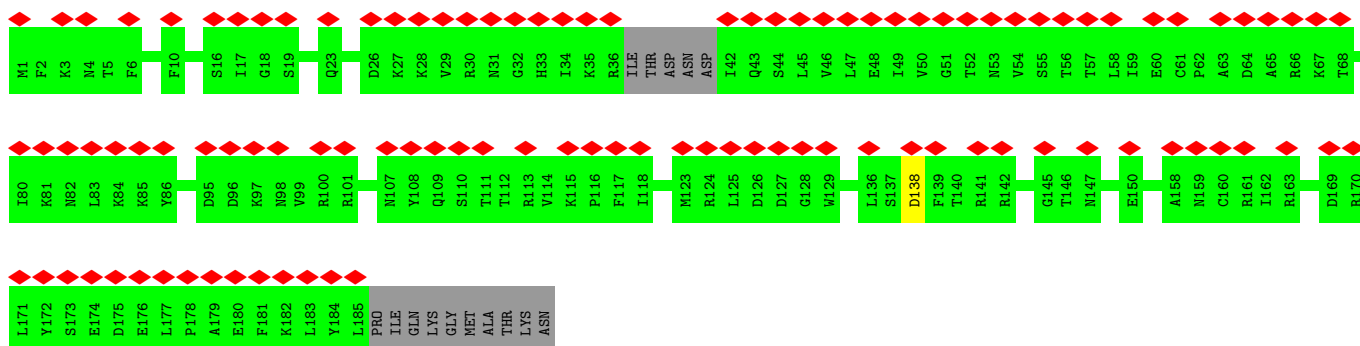
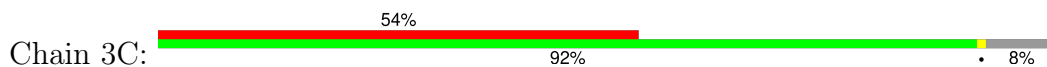
• Molecule 17: Meiosis-specific nuclear structural protein 1



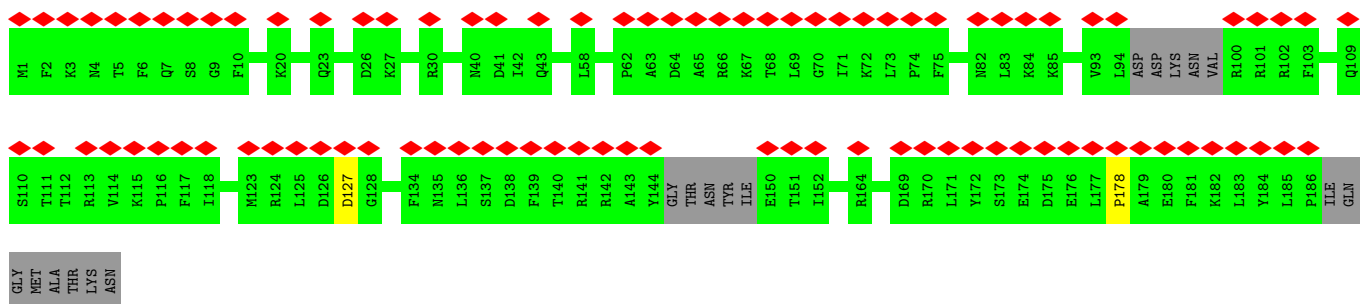
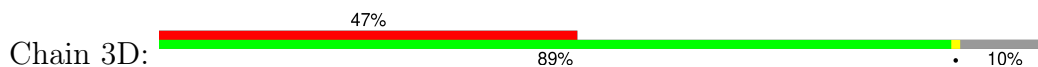
• Molecule 19: CFA20 domain-containing protein



• Molecule 19: CFA20 domain-containing protein

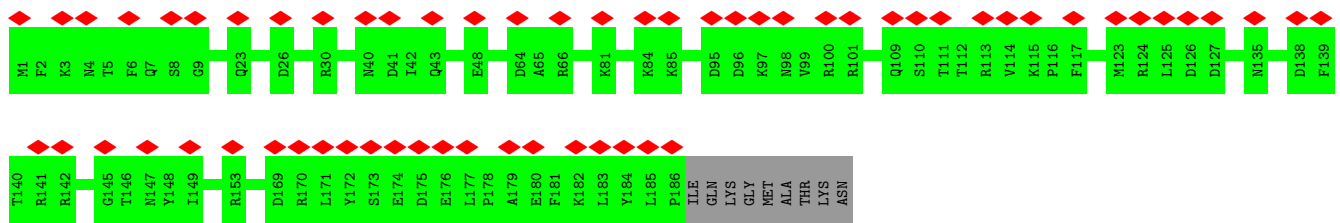


• Molecule 19: CFA20 domain-containing protein

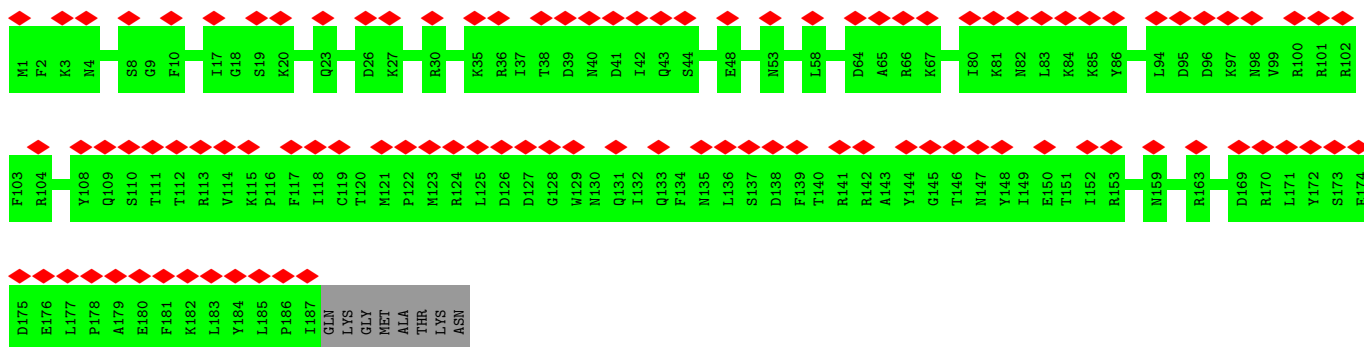


• Molecule 19: CFA20 domain-containing protein

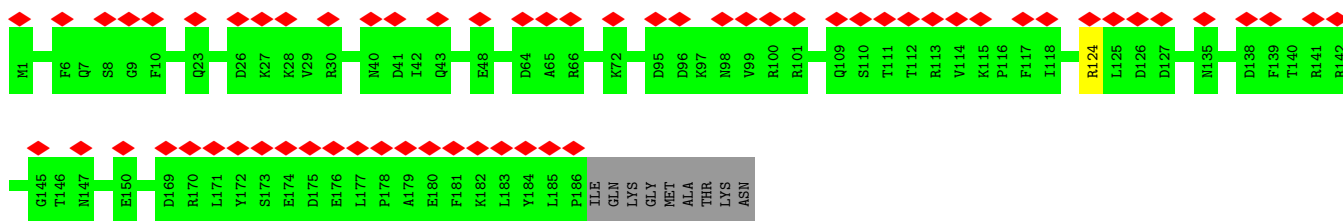




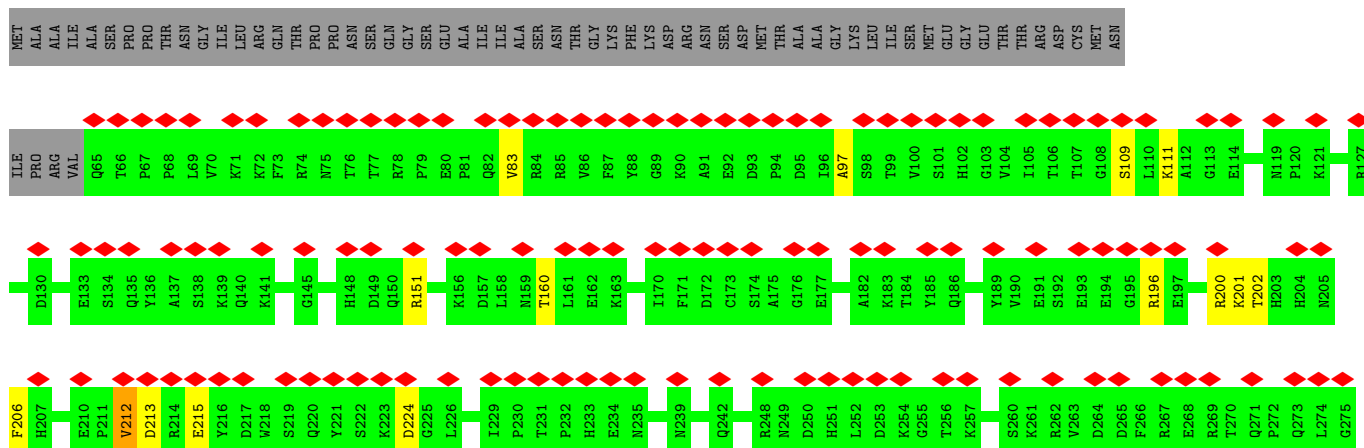
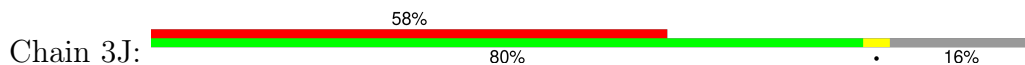
• Molecule 19: CFA20 domain-containing protein



• Molecule 19: CFA20 domain-containing protein



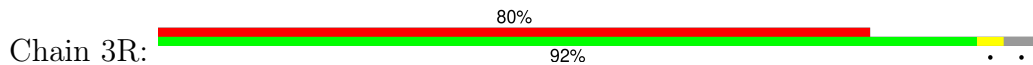
• Molecule 20: EF-hand domain-containing protein



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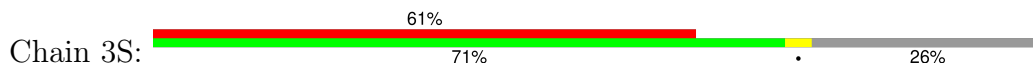
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-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----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

• Molecule 22: CFAP276



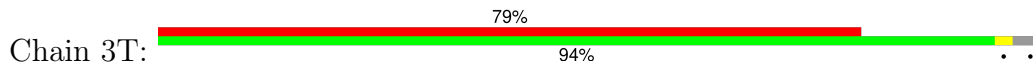
MET	SER	ASN	ILE	GLU	MET	S7	N8	R9	D10	F14	E15	K16	L17	E18	M19	D20	T21	S22	F23	F24	G25	T26	N27	E28	T29	Q30	K31	M32	P33	Y34	G35	E36	P37	T38	H39	I40	A41	Q42	T43	K44	D45	R49	L50	N51	S52	T53	C54	A57	S58	R61	E62	V63	Y64	H65	H66
D67	P68	K69	A70	F71	R72	D73	S74	L75	F77	N82	Y83	D84	H85	H86	G87	E88	L89	L90	R93	S94	E95	M98	Q99	P100	E101	T102	L103	G104	A105	M106	H107	G108	R109	I110	L111	K112	M113	R114	V115	P116	E117	K118	V119	A120	E121	P122	V123	S124	P125	T126	G127	K128	L129	T130	I131
V132	S133	I134	H135	T136	P137	K138	K139	E140	S141	I142	H143	S144	V145	K146	G147	A148	I149	E150	S151	H152	H153	T154	P155	A156	T157	M158	Q159	G160	F161	S162	K164	H166	D166	G167	G168	F169	Y170	T171	THR																

• Molecule 22: CFAP276

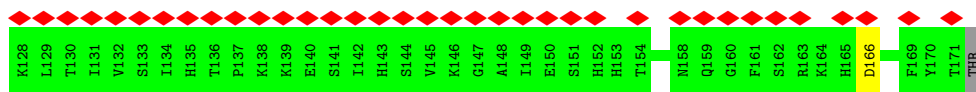


MET	SER	ASN	ILE	GLU	MET	SER	ASN	ARG	ASP	PRO	TYR	PRO	PHE	GLU	LYS	LEU	GLU	ASN	ASP	THR	SER	PHE	PHE	GLY	THR	ASN	GLU	THR	GLN	LYS	MET	PRO	TYR	GLY	GLU	PRO	THR	HIS	ILE	ALA	GLN	THR	LYS	D45	P46	W47	Q48	R49	L50	N51	S52	T53	C54	T55	S58	S59	R60	R61
E62	V63	Y64	H65	H66	D67	P68	K69	A70	P71	R72	D73	D76	K80	A81	N82	Y83	D84	H85	H86	G87	E88	L89	L90	K91	N92	R93	S94	E95	T96	L97	M98	Q99	P100	E101	T102	L103	G104	A105	M106	H107	G108	R109	I110	L111	K112	M113	R114	V115	P116	E117	K118	V119	A120	E121	P122	V123	S124	
P125	T126	G127	K128	L129	T130	I131	S132	S133	I134	H135	P136	K138	K139	E140	S141	I142	H143	V145	K146	G147	A148	I149	S151	H152	H153	T154	P155	A156	T157	N158	Q159	G160	F161	S162	K164	H166	D166	F169	Y170	T171	THR																	

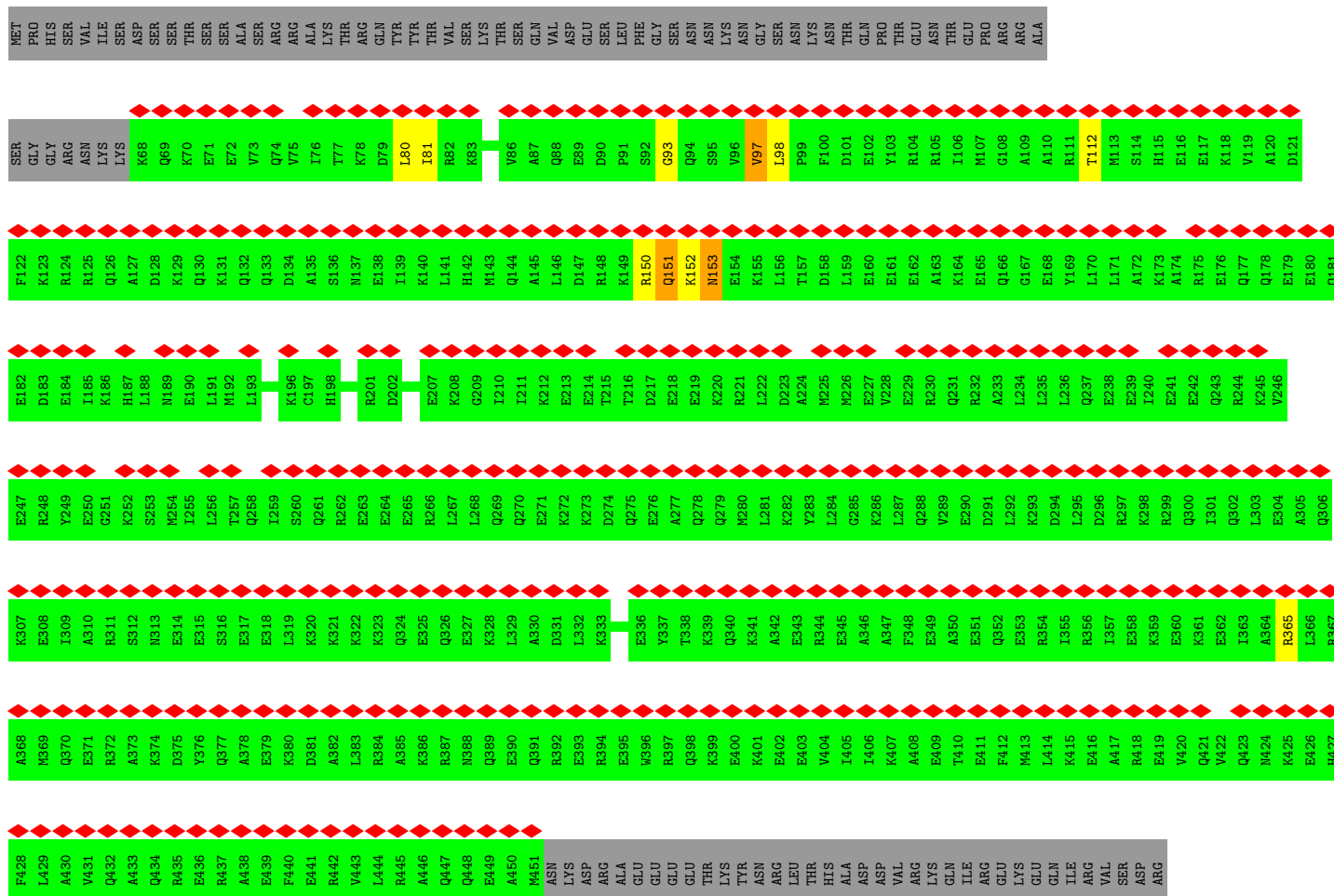
• Molecule 22: CFAP276



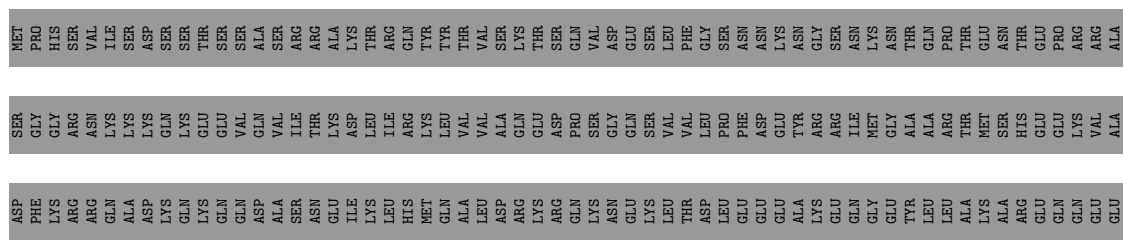
MET	SER	ASN	ILE	GLU	MET	S7	N8	R9	D10	P11	Y12	P13	F14	E15	K16	L17	E18	M19	D20	T21	S22	F23	F24	G25	T26	N27	E28	T29	Q30	K31	M32	P33	Y34	G35	E36	P37	T38	H39	I40	A41	Q42	T43	K44	D45	Q48	R49	T53	C54	A57	R60	R61	E62	V63	Y64	H65		
H66	D67	P68	K69	A70	F71	R72	D73	S74	L75	D76	K80	A81	N82	Y83	D84	H85	H86	E88	L89	L90	K91	N92	R93	S94	E95	T96	L97	M98	Q99	P100	E101	T102	L103	G104	A105	M106	H107	G108	I109	I110	L111	K112	M113	R114	V115	P116	E117	K118	V119	A120	E121	P122	V123	S124	P125	T126	G127



• Molecule 23: Cilia- and flagella-associated protein 45



• Molecule 23: Cilia- and flagella-associated protein 45

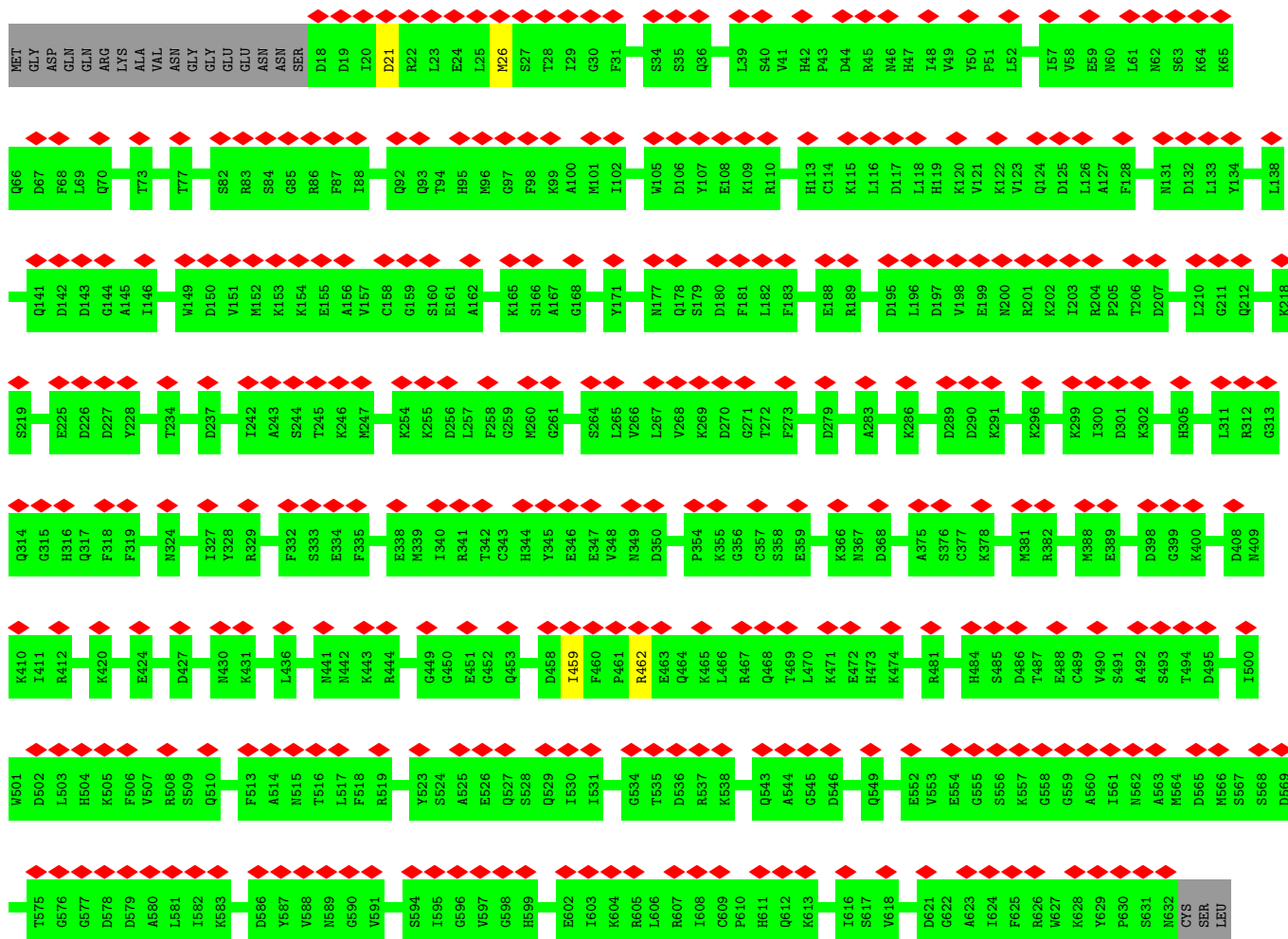


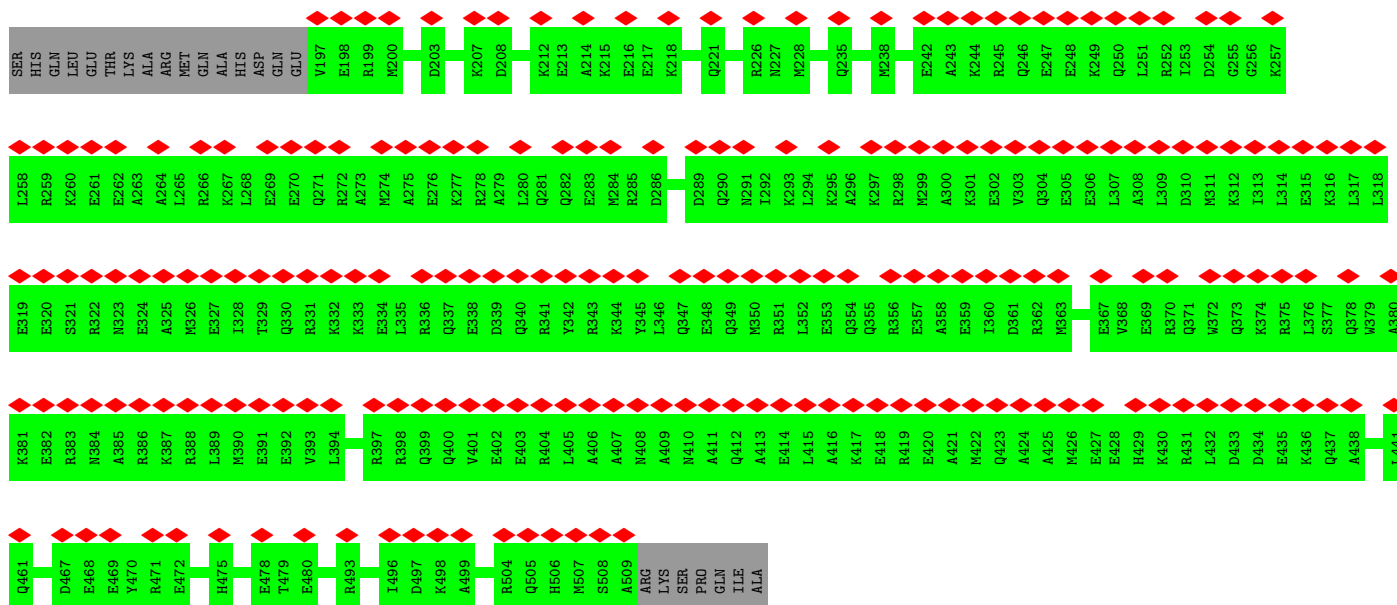


• Molecule 24: Cilia- and flagella-associated protein 52

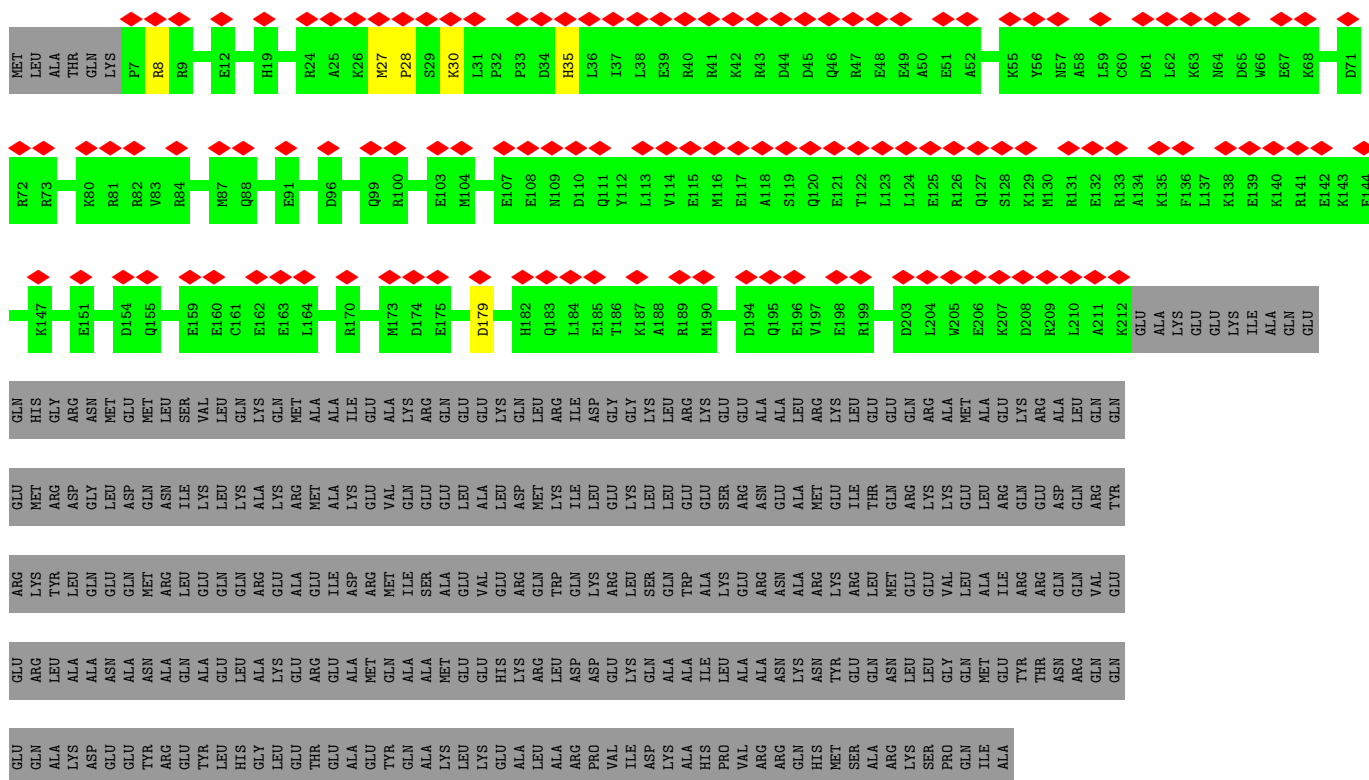


Chain 4B:



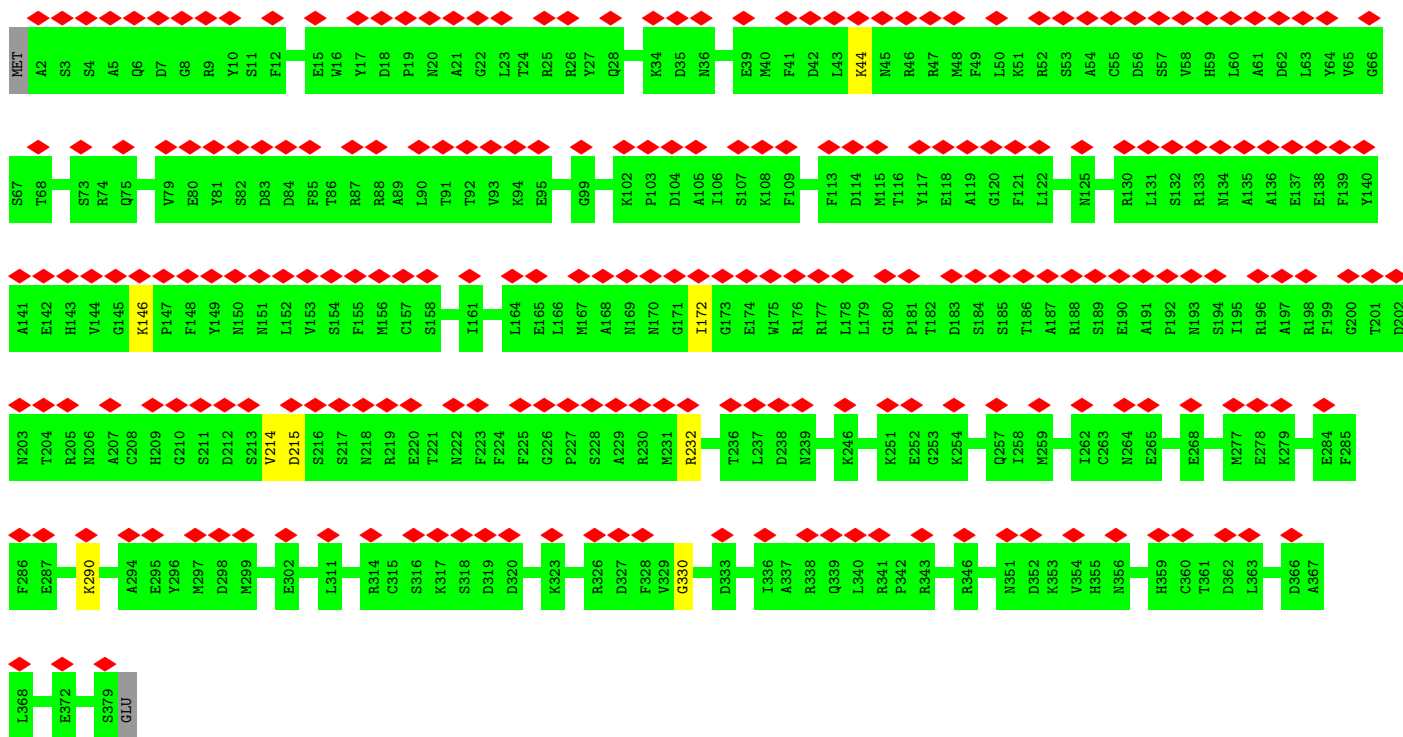


• Molecule 25: Trichohyalin-plectin-homology domain-containing protein

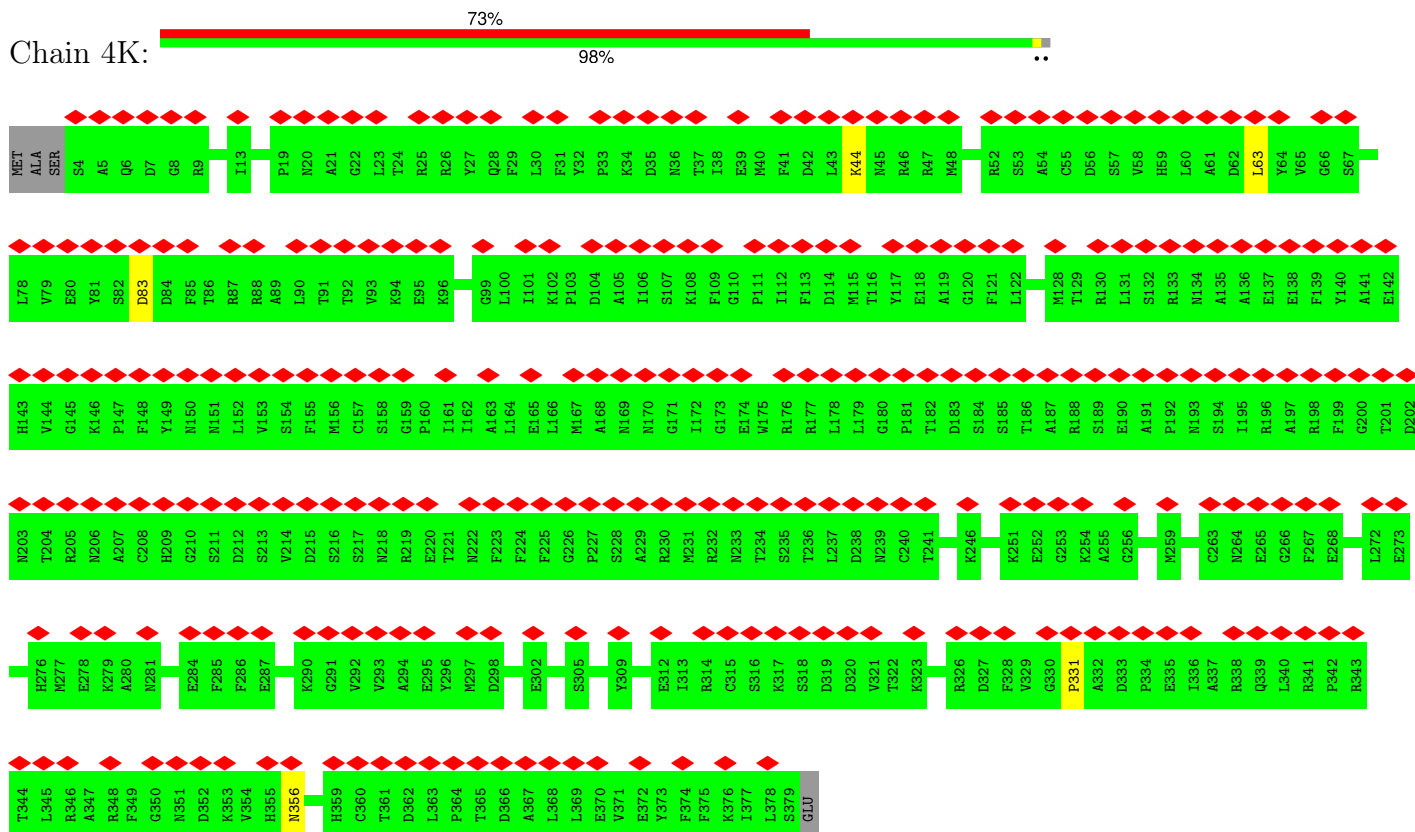


• Molecule 26: Nucleoside diphosphate kinase

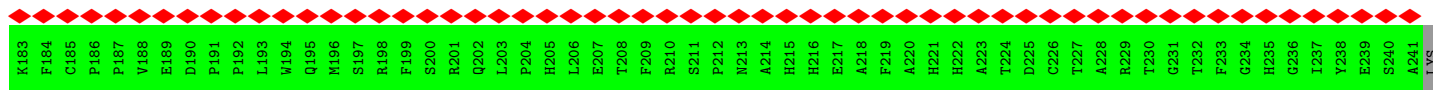




- Molecule 26: Nucleoside diphosphate kinase

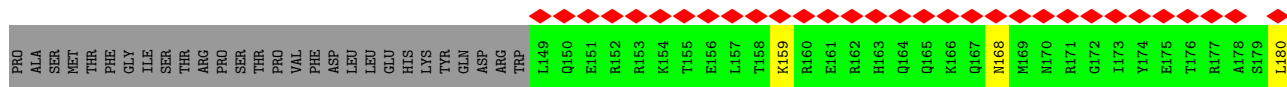
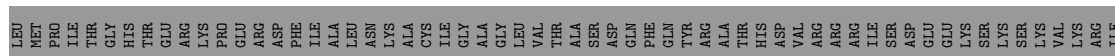
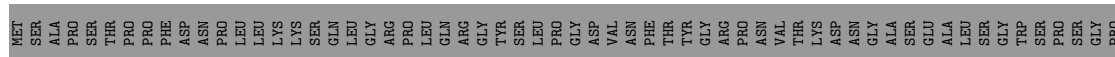


- Molecule 27: Cilia- and flagella-associated protein 77



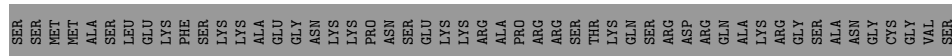
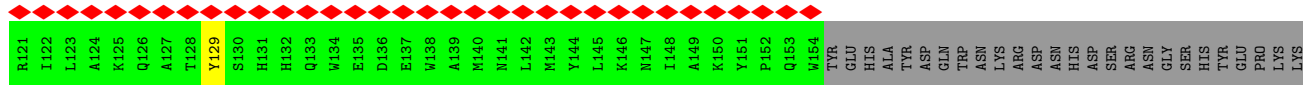
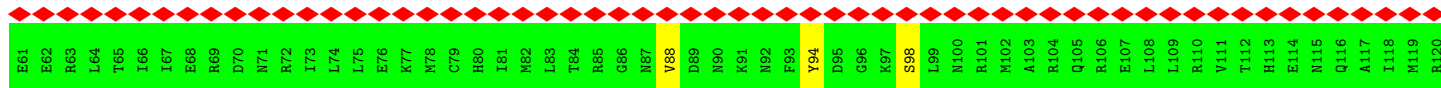
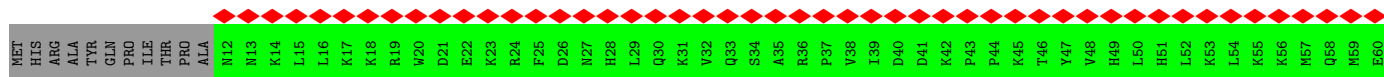
SER

• Molecule 27: Cilia- and flagella-associated protein 77

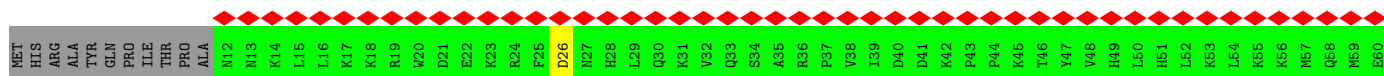


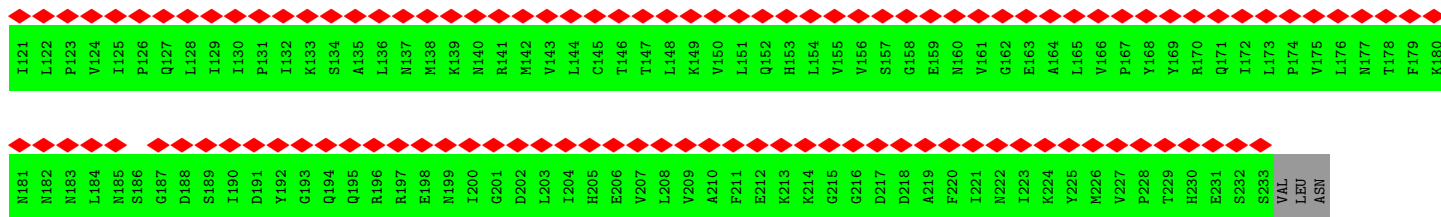
A241
LYS
SER

• Molecule 28: Cilia- and flagella-associated protein 97

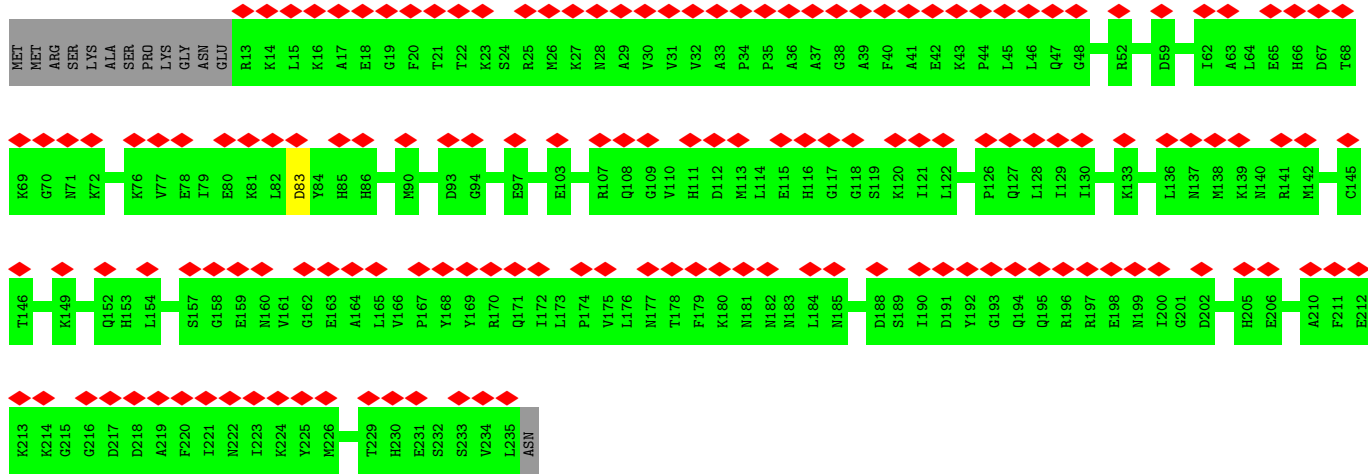


• Molecule 28: Cilia- and flagella-associated protein 97

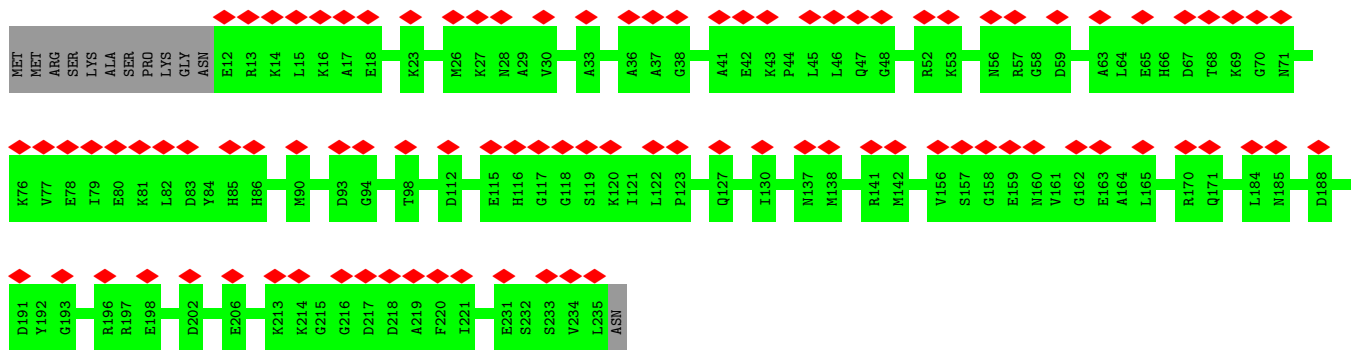
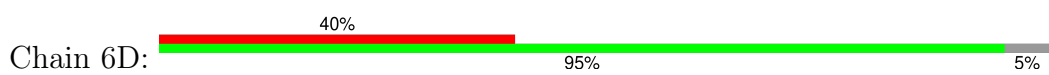




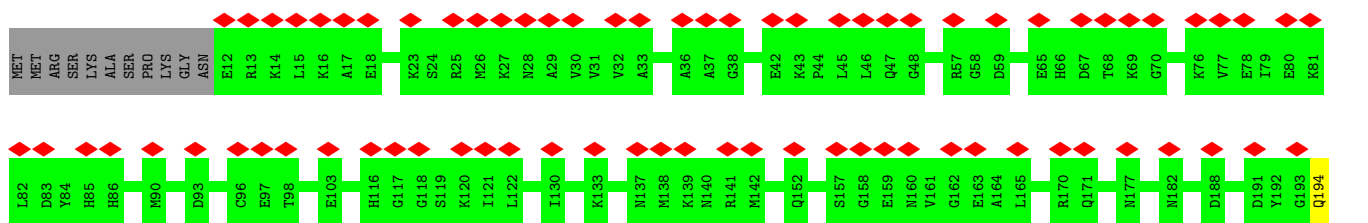
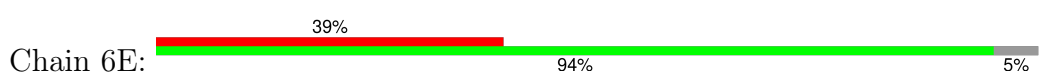
• Molecule 31: PACRG

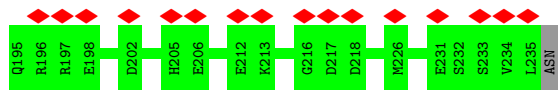


• Molecule 31: PACRG

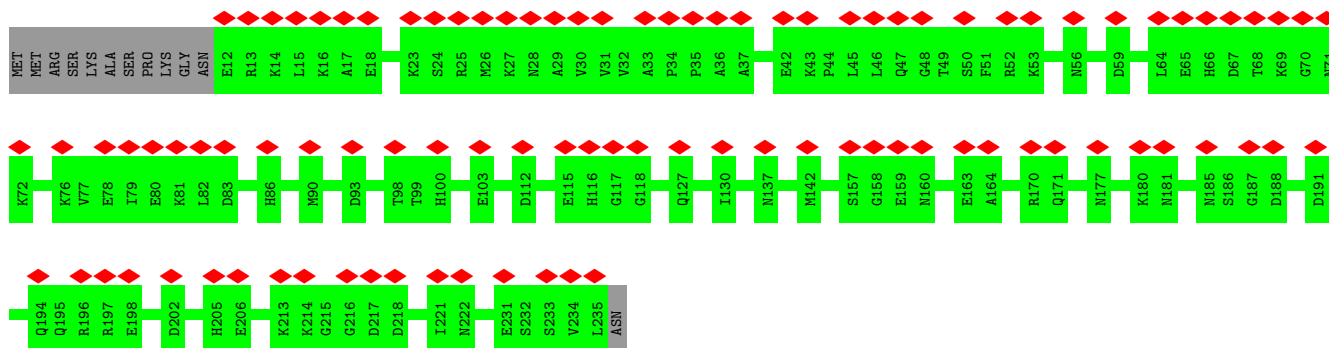
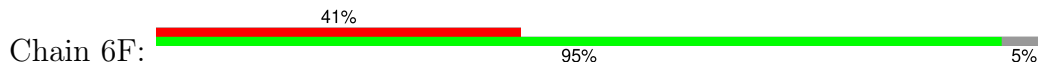


• Molecule 31: PACRG

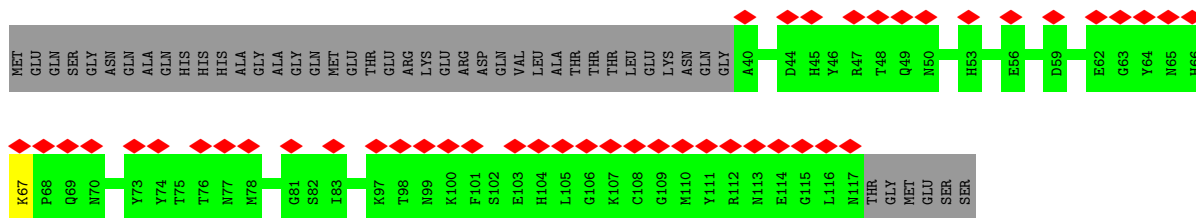




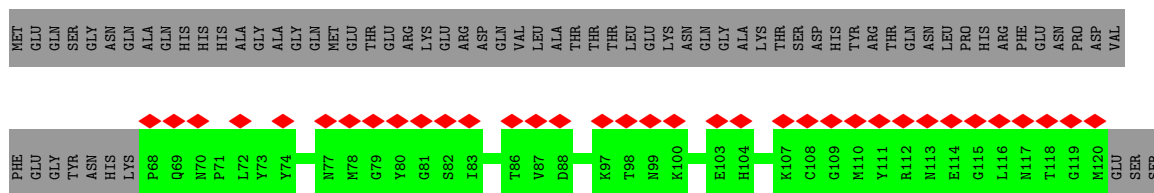
• Molecule 31: PACRG



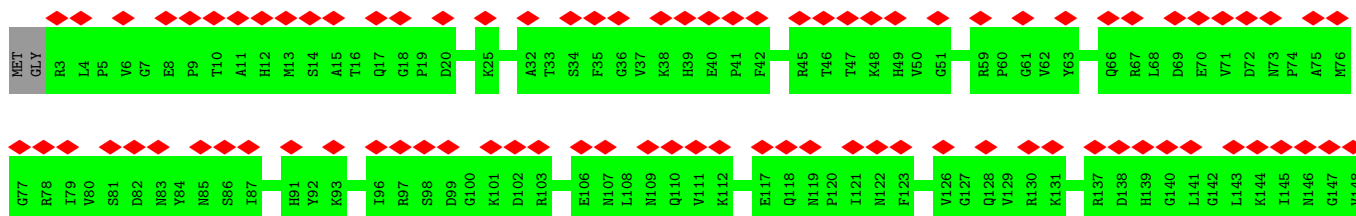
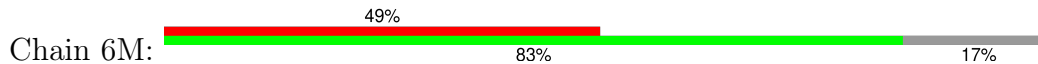
• Molecule 32: Piercel

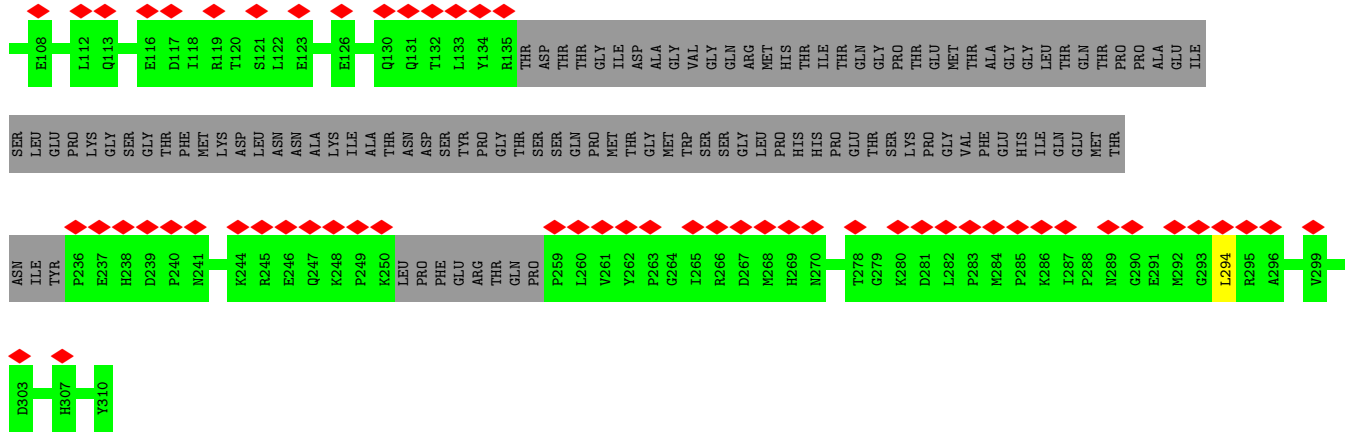


• Molecule 32: Piercel

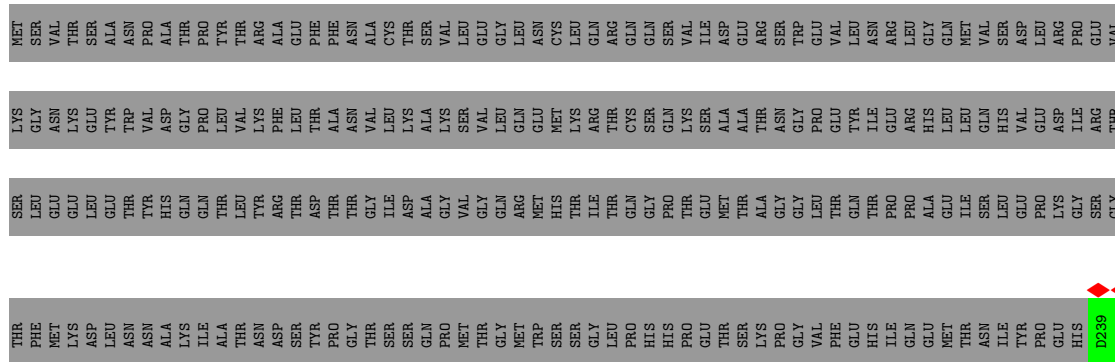


• Molecule 33: Protein phosphatase 1 regulatory subunit 32

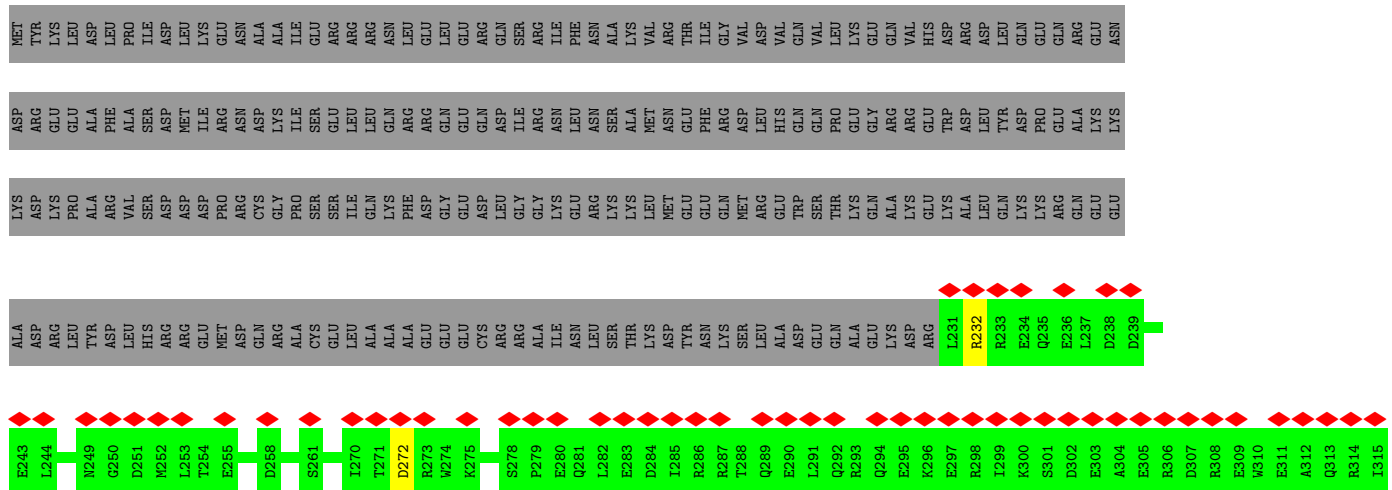


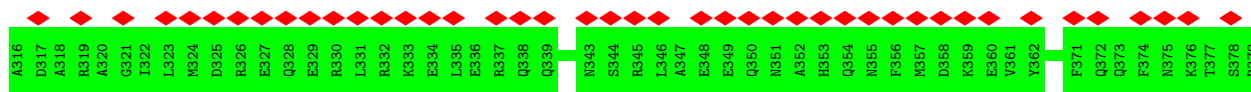


• Molecule 34: RIB35

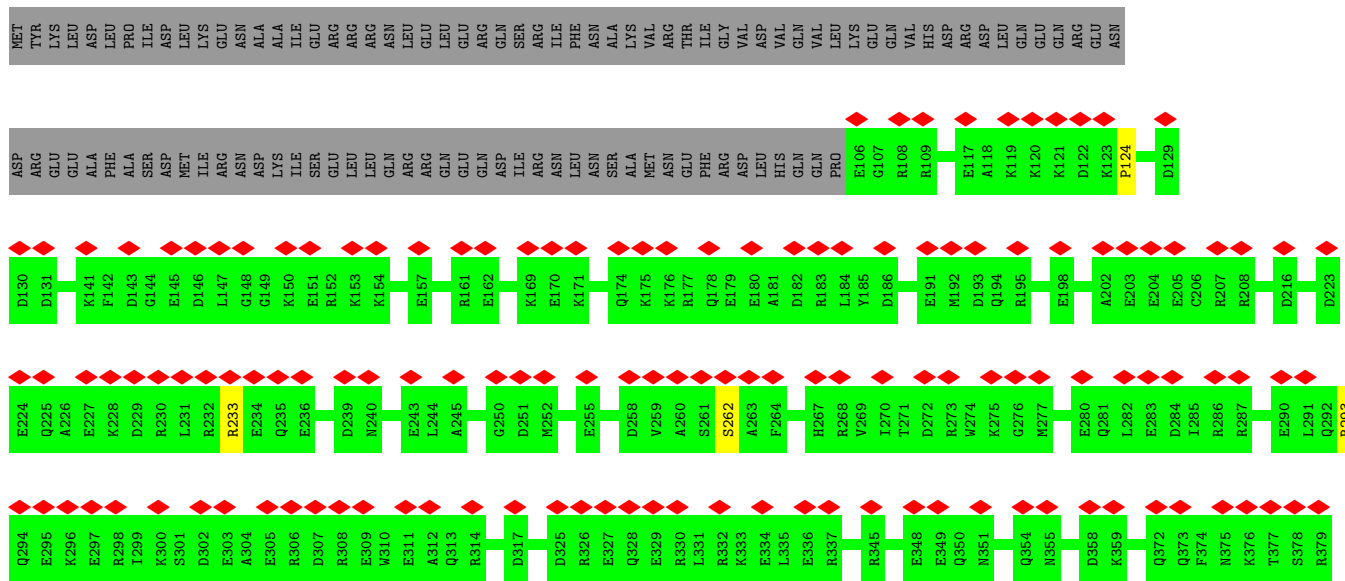
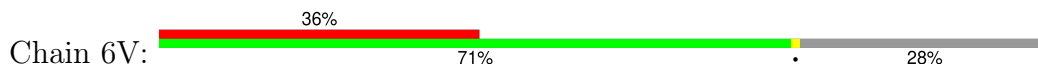


• Molecule 35: RIB43A-like with coiled-coils protein 2

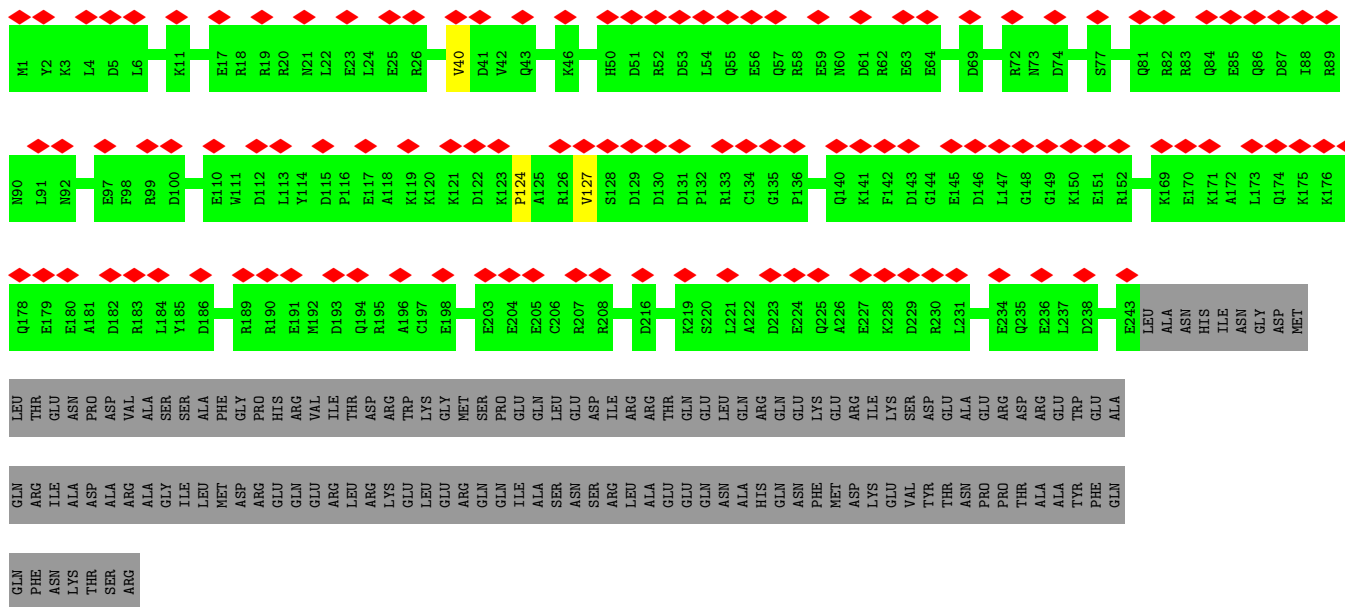




• Molecule 35: RIB43A-like with coiled-coils protein 2



• Molecule 35: RIB43A-like with coiled-coils protein 2

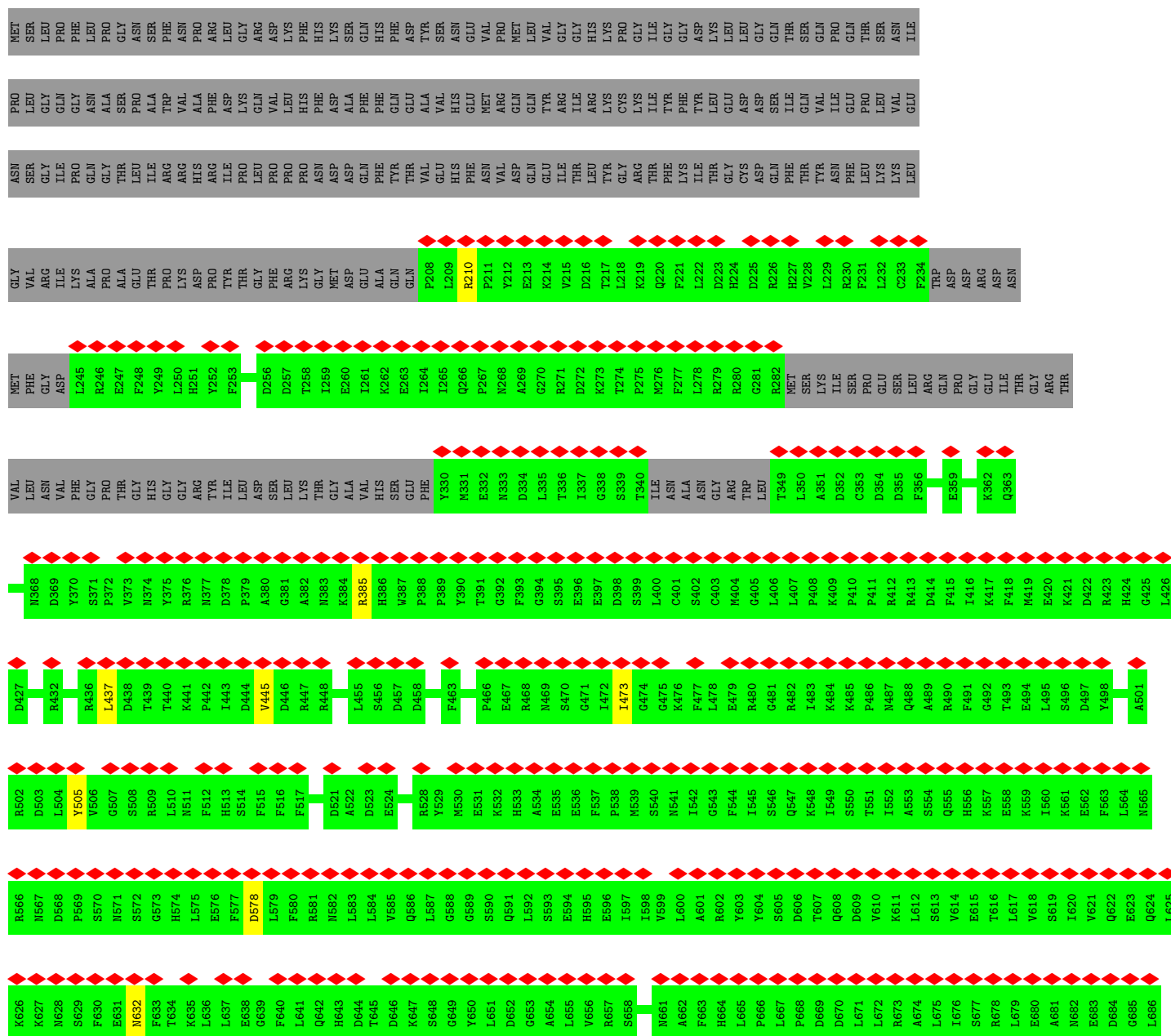


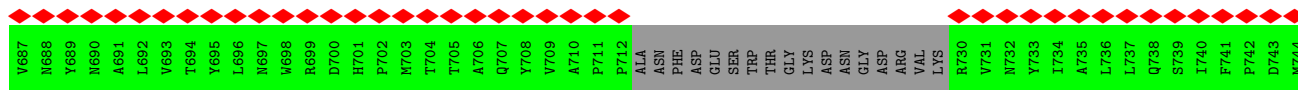
• Molecule 35: RIB43A-like with coiled-coils protein 2



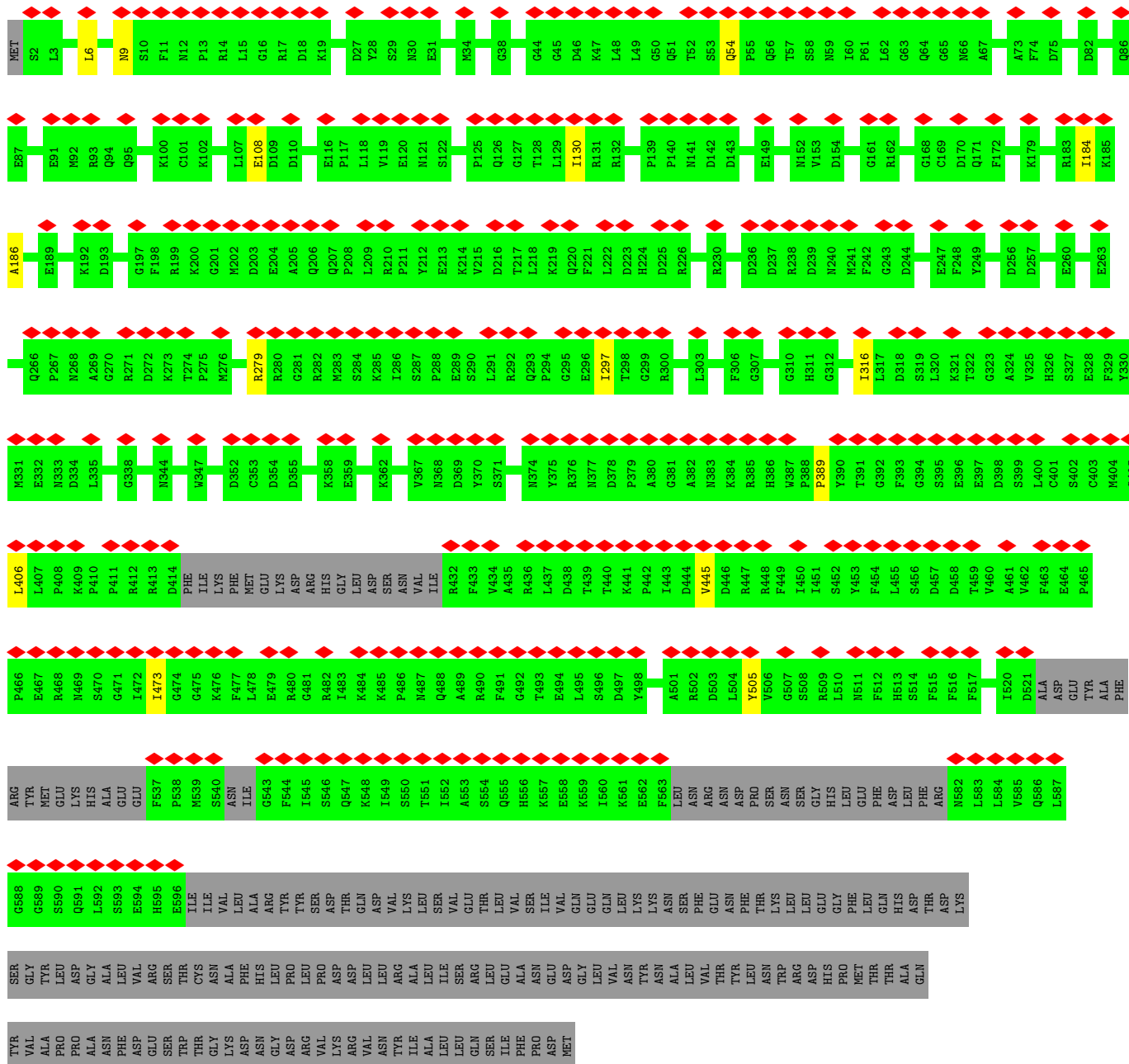
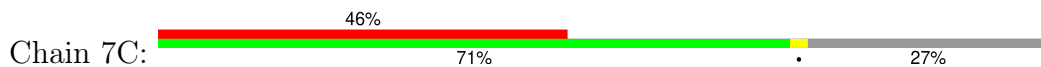


● Molecule 36: EF-hand domain-containing family member C2



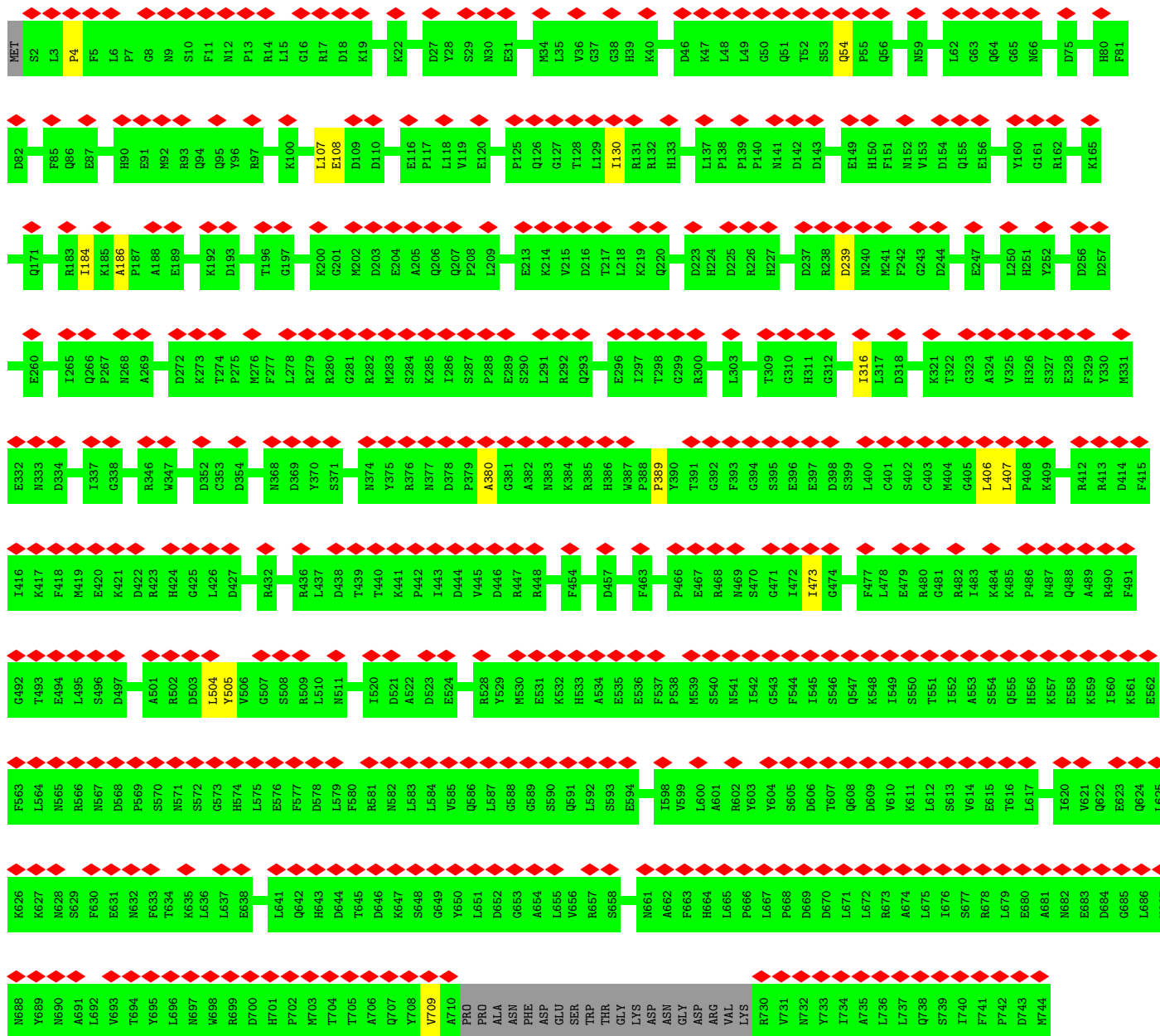


• Molecule 36: EF-hand domain-containing family member C2

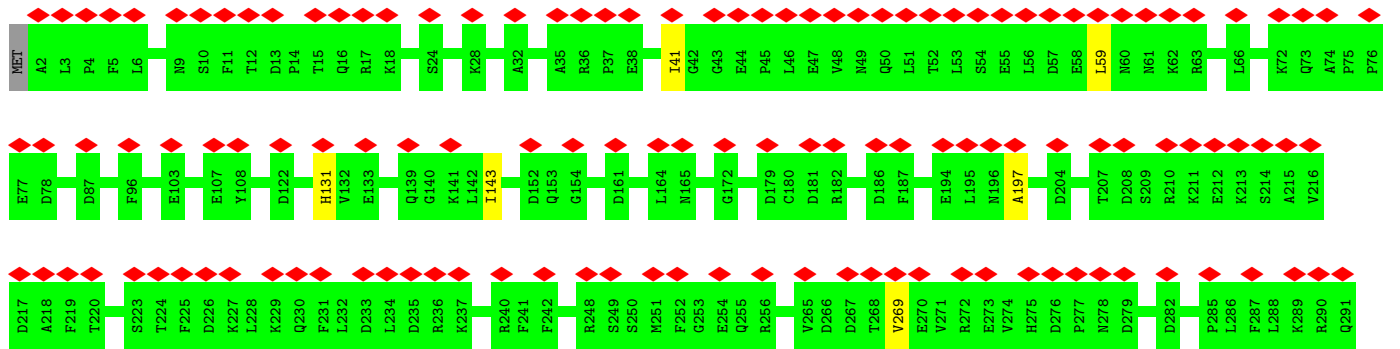
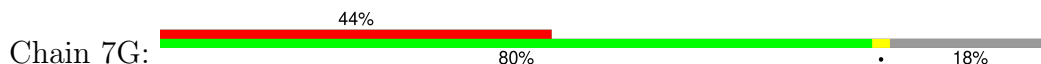


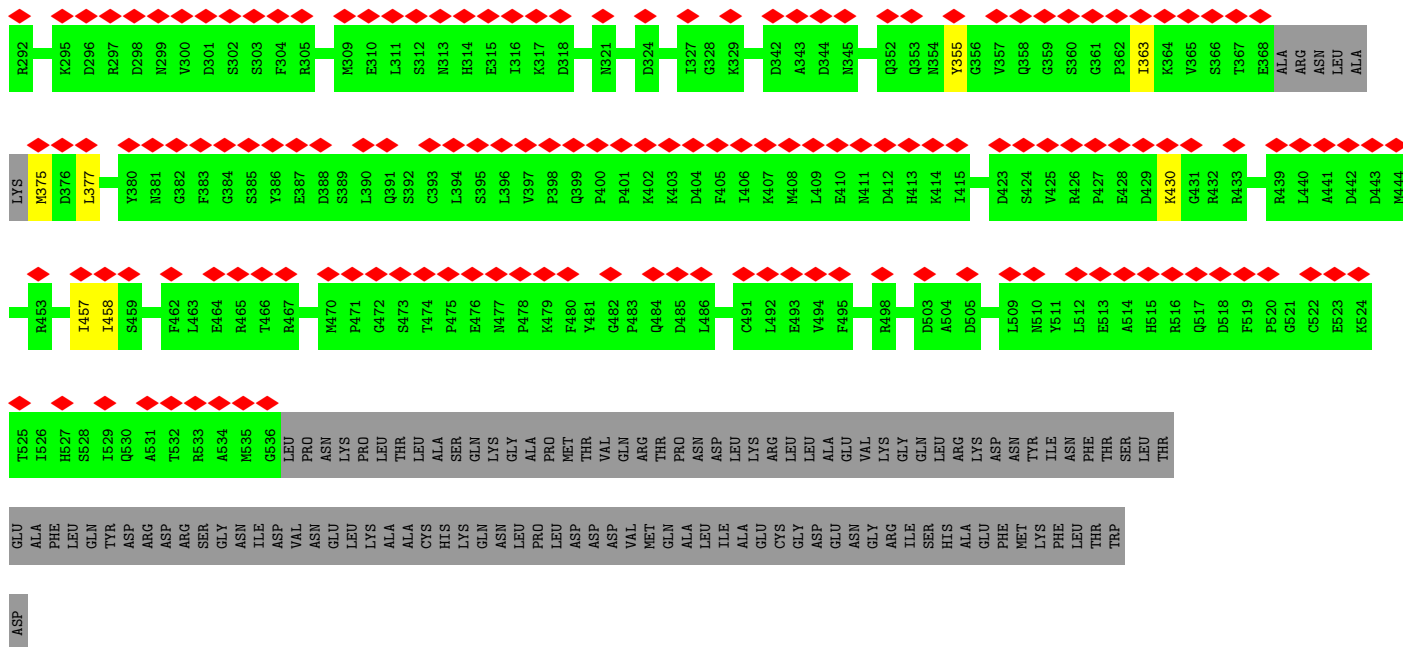
• Molecule 36: EF-hand domain-containing family member C2



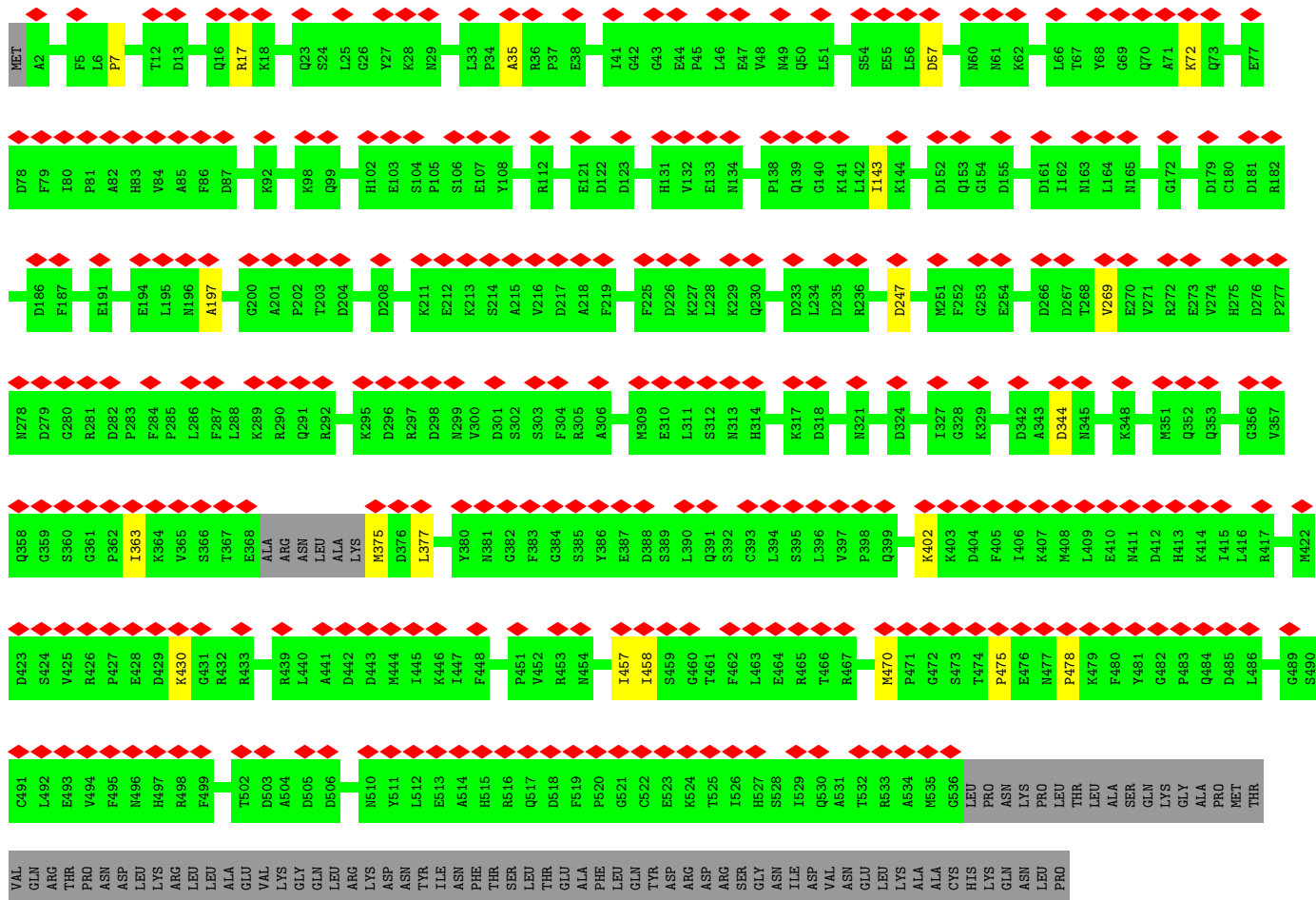
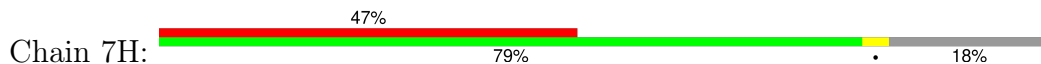


● Molecule 37: Flagellar protofilament ribbon protein rib74



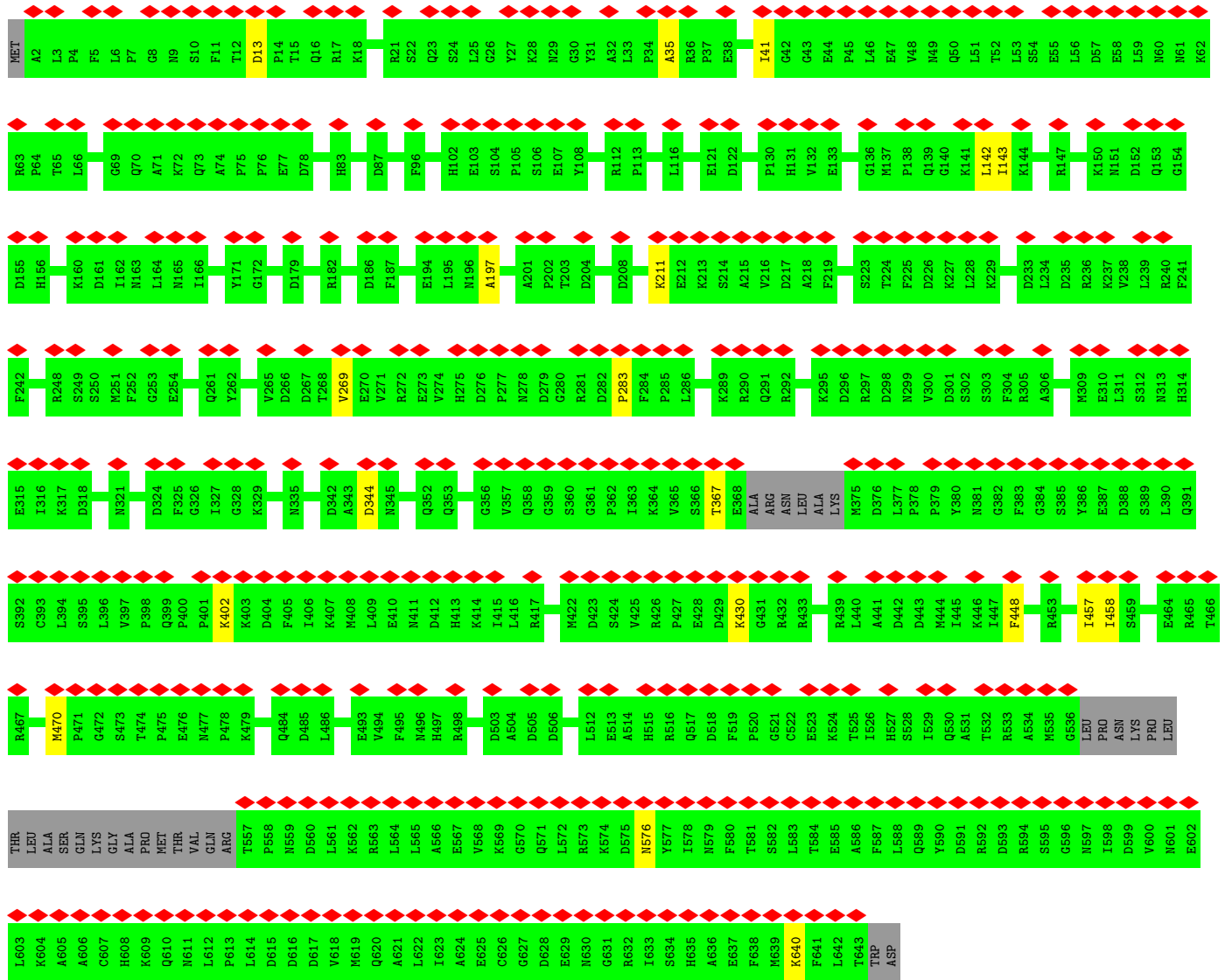
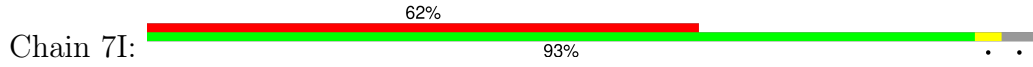


● Molecule 37: Flagellar protofilament ribbon protein rib74

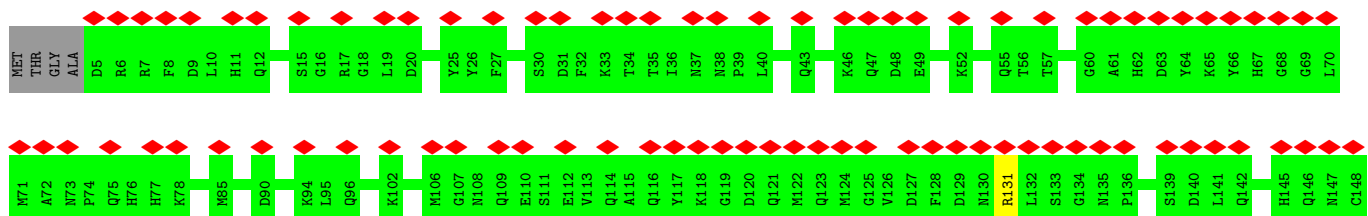
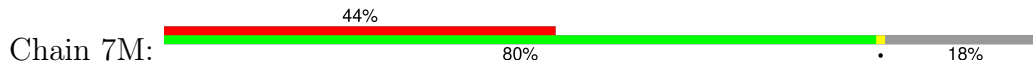


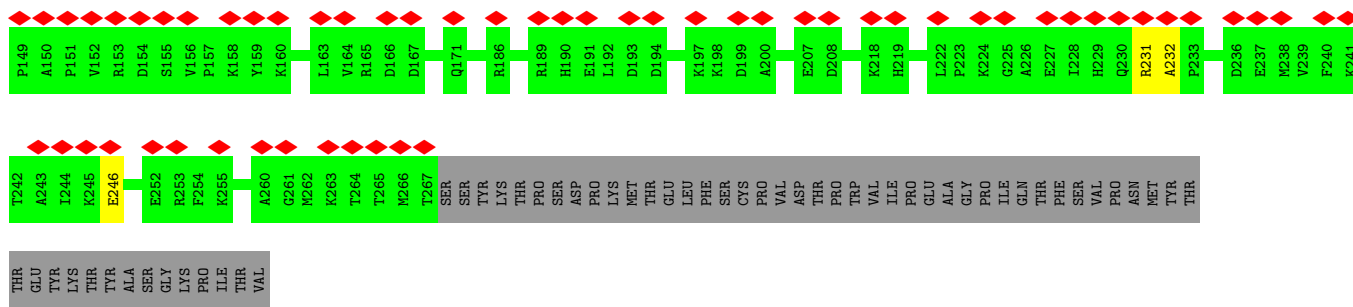
LEU ASP ASP VAL MET MET GLN ALA LEU LEU LEU LEU LEU CYS GLY ASP ASP GLU ASN GLY ARG ILE SER HIS ALA ALA GLU PHE MET LYS PHE LEU THR THR ASP

• Molecule 37: Flagellar protofilament ribbon protein rib74

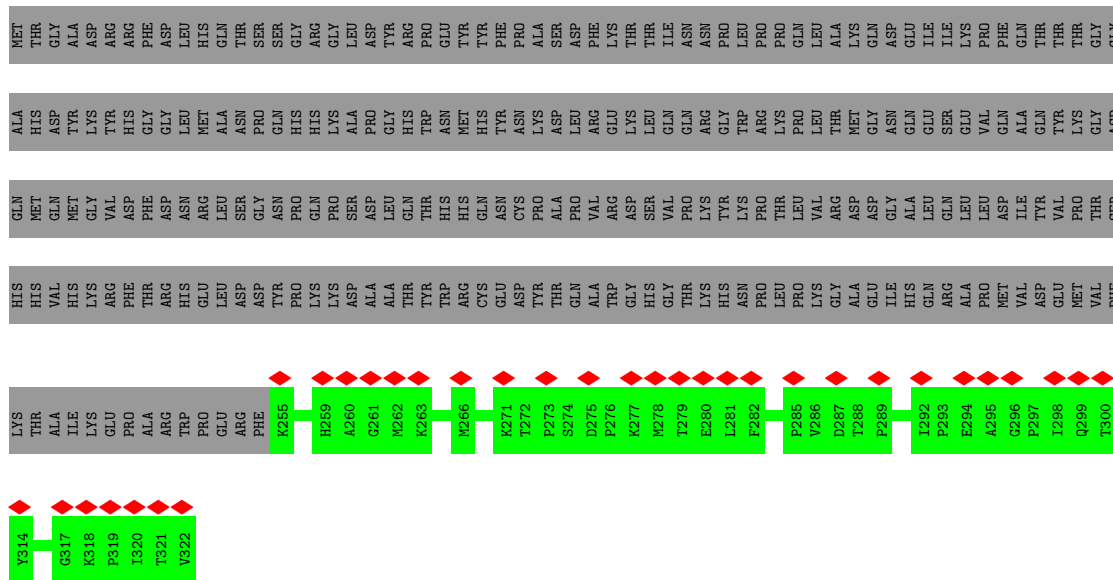


• Molecule 38: SAXO3(LOC115918676)

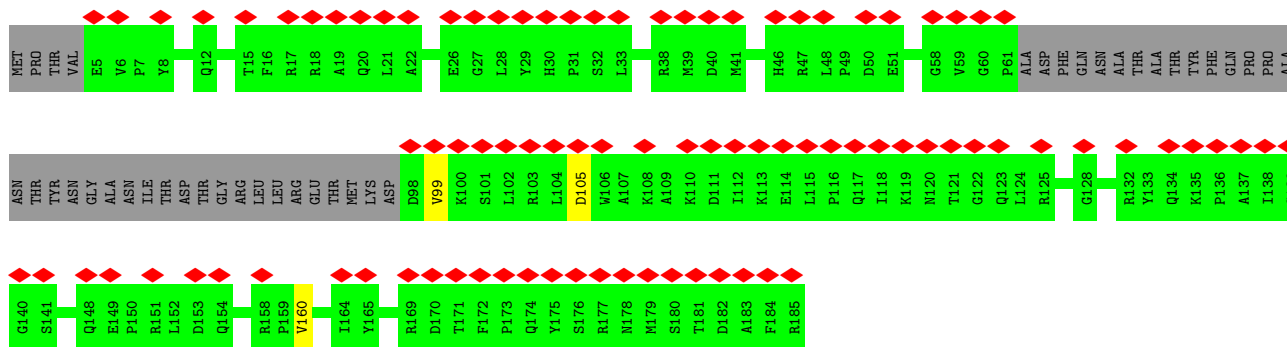
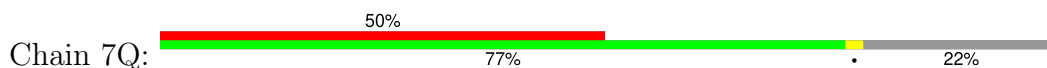




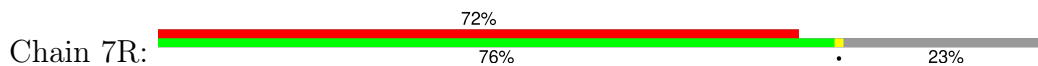
• Molecule 38: SAXO3(LOC115918676)

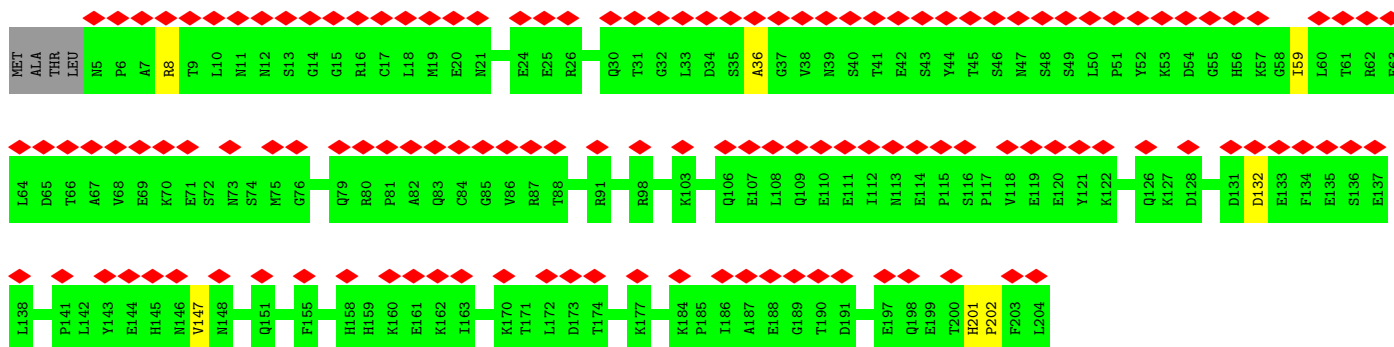


• Molecule 39: TEPP protein

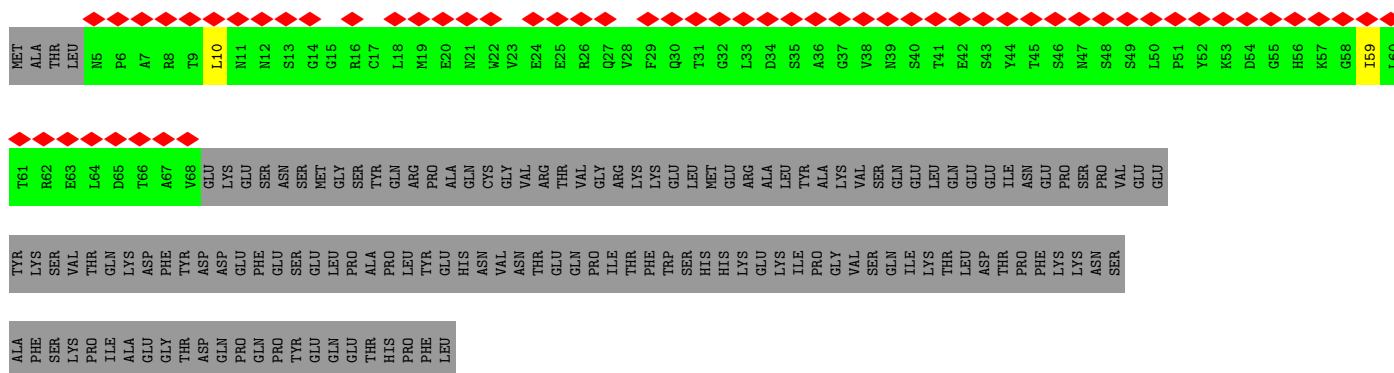


• Molecule 39: TEPP protein

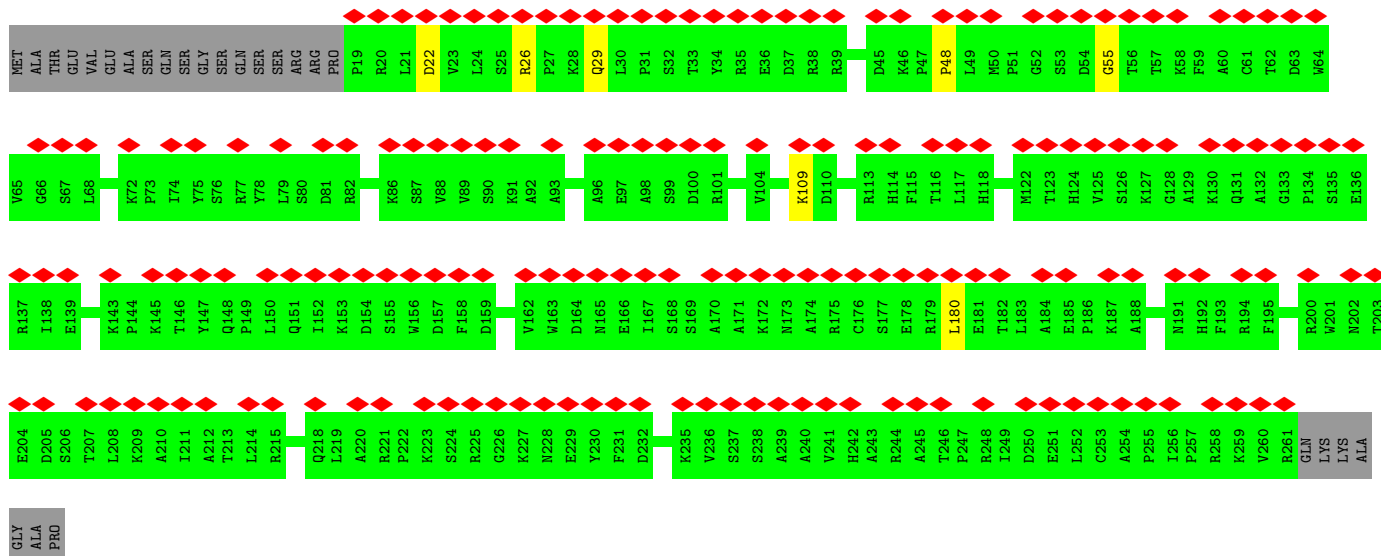
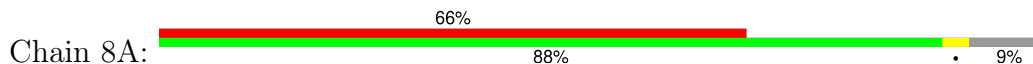




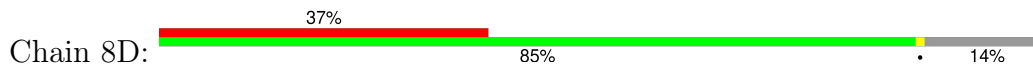
• Molecule 41: Sperm-associated antigen 8



• Molecule 42: Testicular haploid expressed gene protein-like

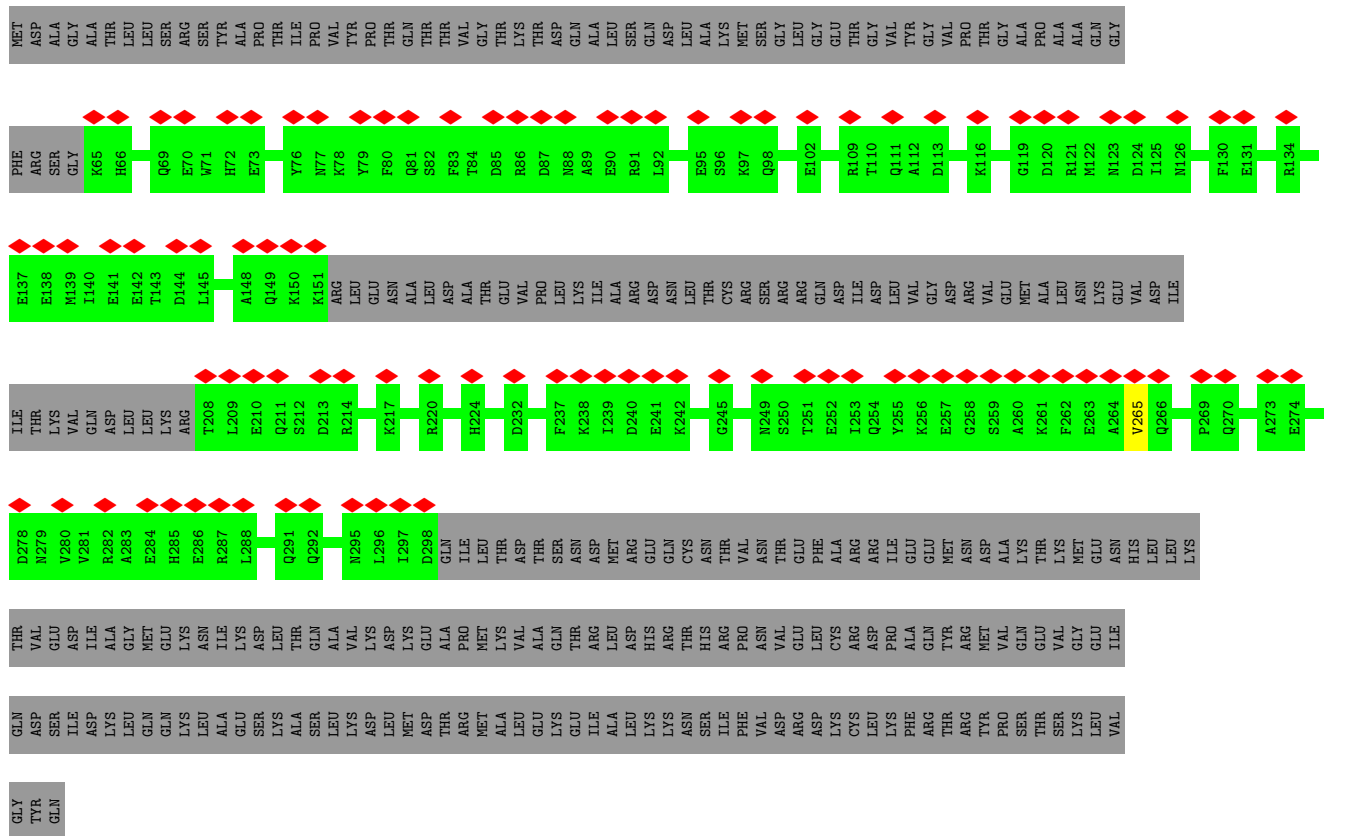


• Molecule 43: Tektin

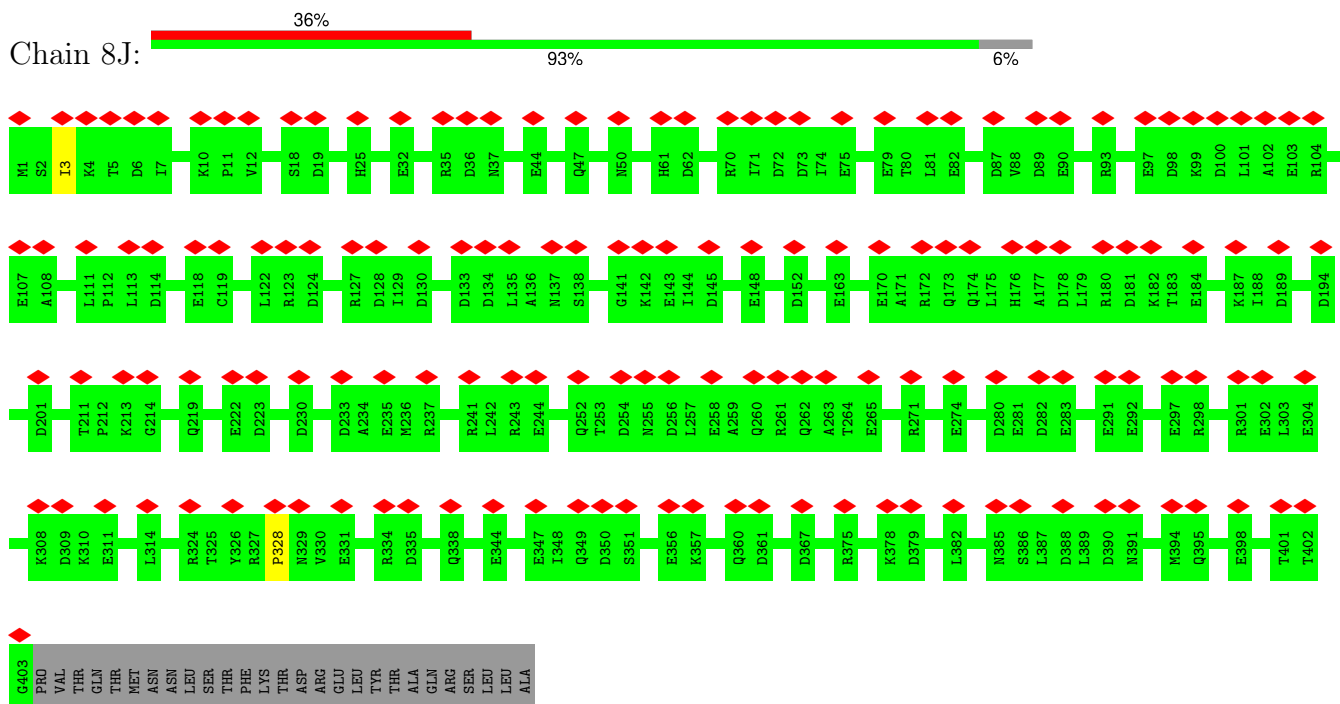




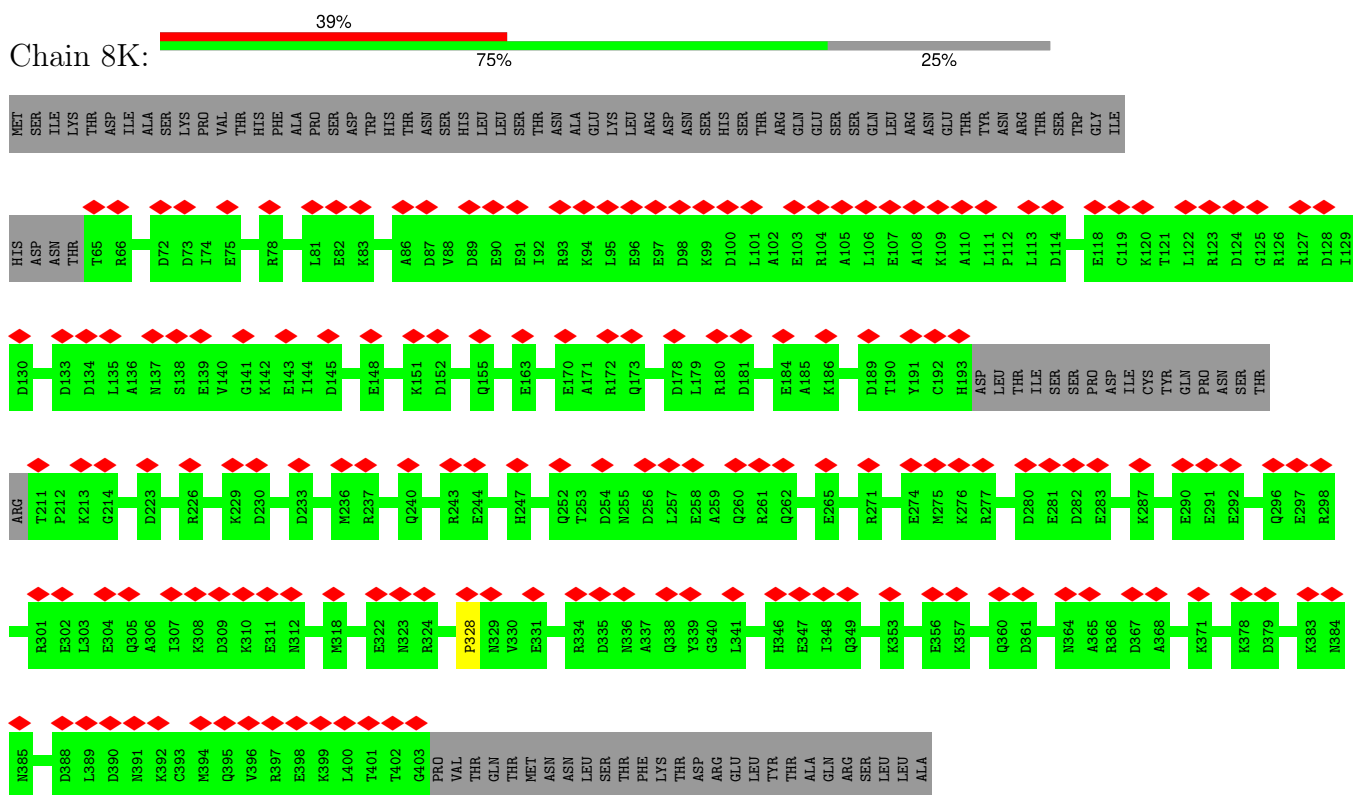
• Molecule 43: Tektin



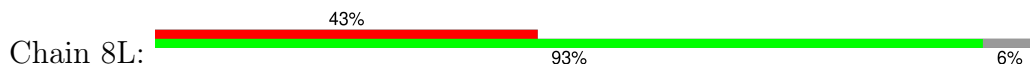
• Molecule 43: Tektin



• Molecule 44: Tektin

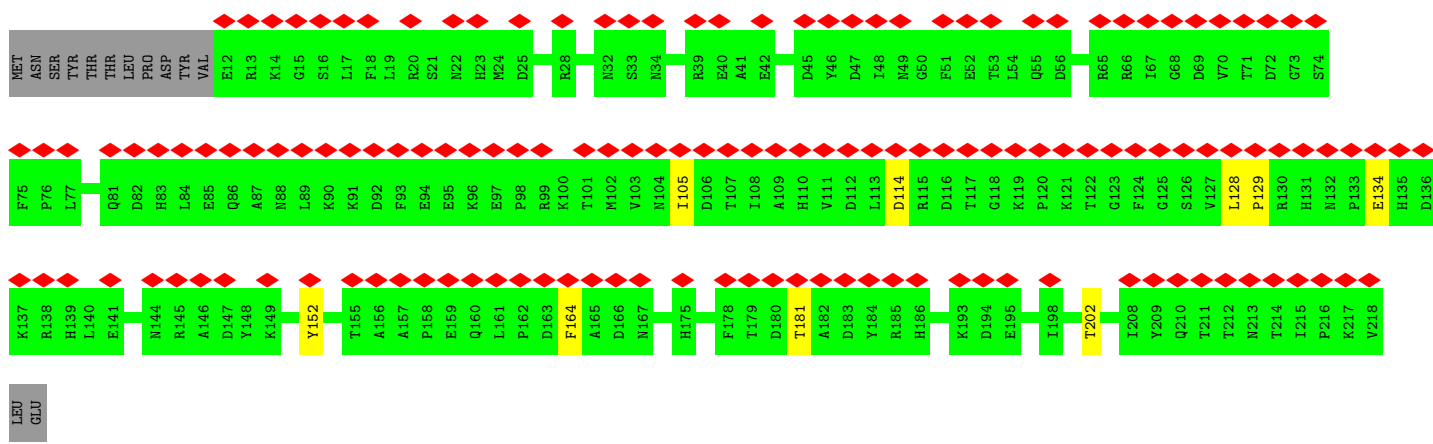
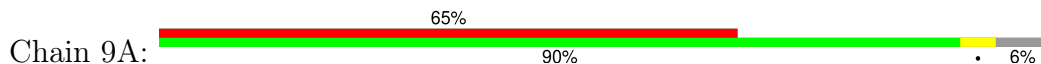


• Molecule 44: Tektin

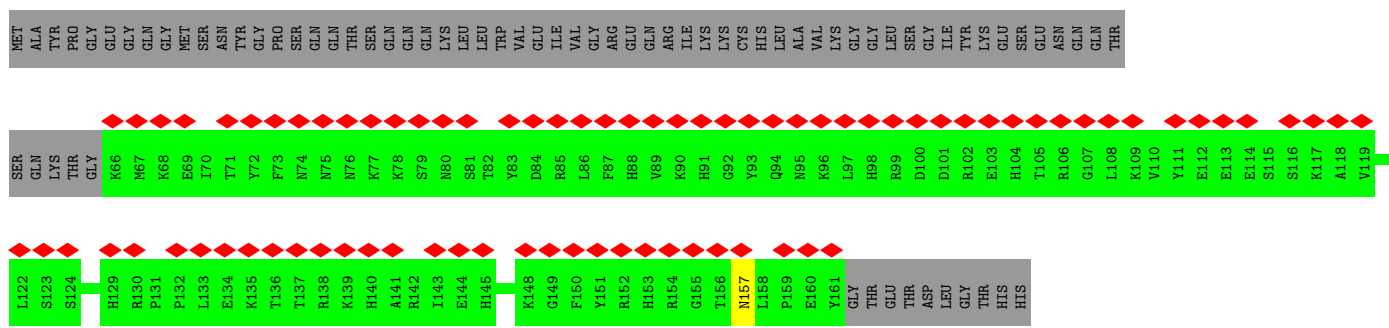




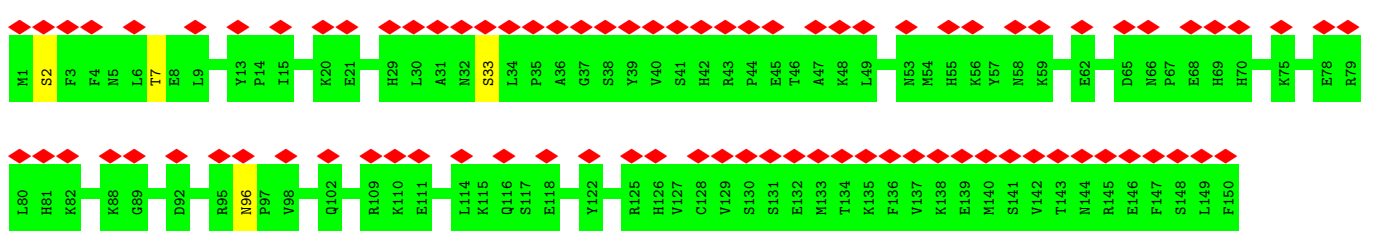
• Molecule 47: Tex36(CFAP95, C9orf135)



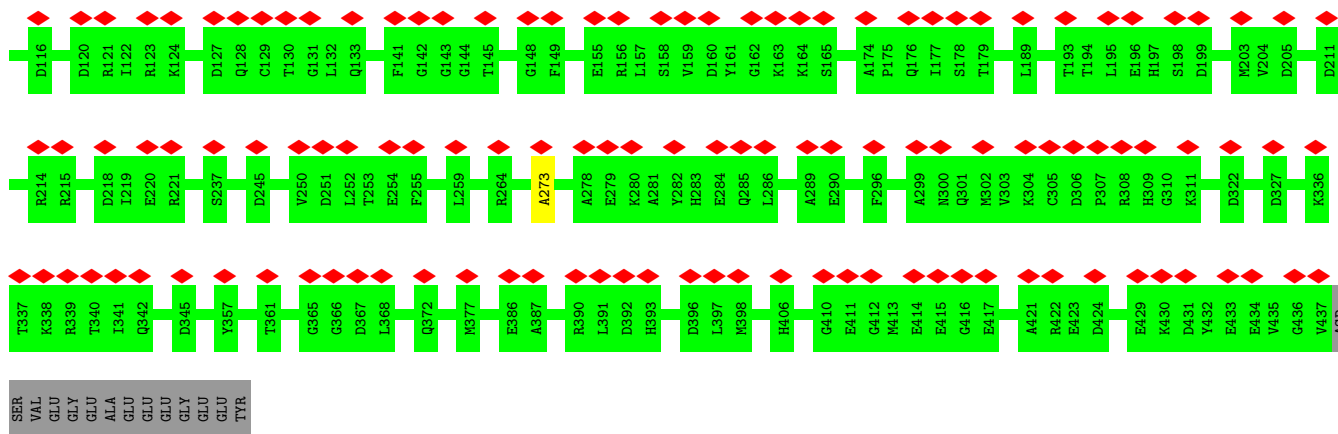
• Molecule 48: CFAP90(C5orf49)



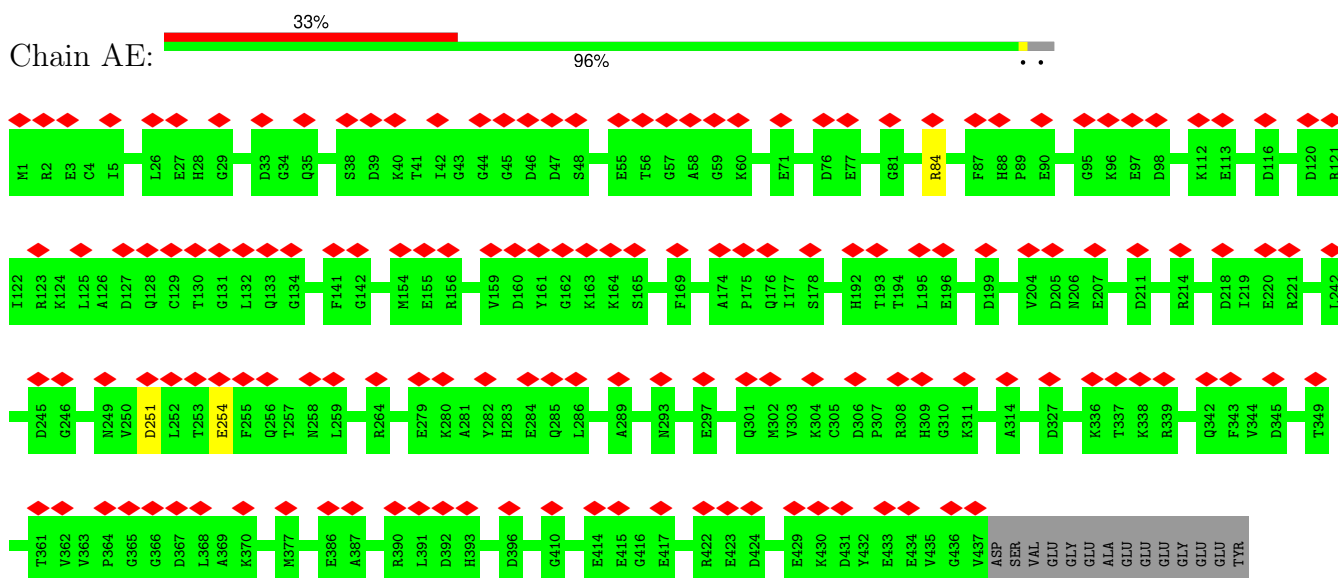
• Molecule 49: Tex49



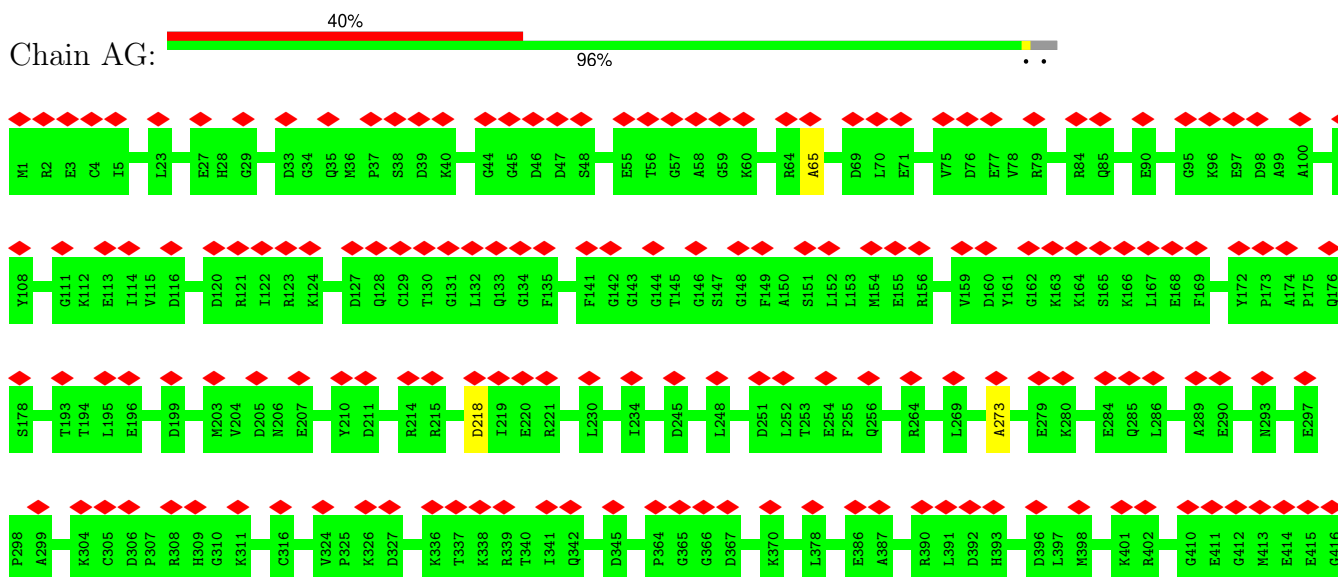
• Molecule 50: Tex49_homologue(LOC580808)

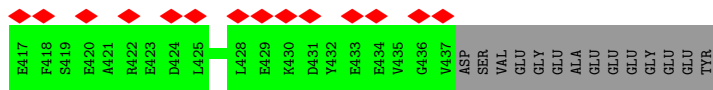


• Molecule 54: Tubulin alpha chain

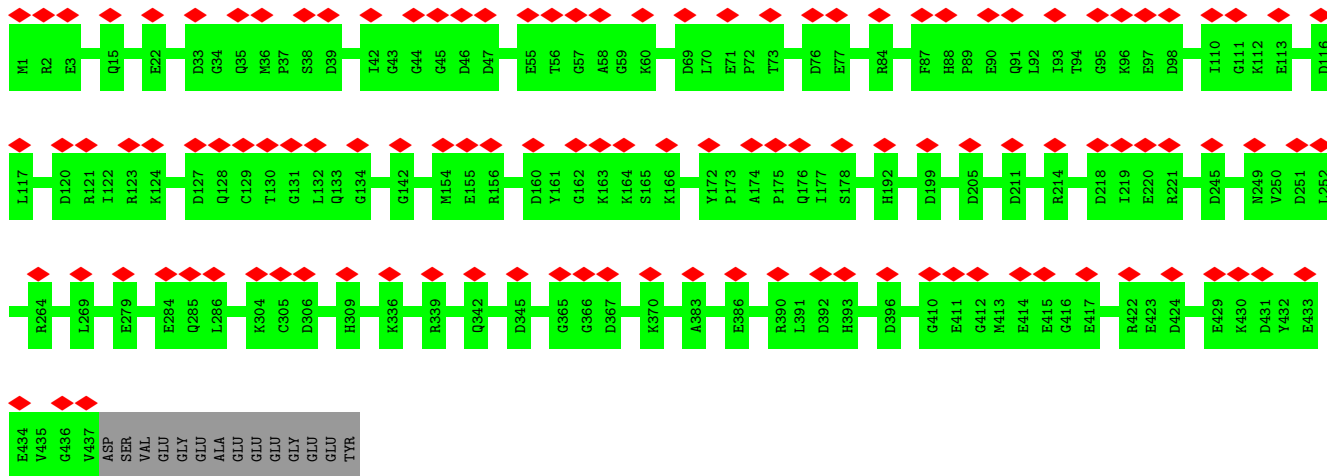


• Molecule 54: Tubulin alpha chain

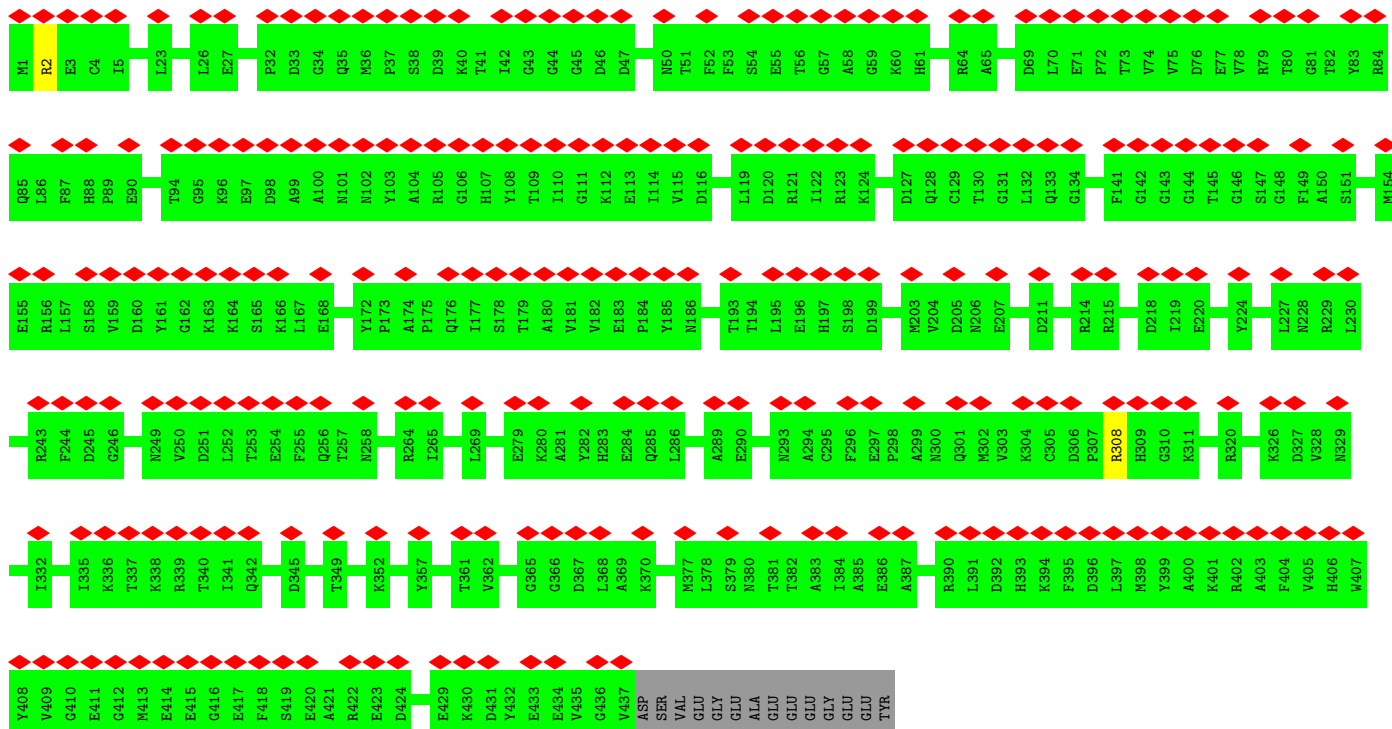




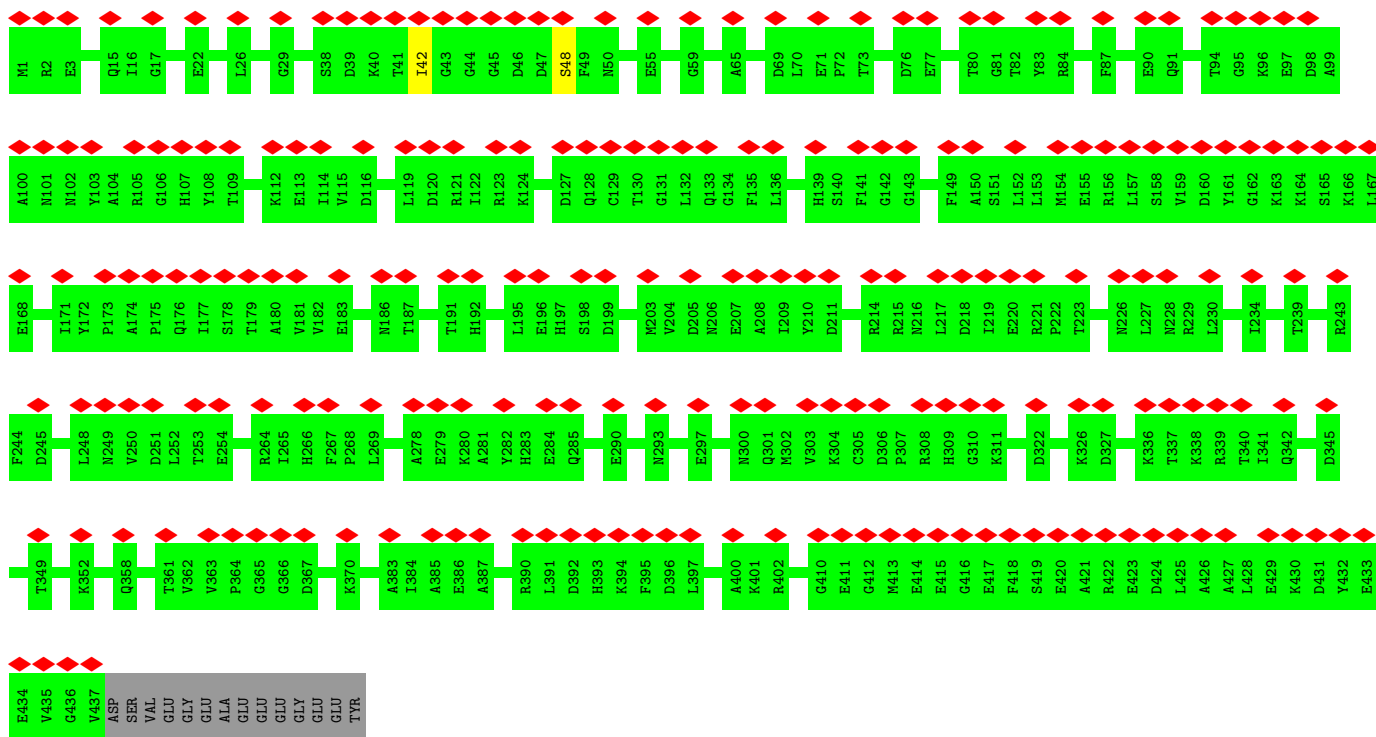
• Molecule 54: Tubulin alpha chain



• Molecule 54: Tubulin alpha chain



• Molecule 54: Tubulin alpha chain

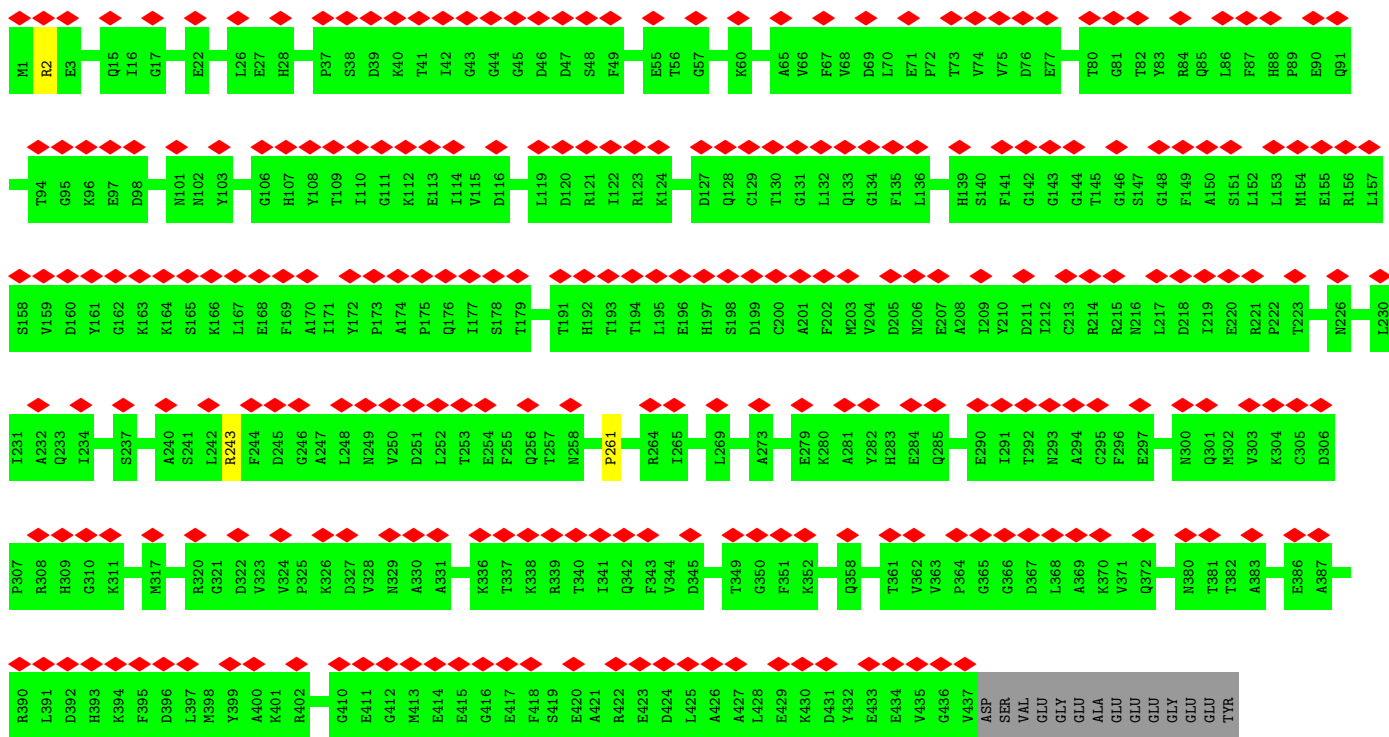


• Molecule 54: Tubulin alpha chain



• Molecule 54: Tubulin alpha chain

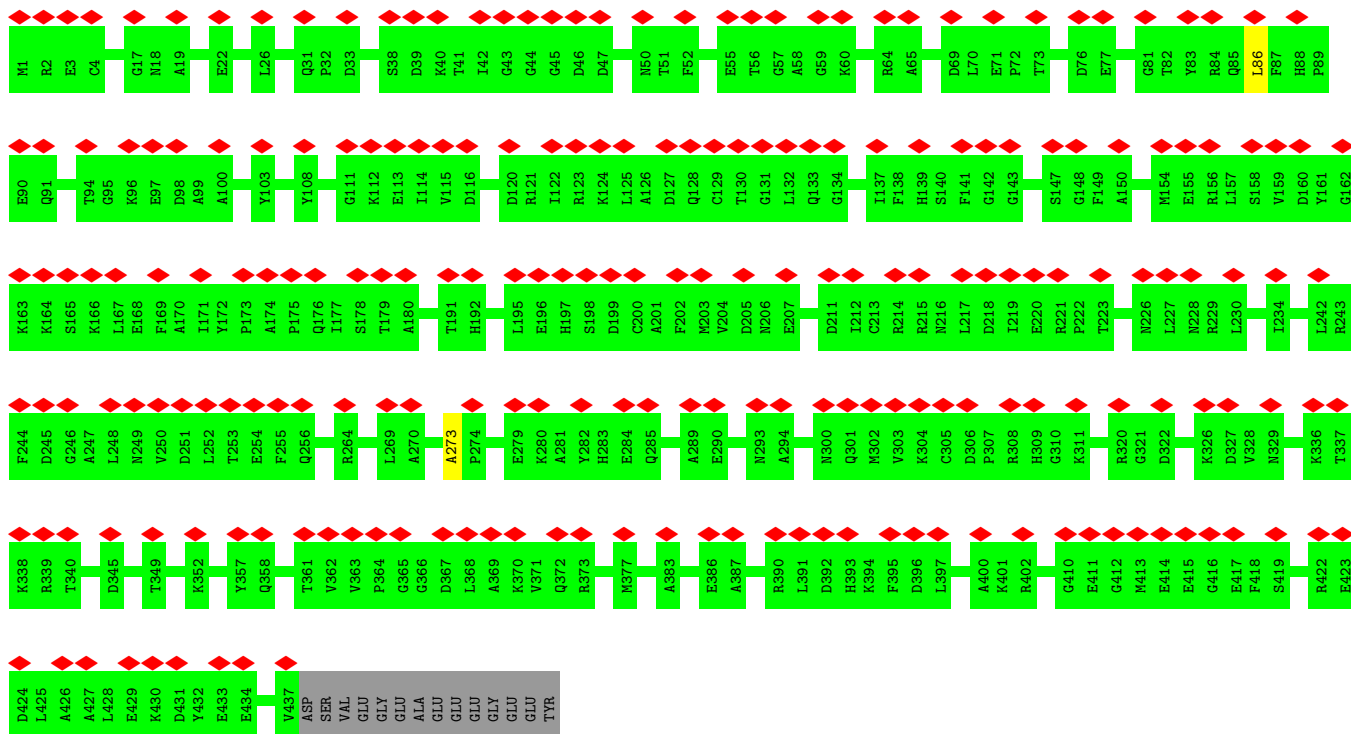




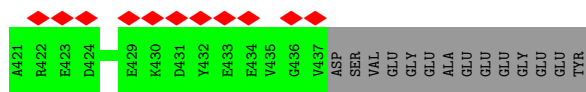
• Molecule 54: Tubulin alpha chain



Chain BI:



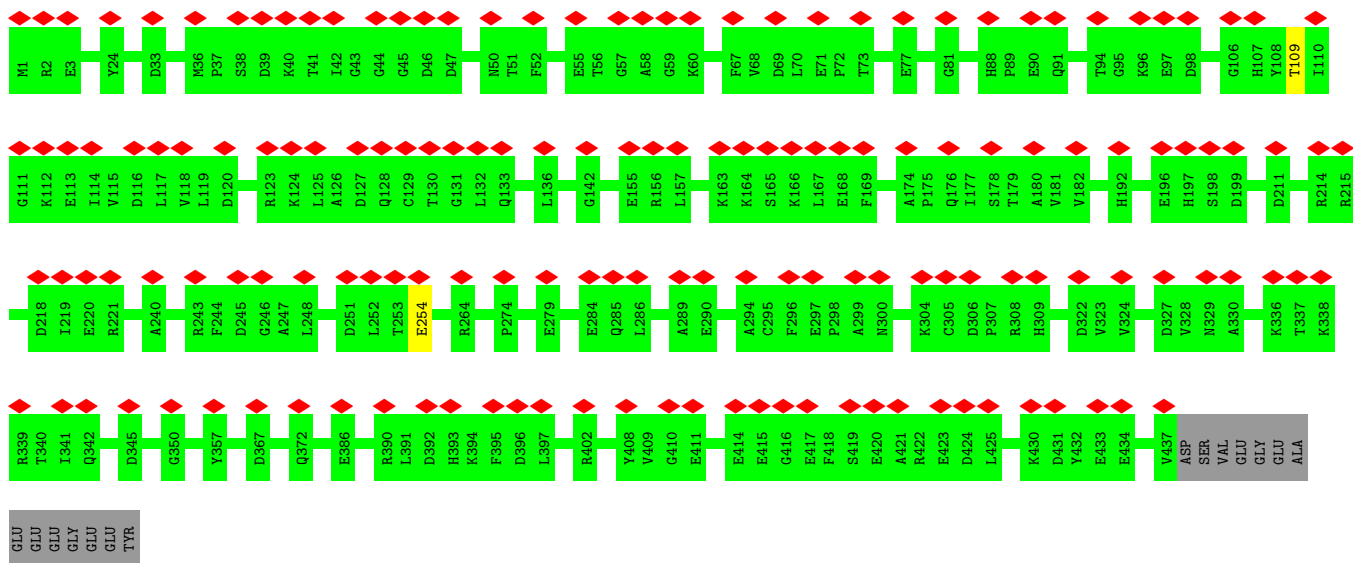
• Molecule 54: Tubulin alpha chain



• Molecule 54: Tubulin alpha chain



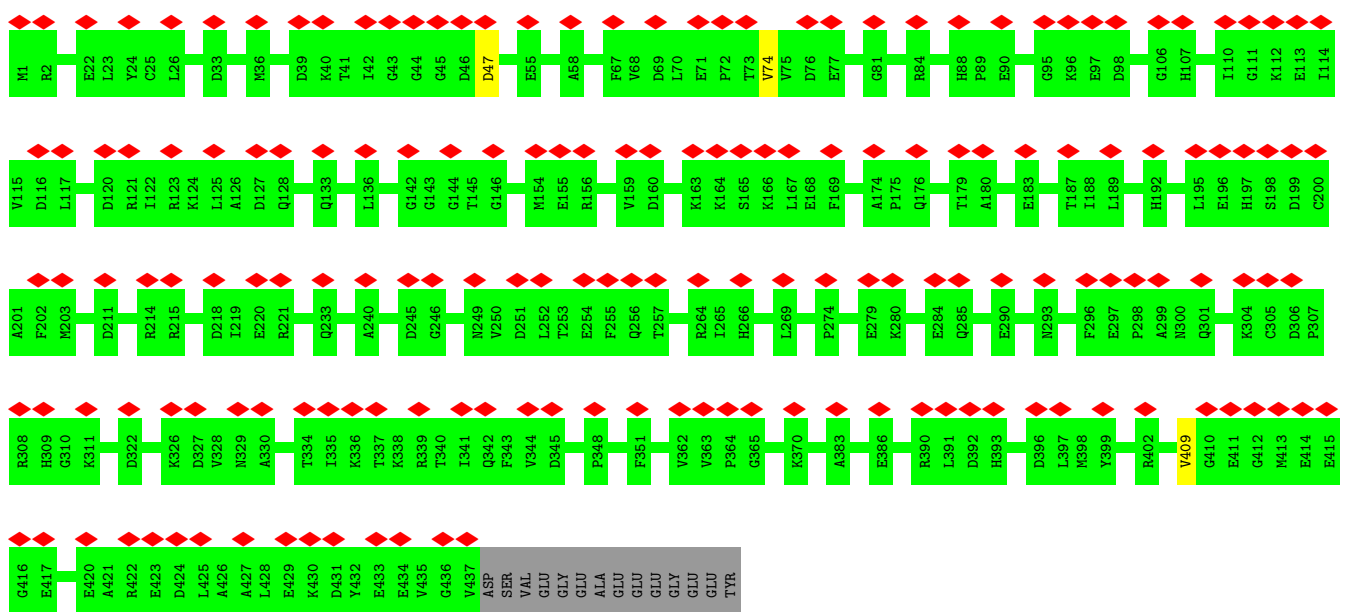
Chain CA:



• Molecule 54: Tubulin alpha chain



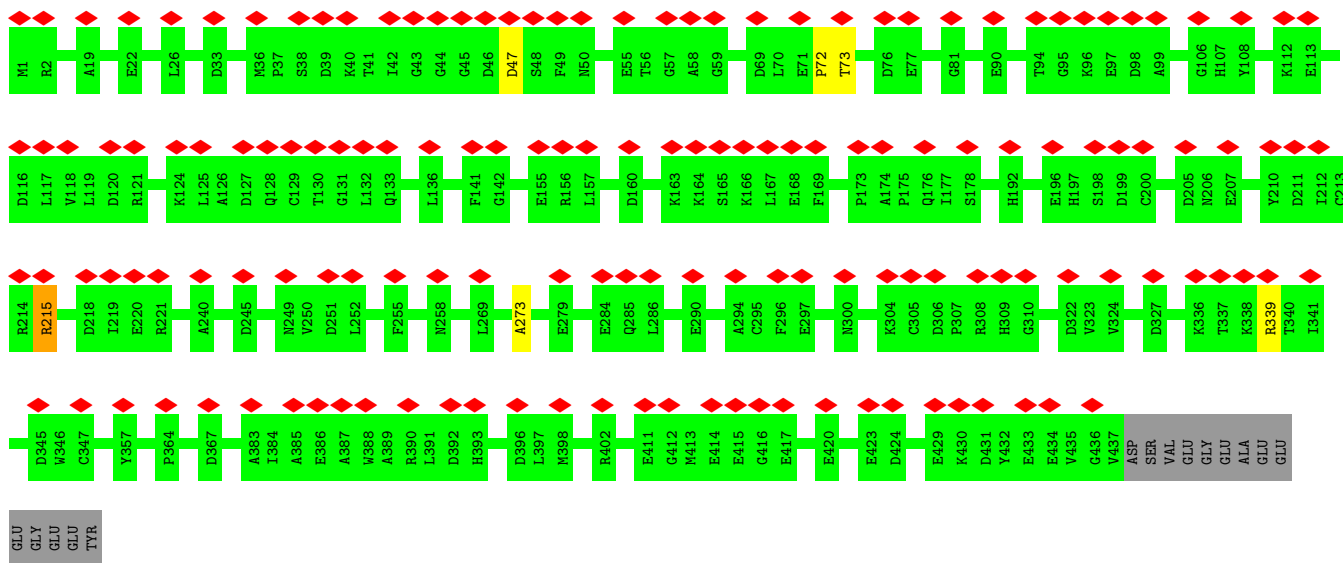
Chain CB:



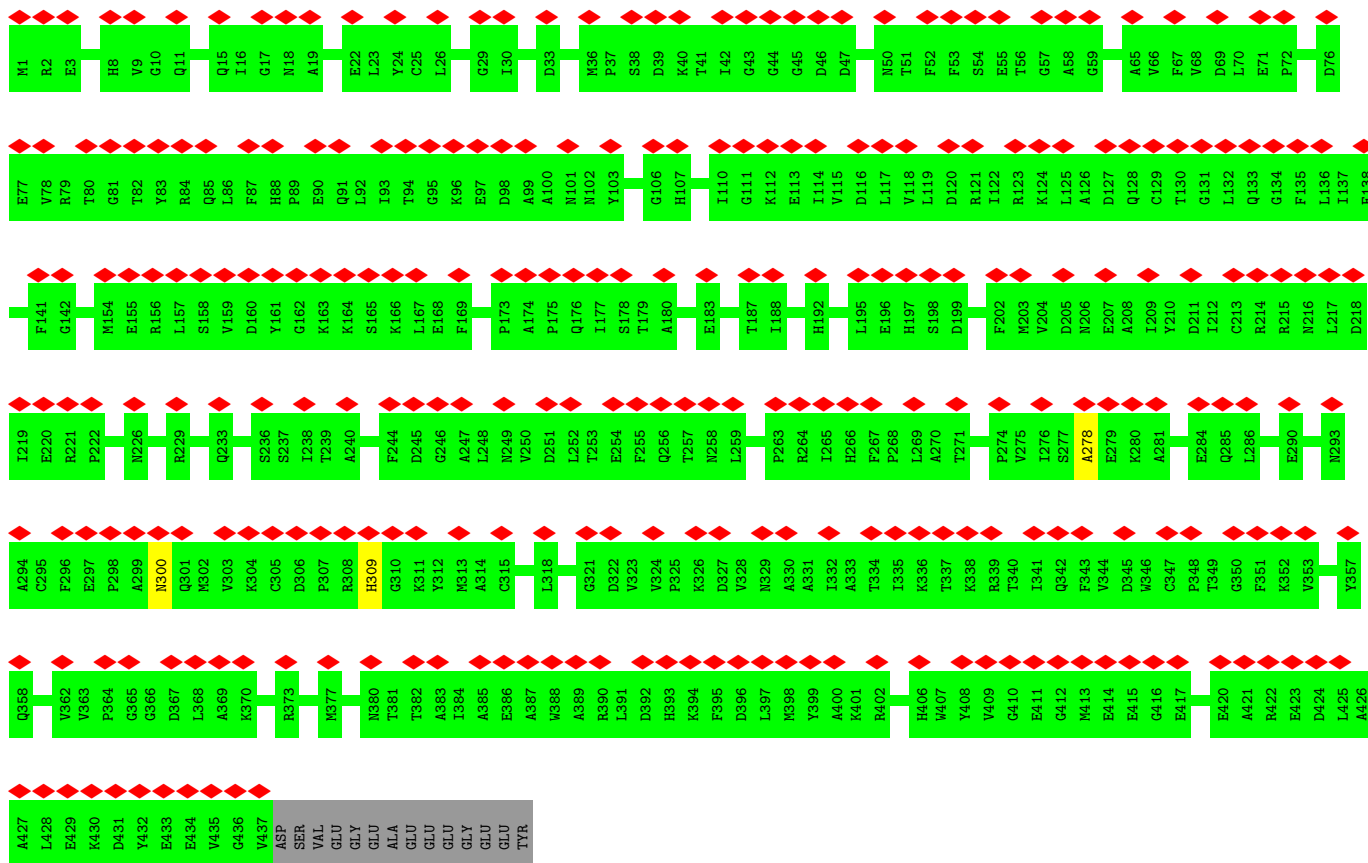
• Molecule 54: Tubulin alpha chain



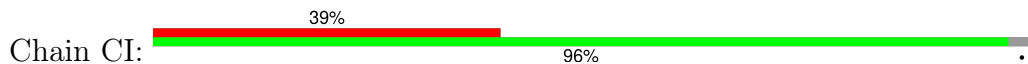
Chain CE:

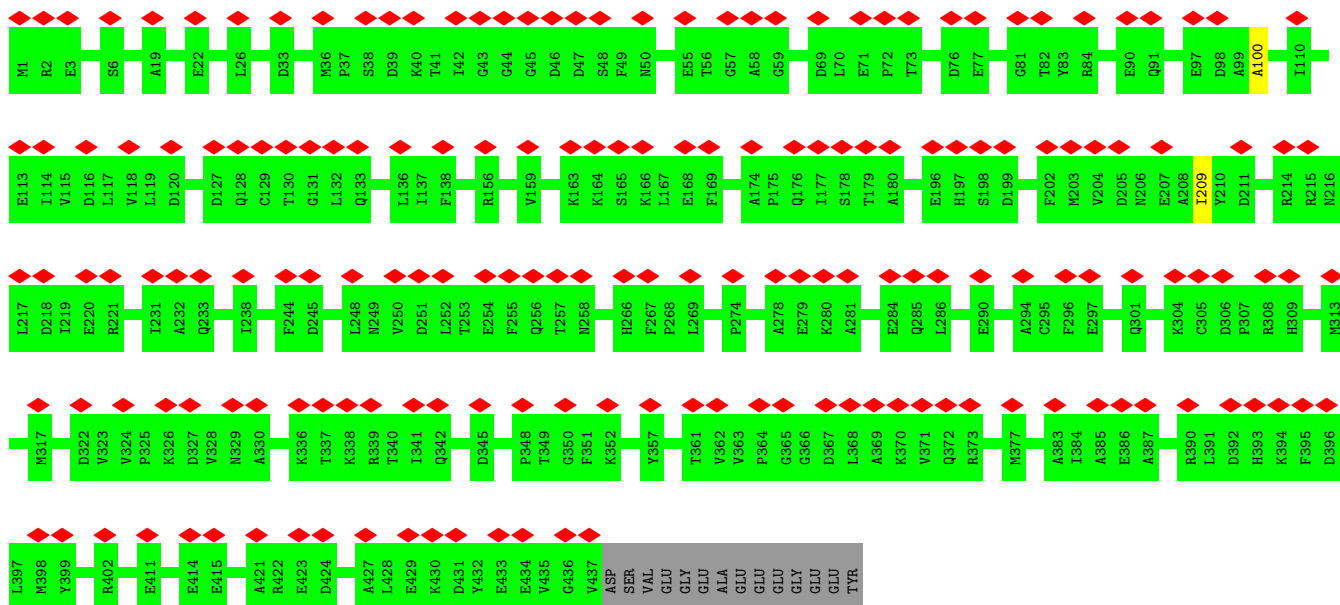


• Molecule 54: Tubulin alpha chain

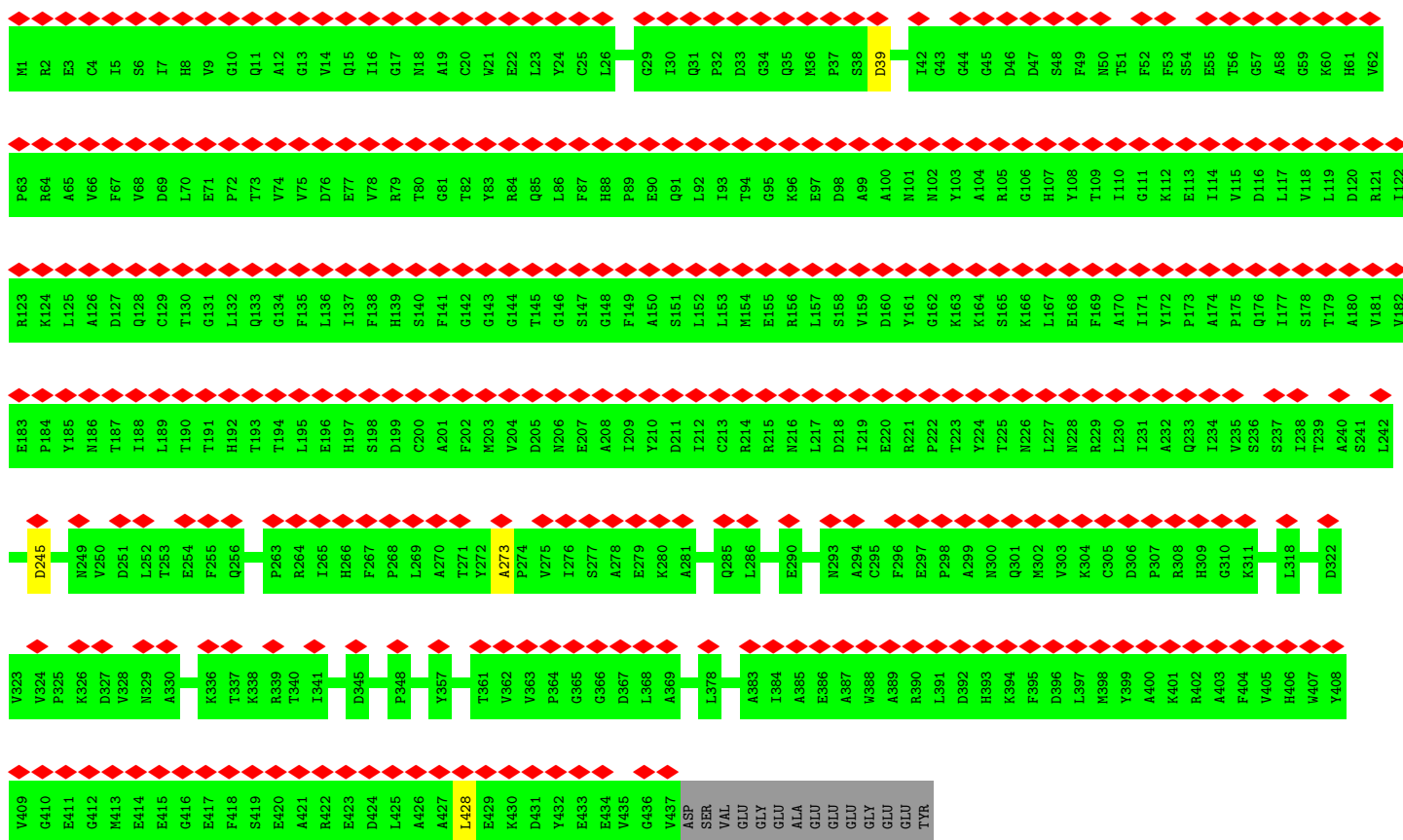
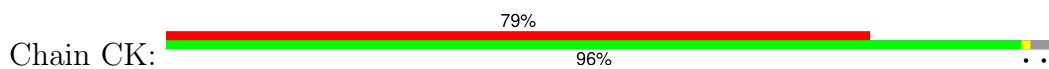


• Molecule 54: Tubulin alpha chain

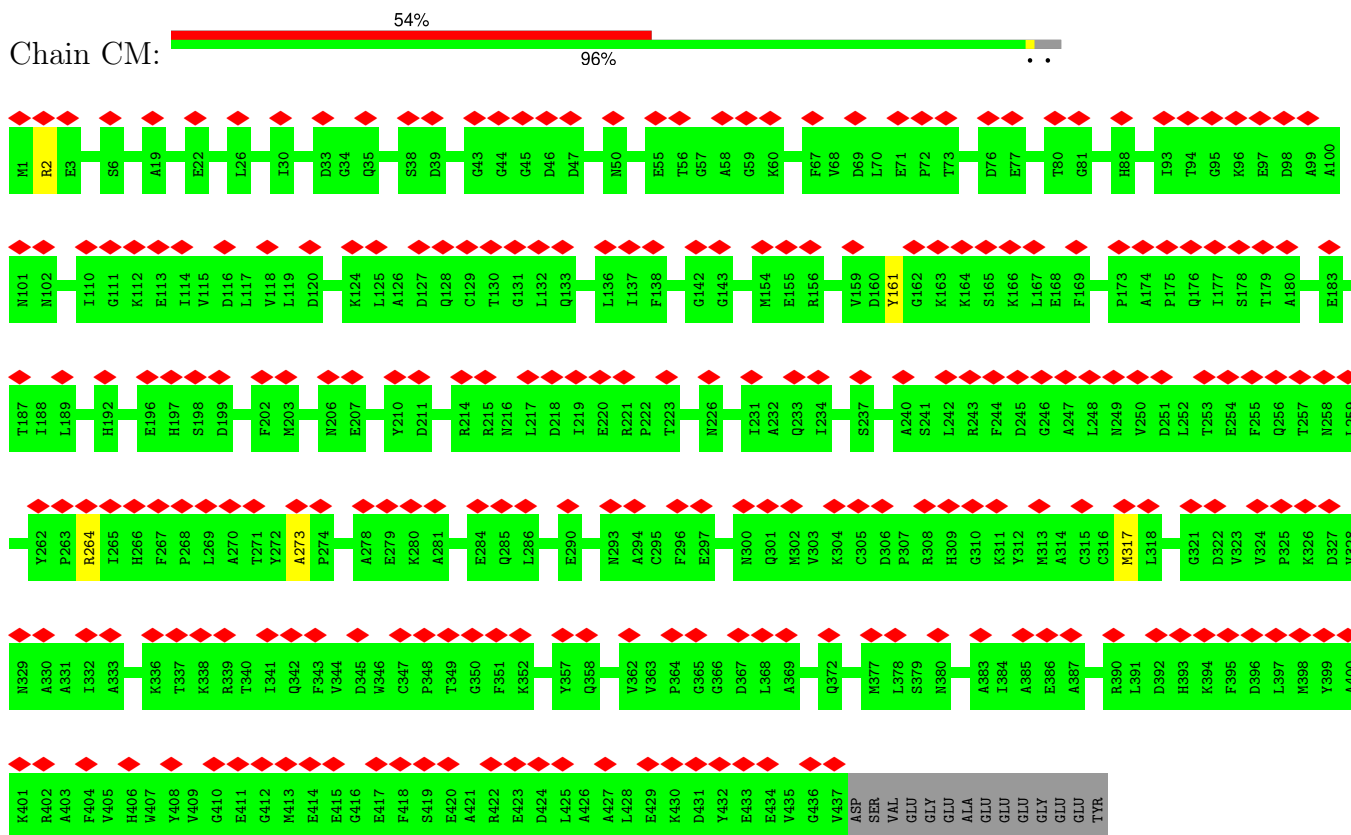




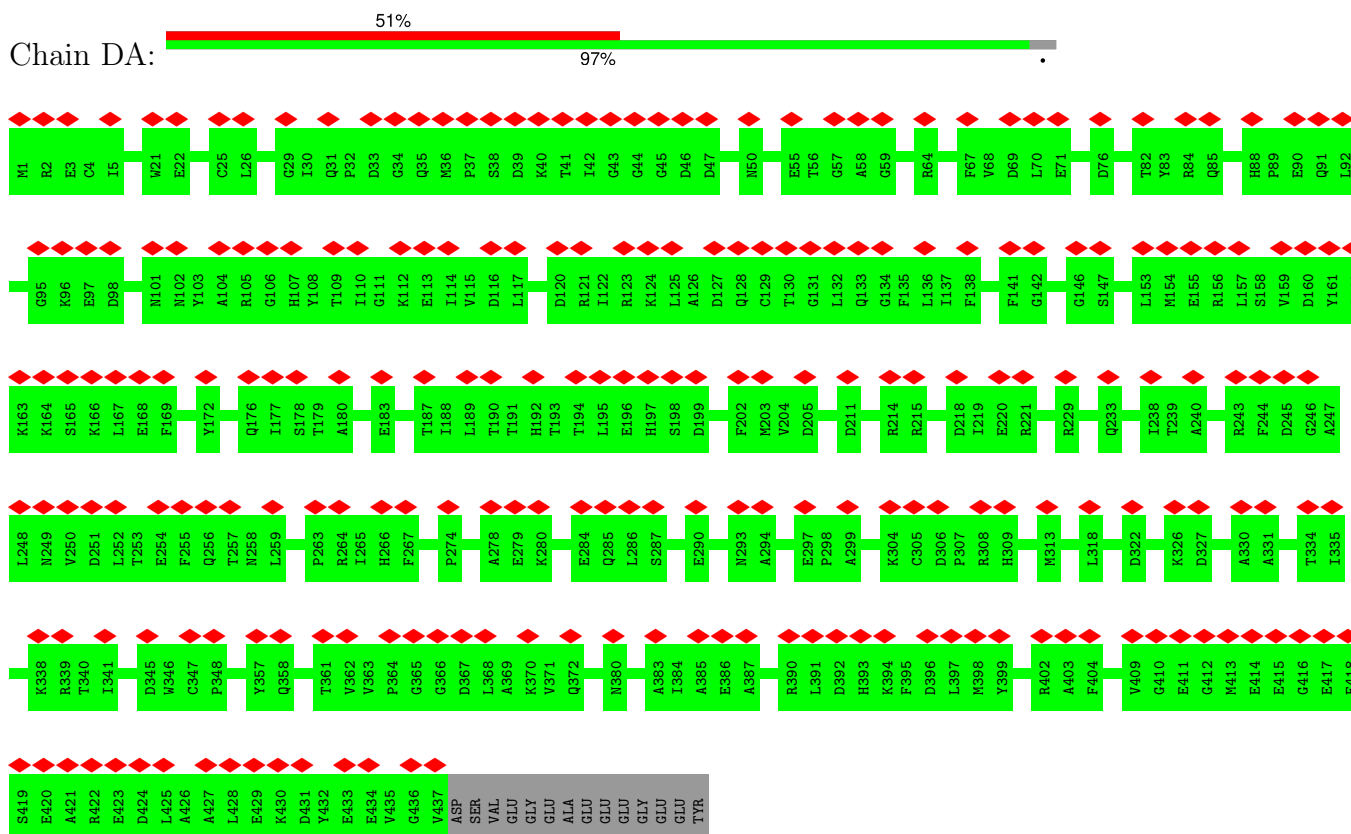
• Molecule 54: Tubulin alpha chain



• Molecule 54: Tubulin alpha chain

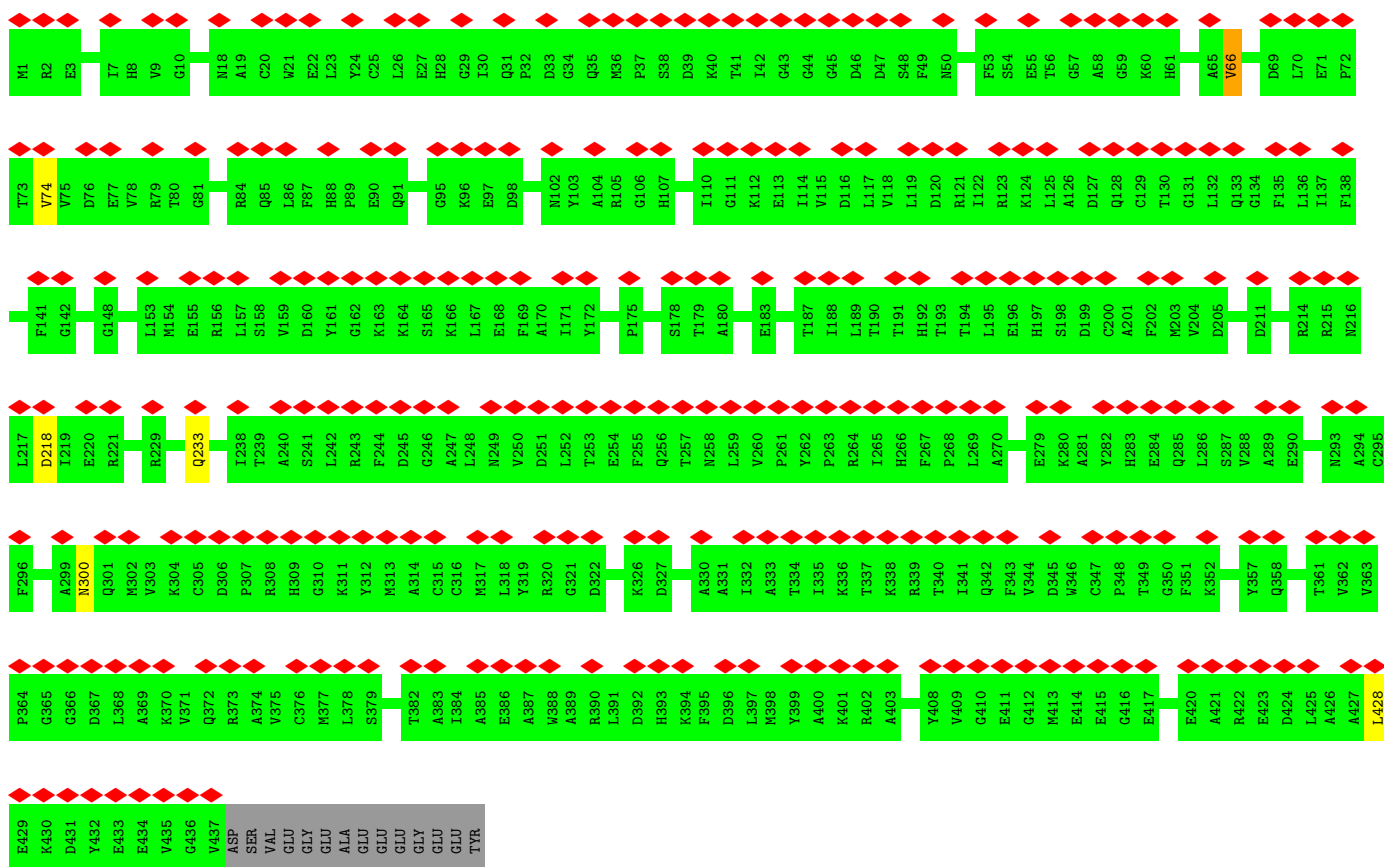


• Molecule 54: Tubulin alpha chain

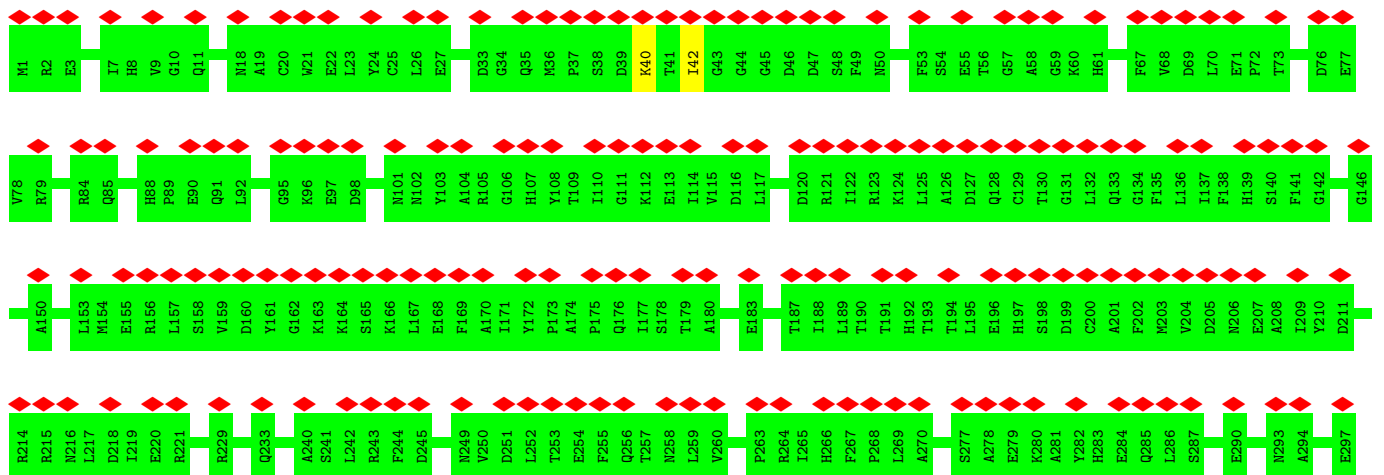


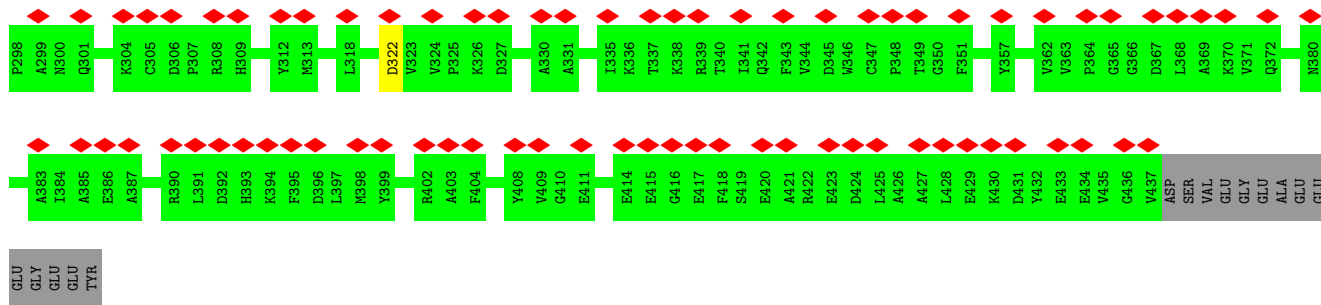
GLU
TYR

• Molecule 54: Tubulin alpha chain

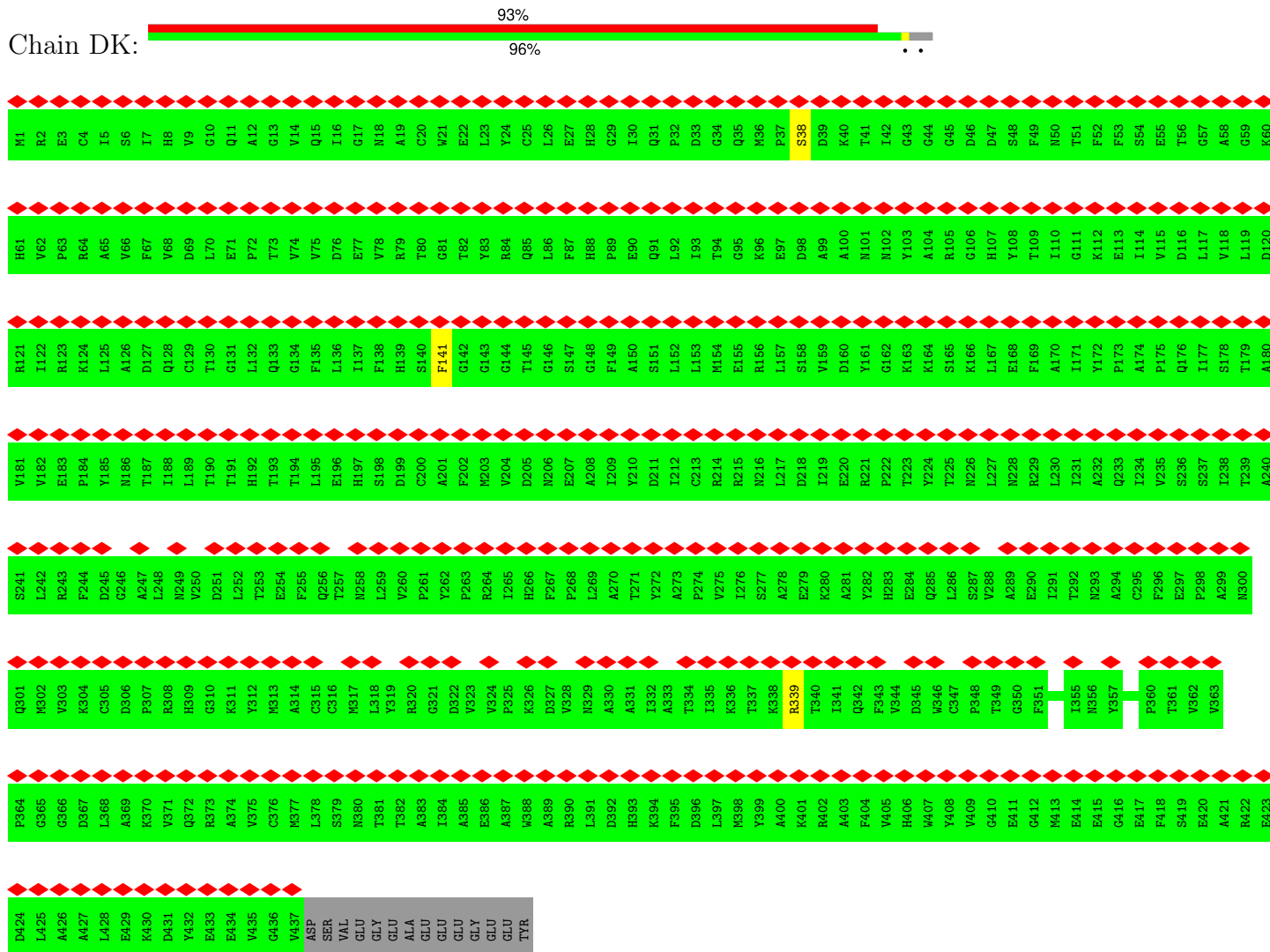


• Molecule 54: Tubulin alpha chain

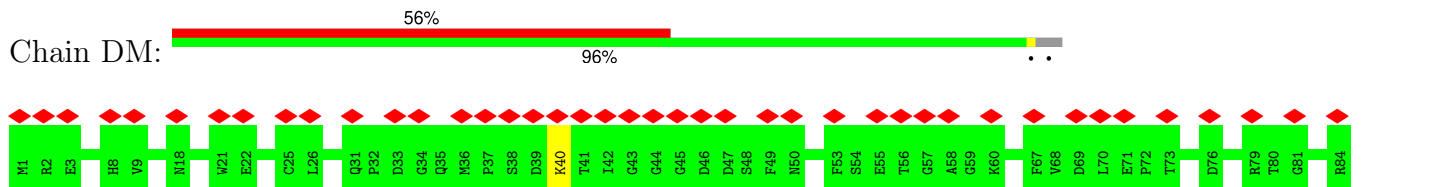


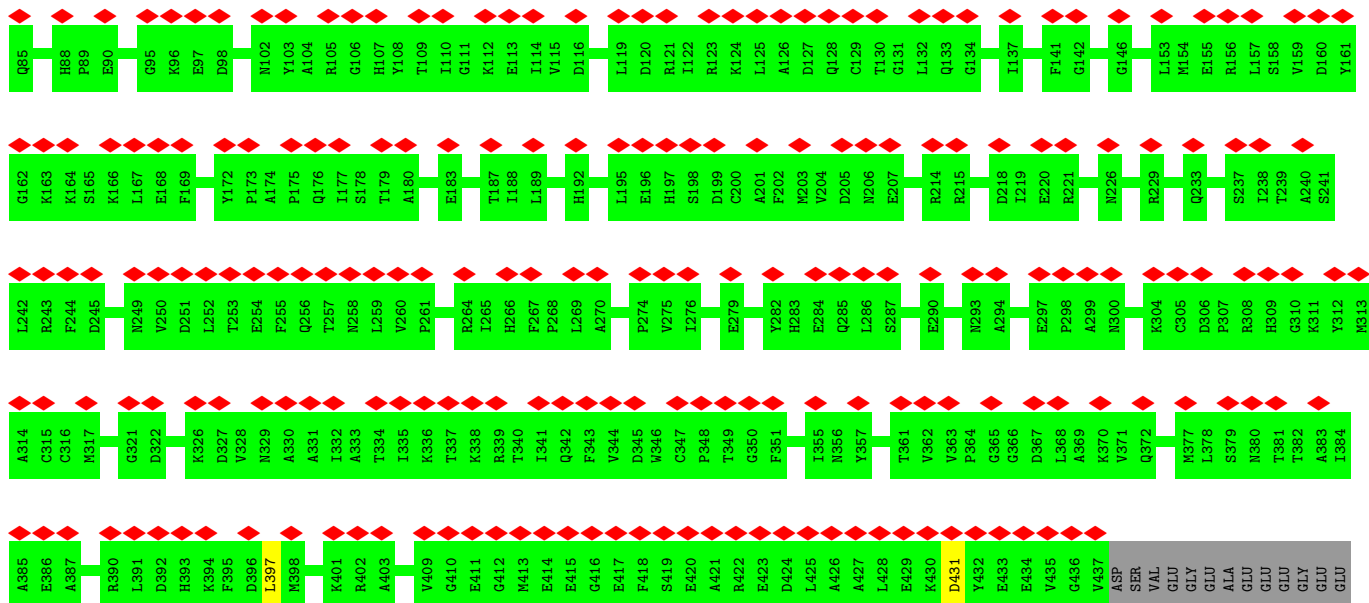


• Molecule 54: Tubulin alpha chain



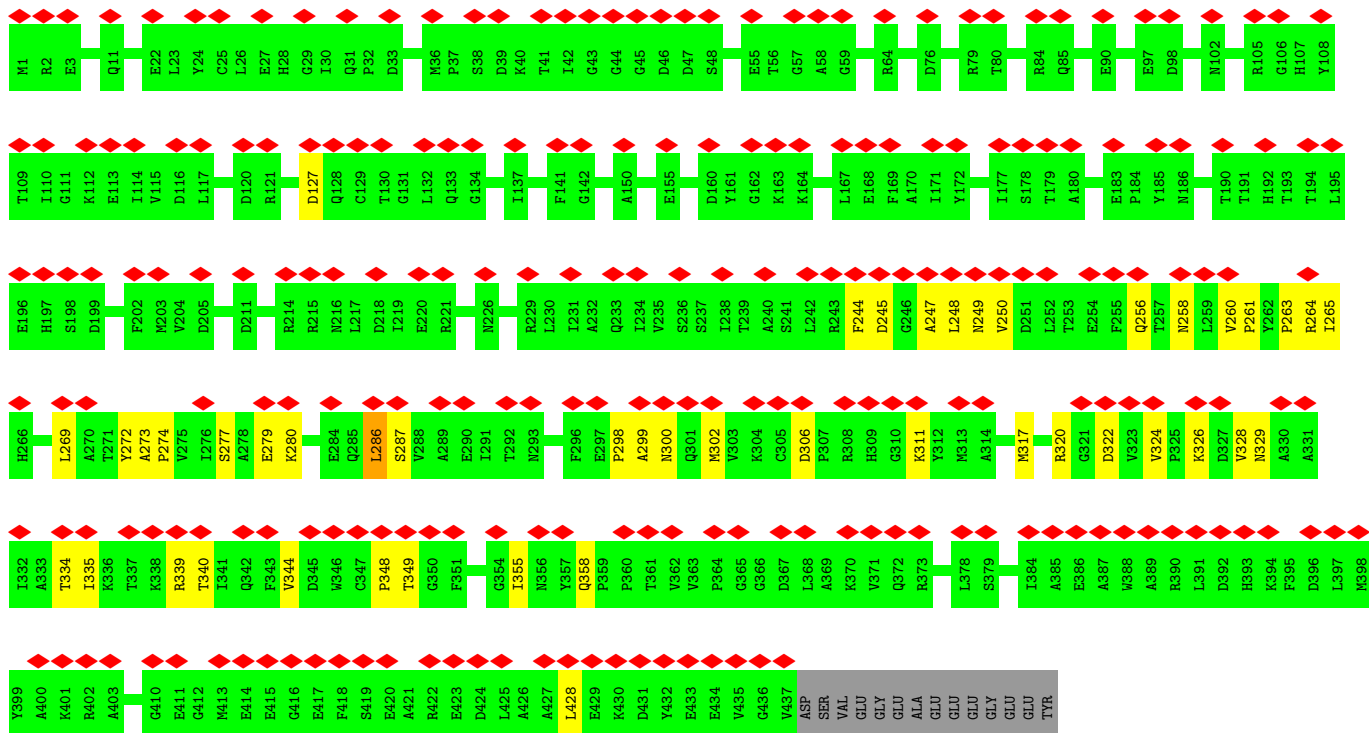
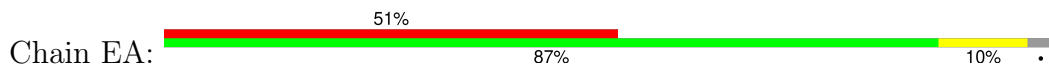
• Molecule 54: Tubulin alpha chain





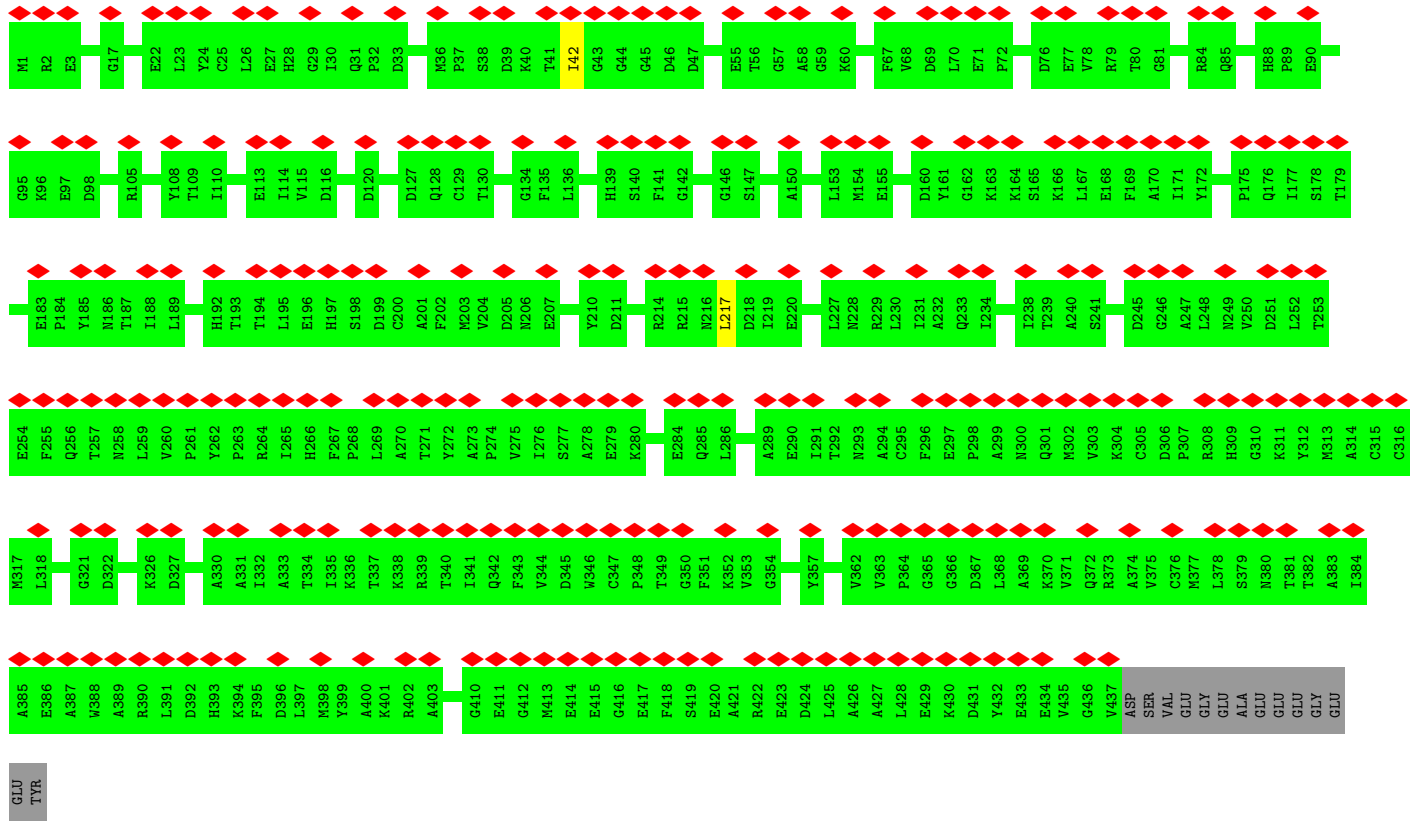
TYR

• Molecule 54: Tubulin alpha chain

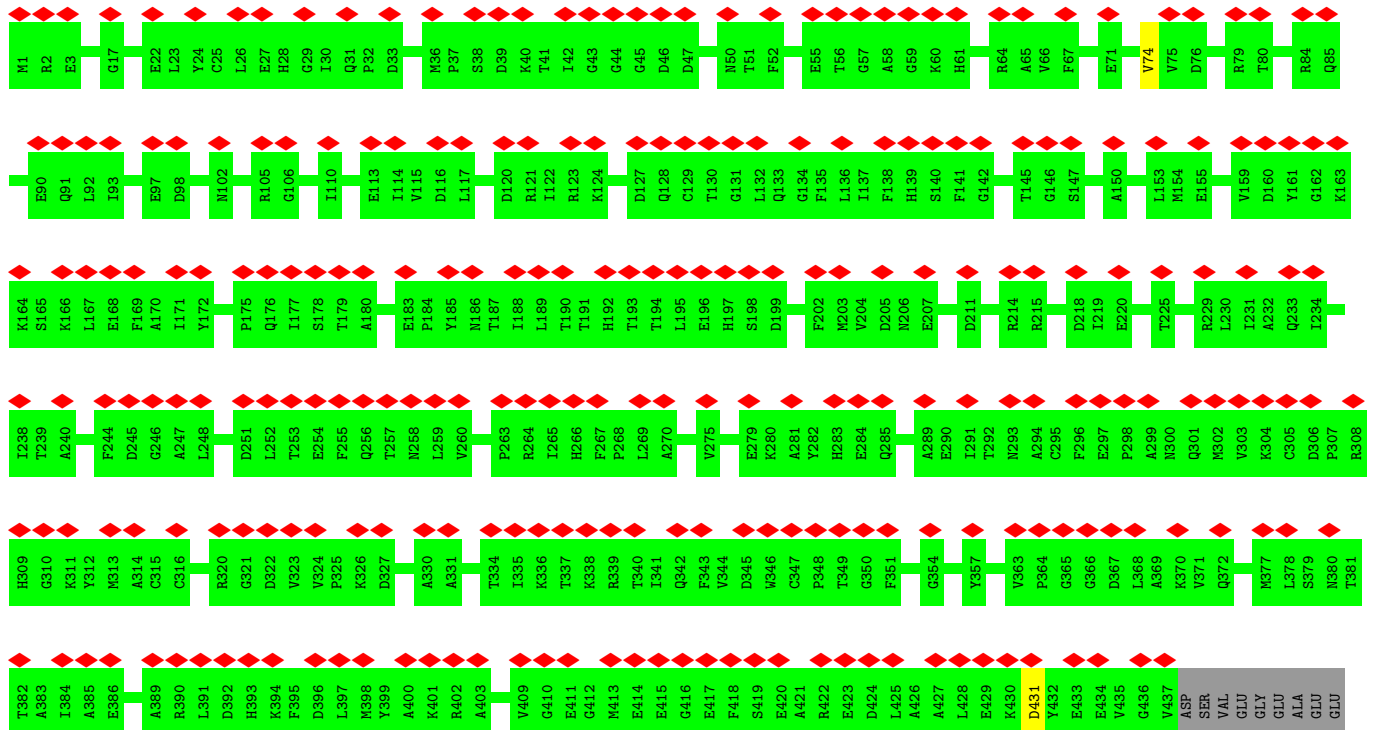


• Molecule 54: Tubulin alpha chain



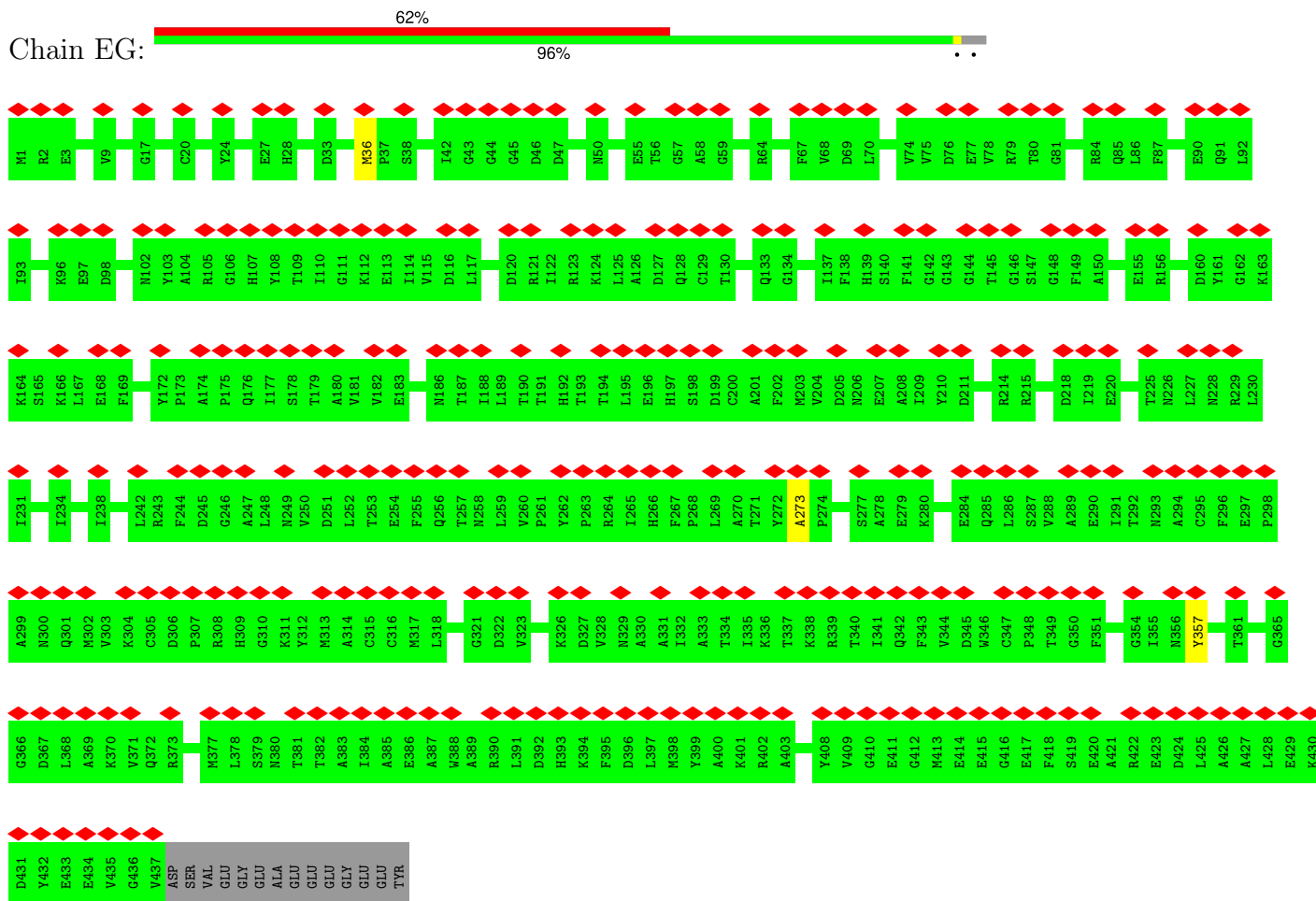


- Molecule 54: Tubulin alpha chain

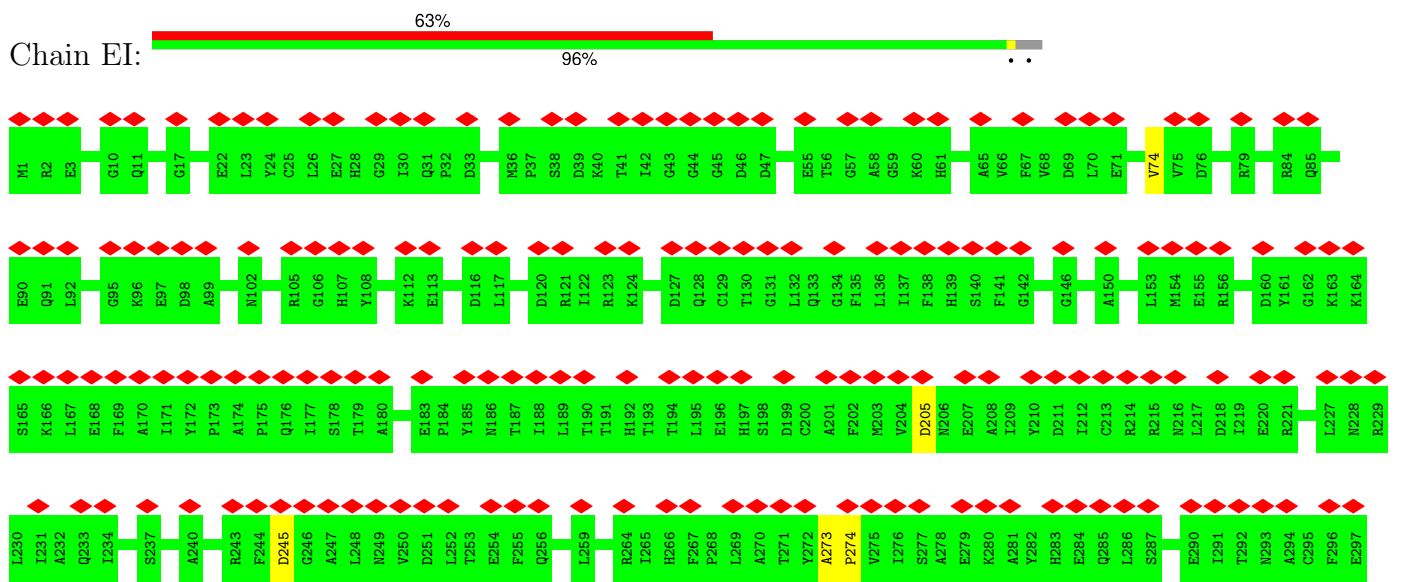


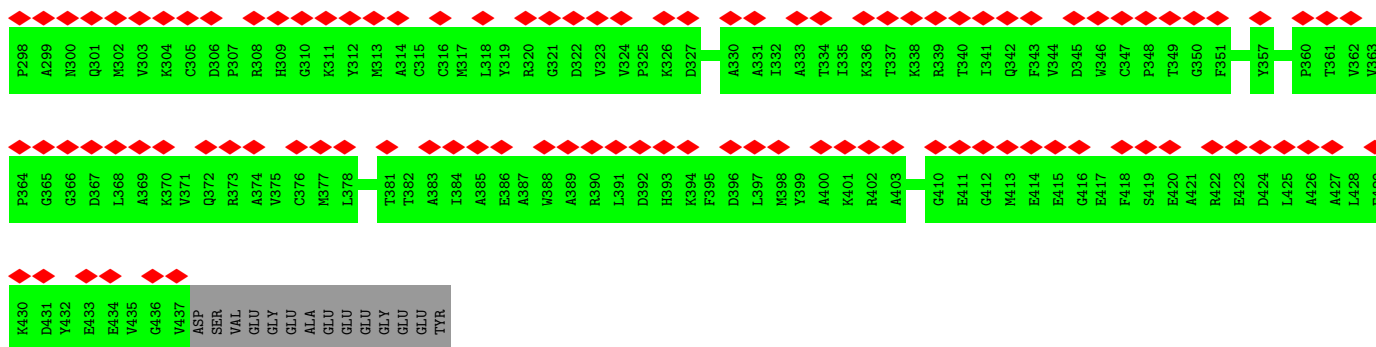
GLU
GLY
GLU
TYR

• Molecule 54: Tubulin alpha chain

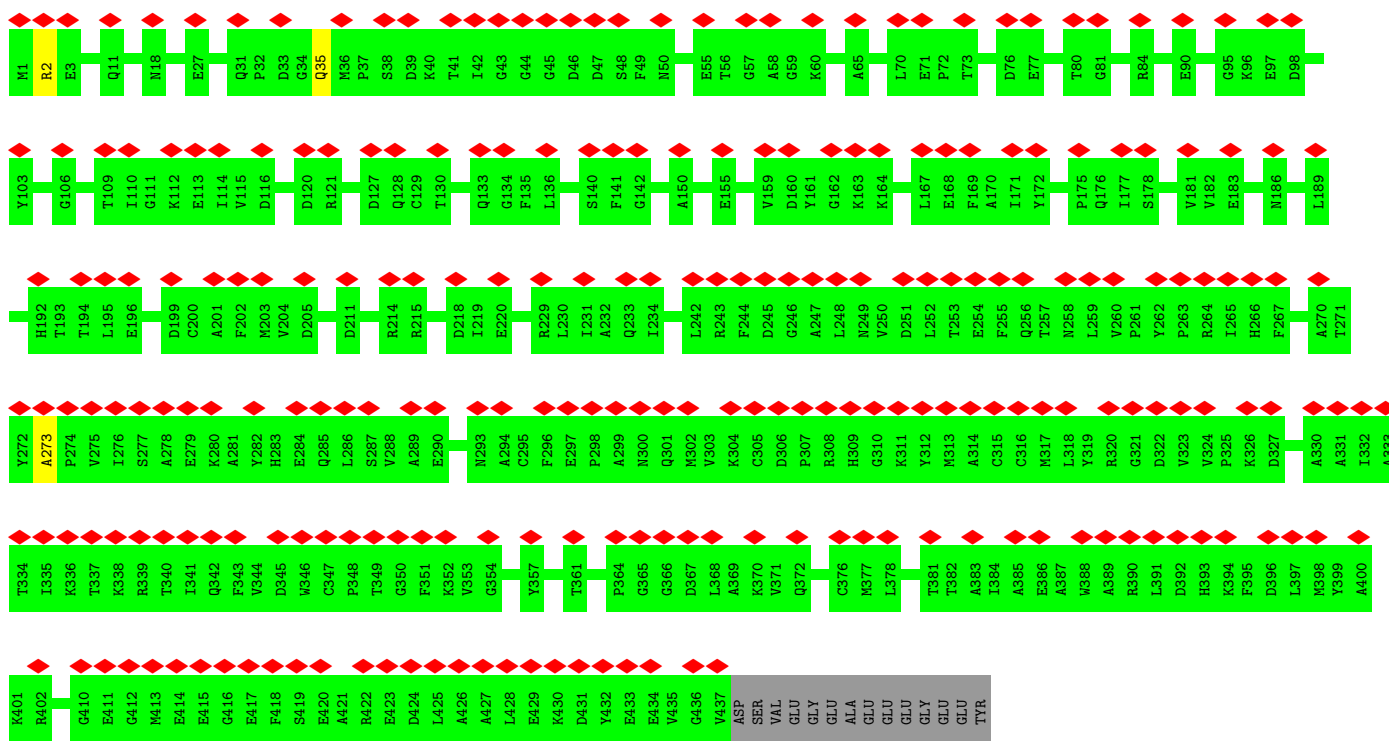


• Molecule 54: Tubulin alpha chain

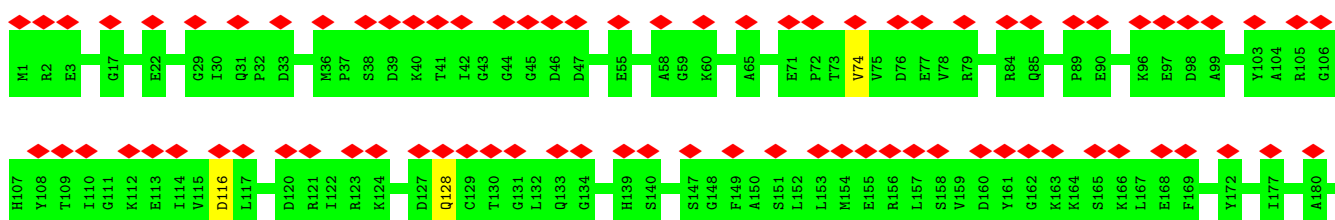
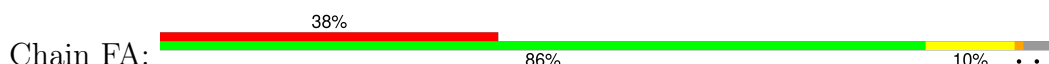


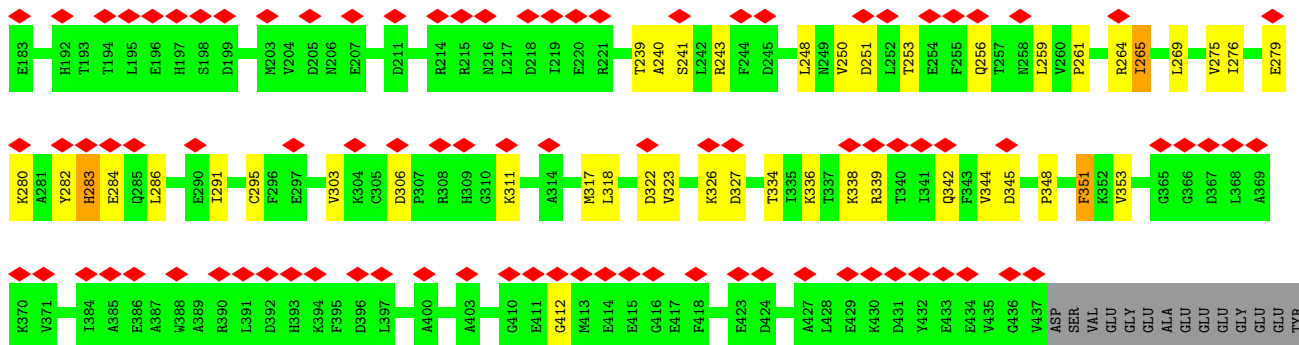


• Molecule 54: Tubulin alpha chain

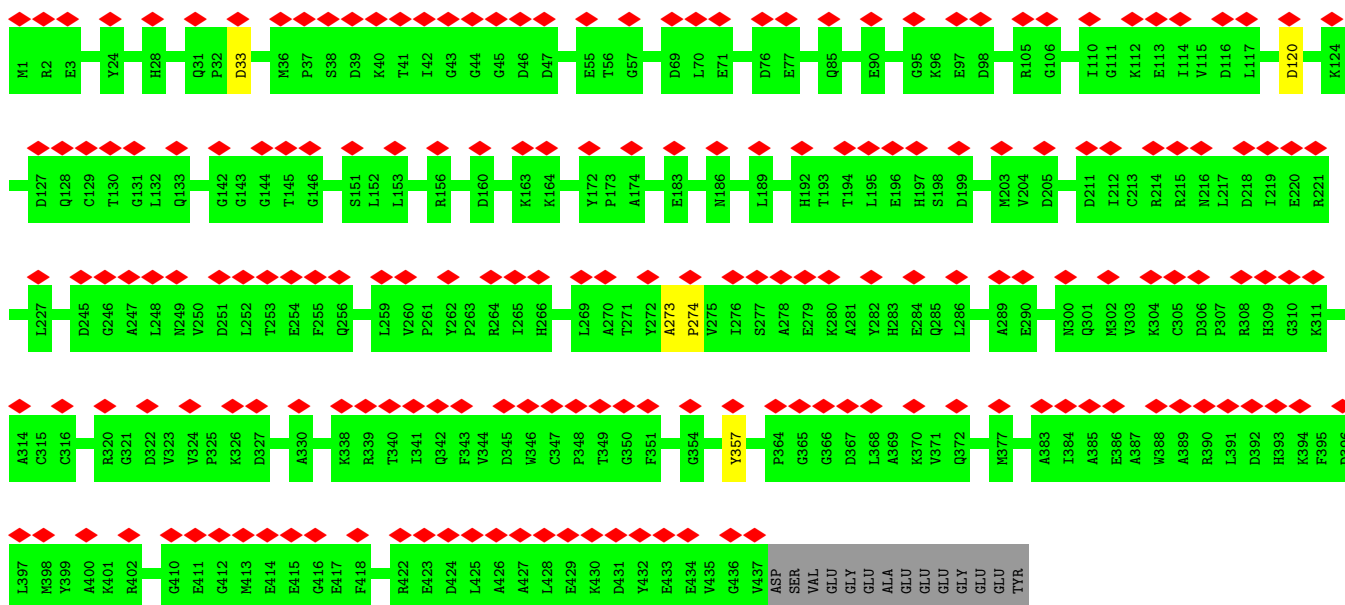
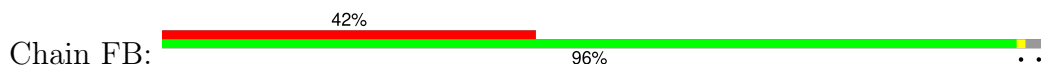


• Molecule 54: Tubulin alpha chain

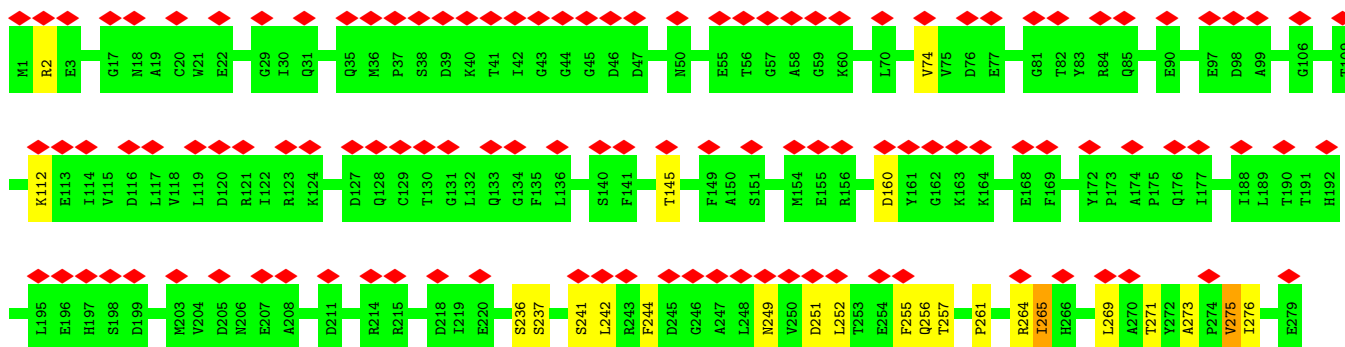
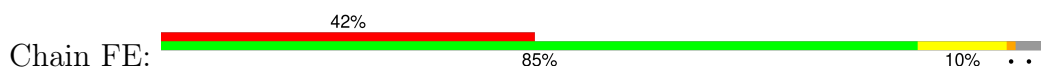


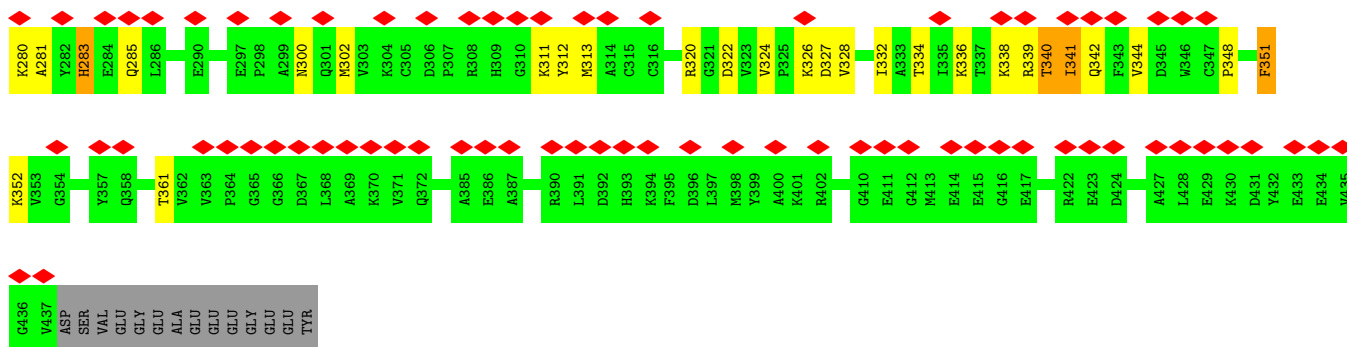


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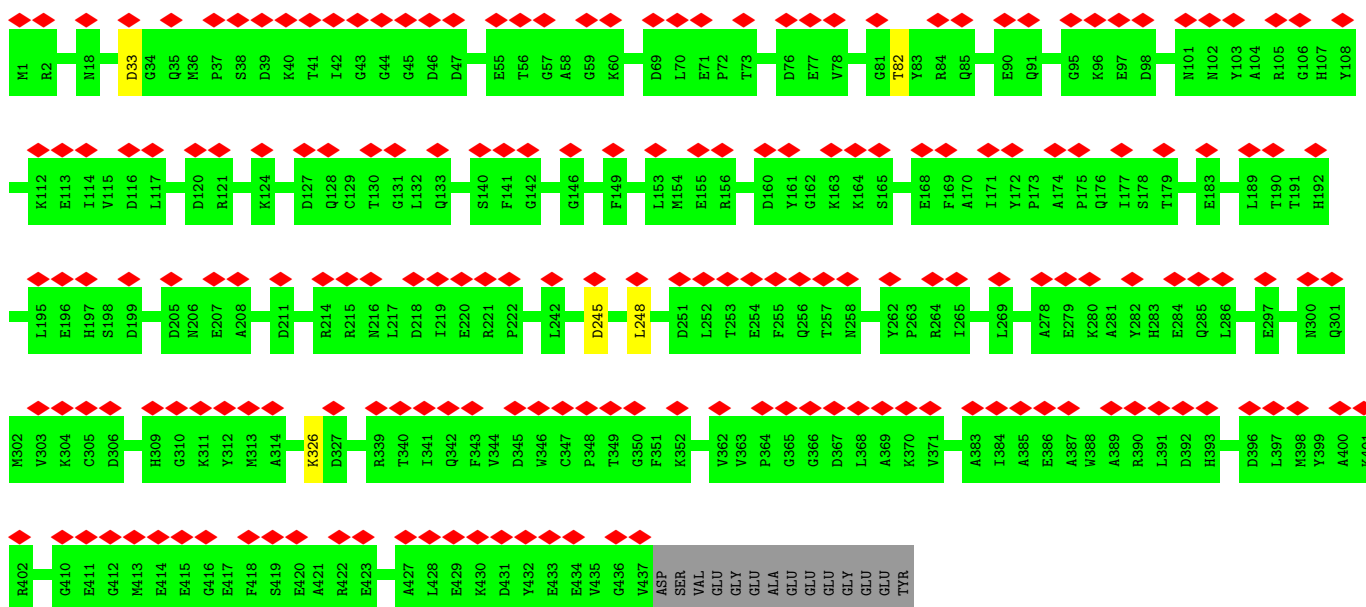
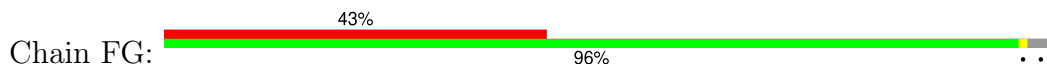


• Molecule 54: Tubulin alpha chain

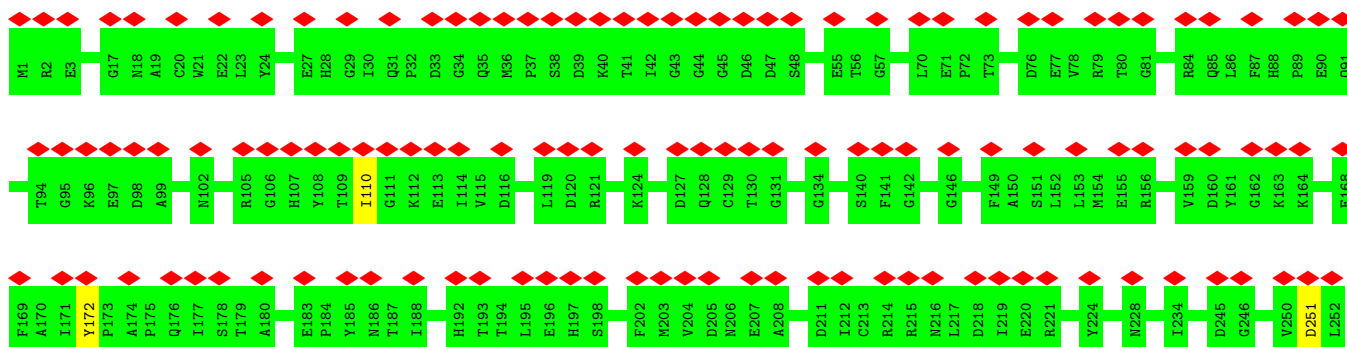
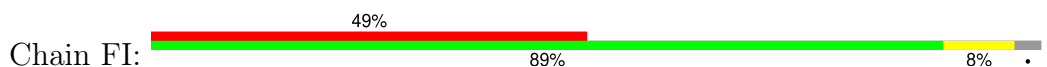


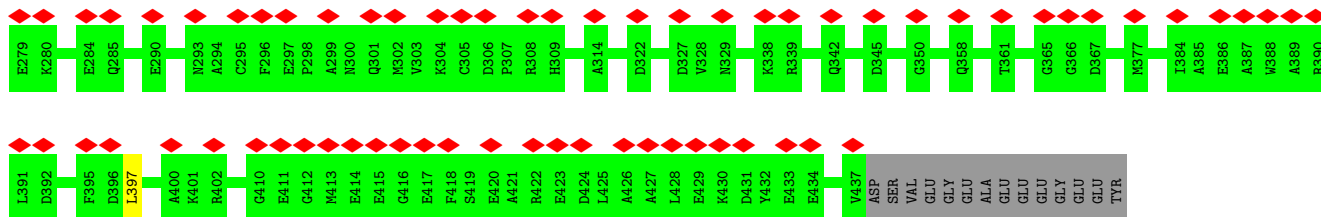


• Molecule 54: Tubulin alpha chain

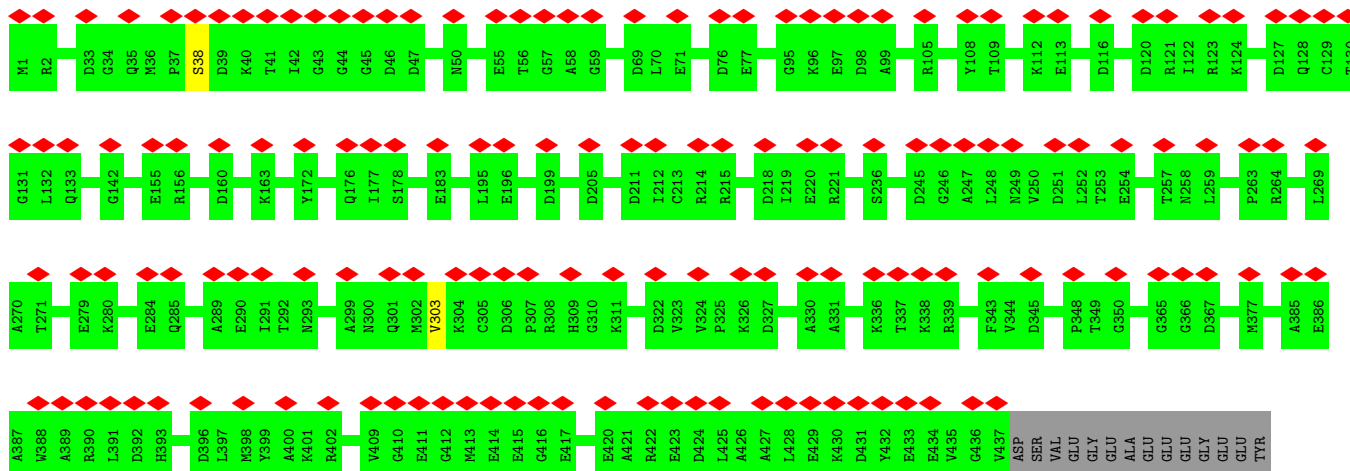


• Molecule 54: Tubulin alpha chain

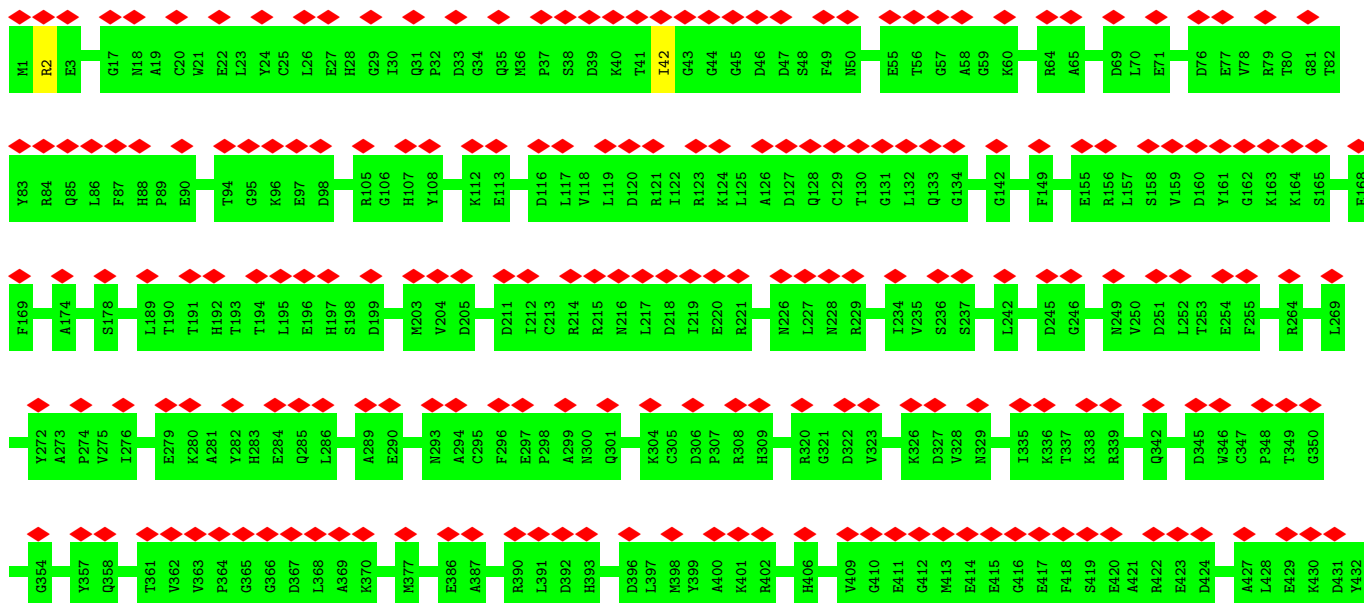


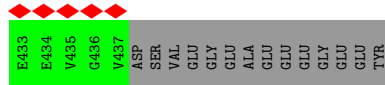


• Molecule 54: Tubulin alpha chain

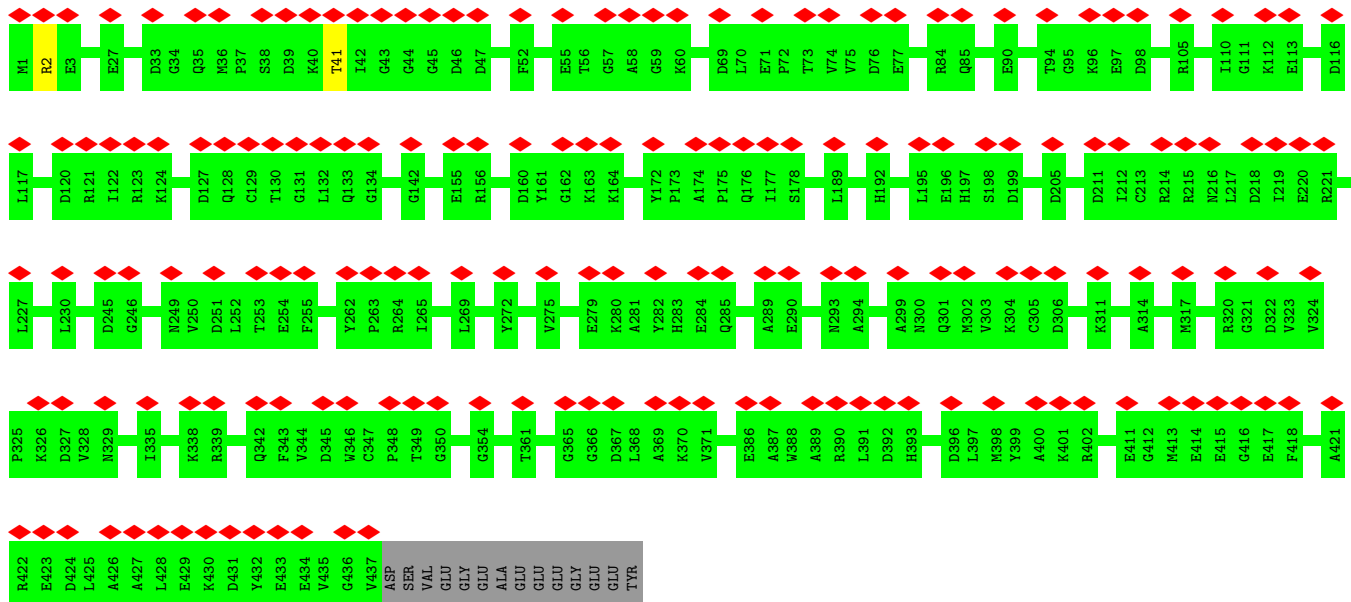
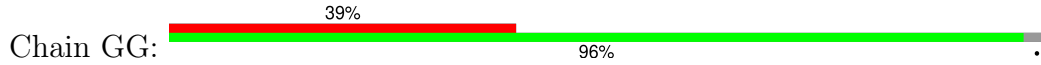


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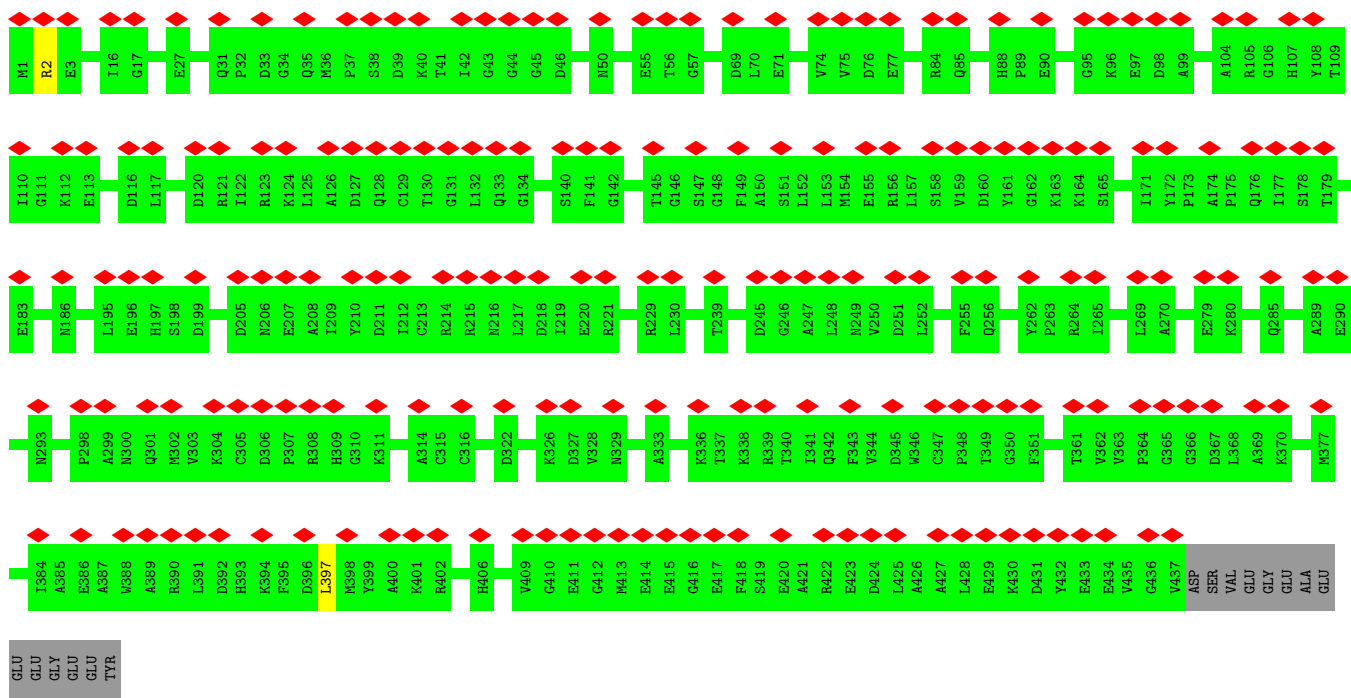


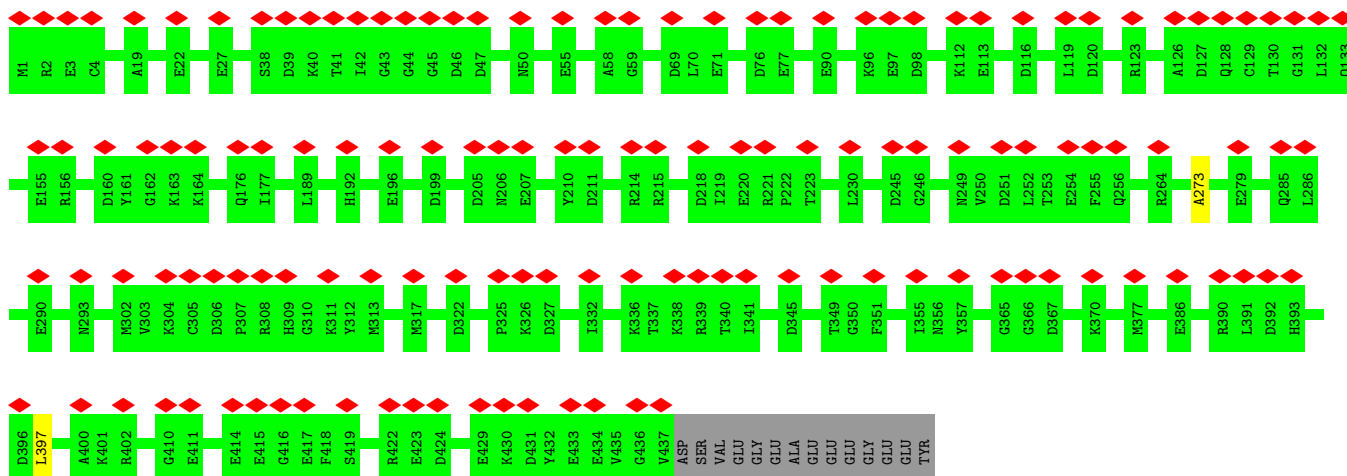


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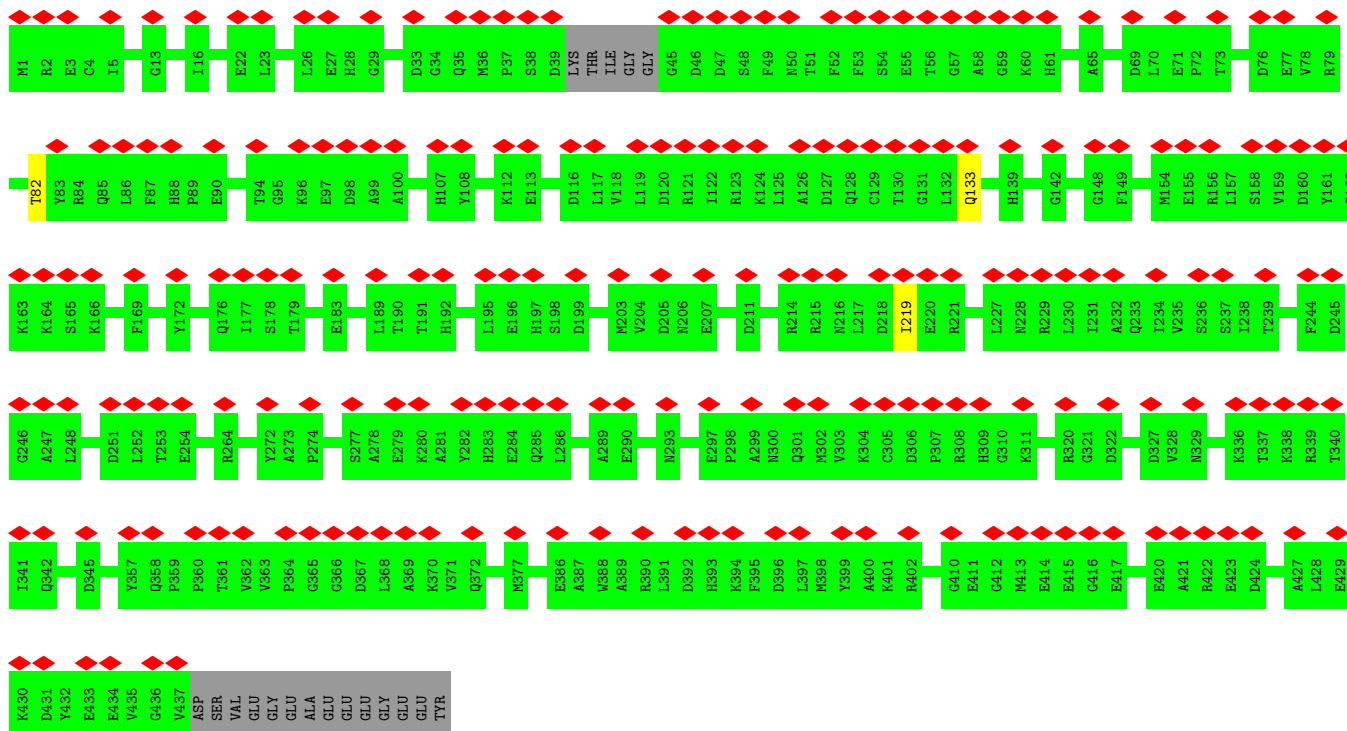


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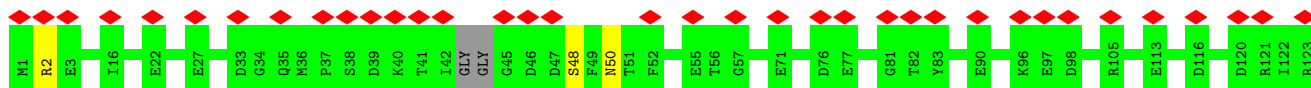


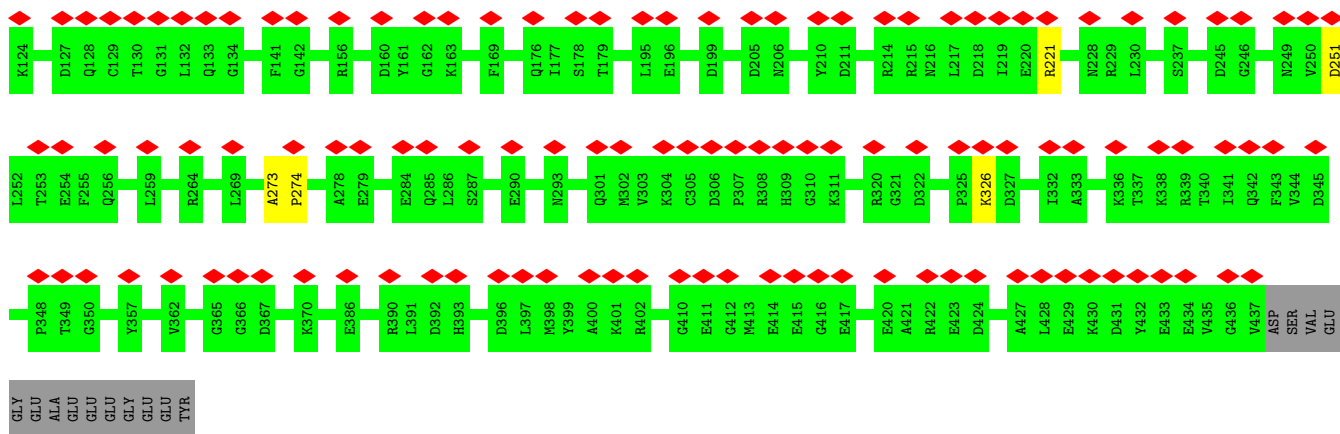


• Molecule 54: Tubulin alpha chain

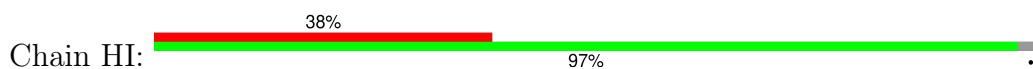


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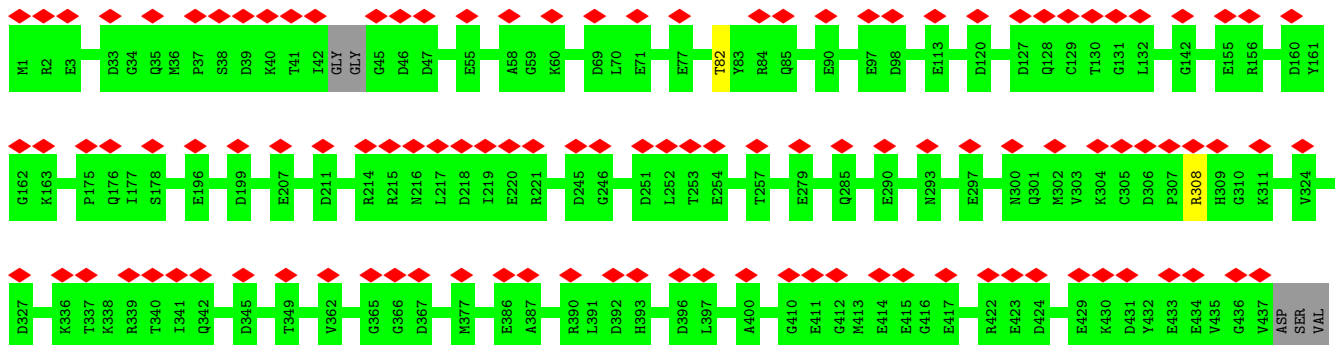




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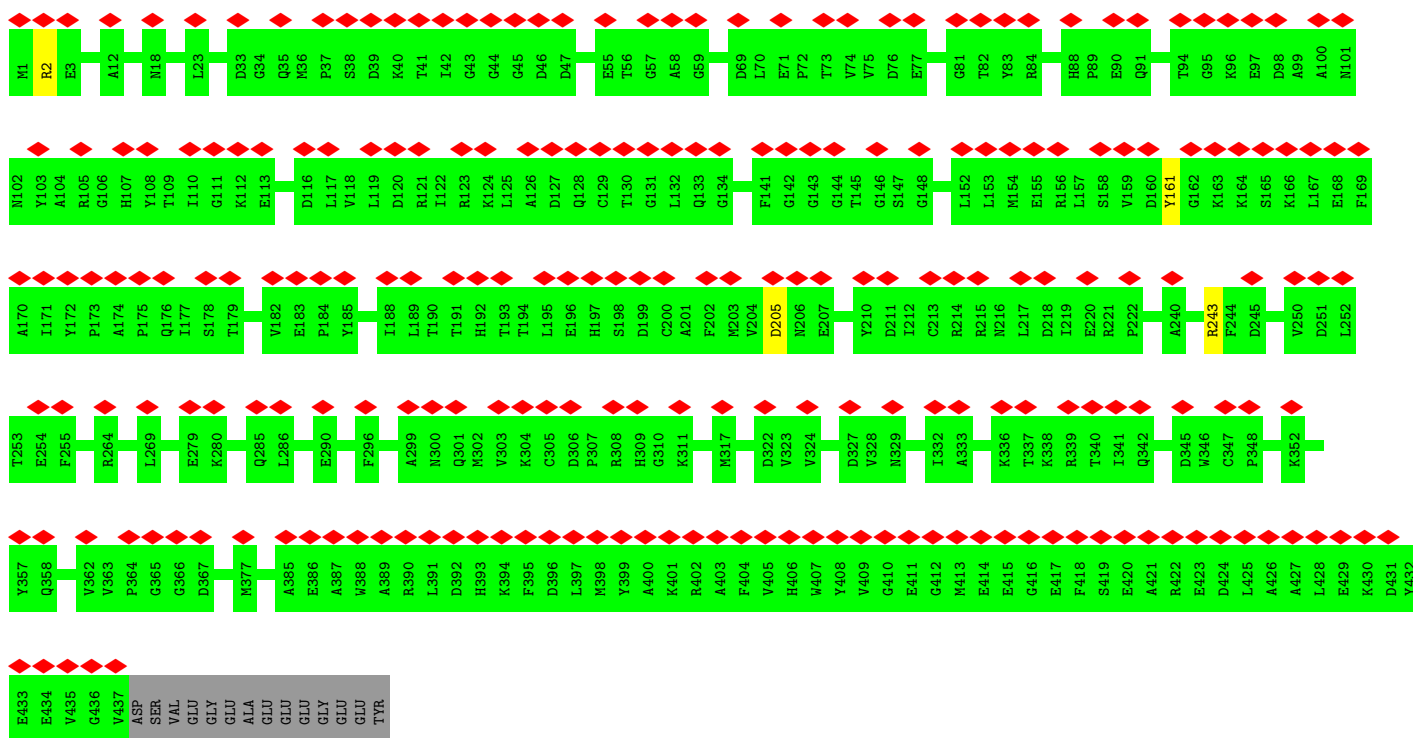


• Molecule 54: Tubulin alpha chain

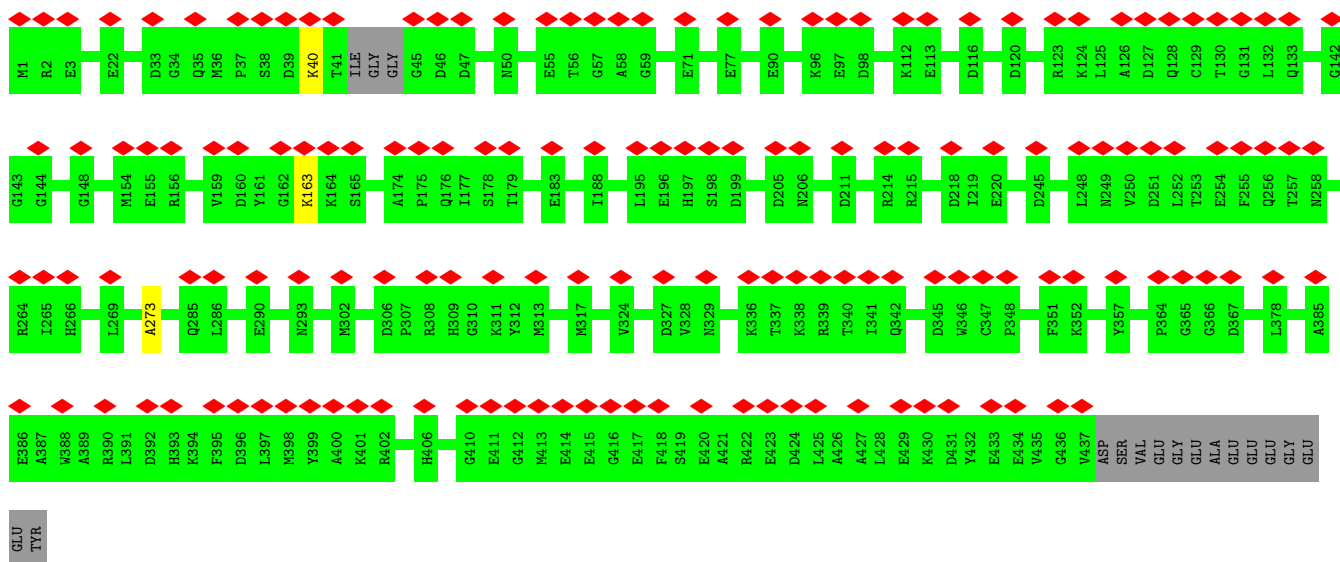


GLU
GLY
GLU
ALA
GLU
GLU
GLU
GLY
GLU
GLU
TYR

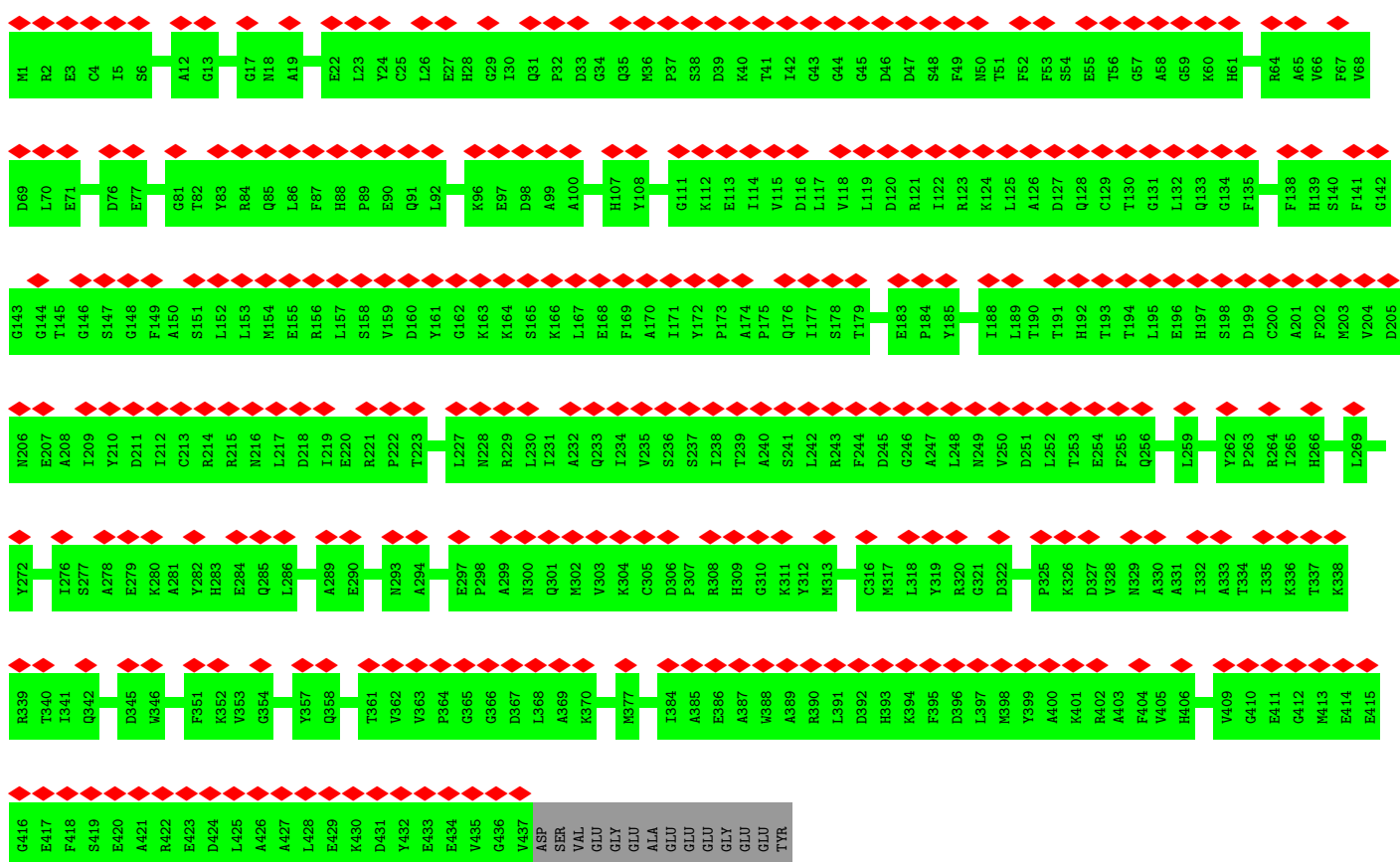
• Molecule 54: Tubulin alpha chain



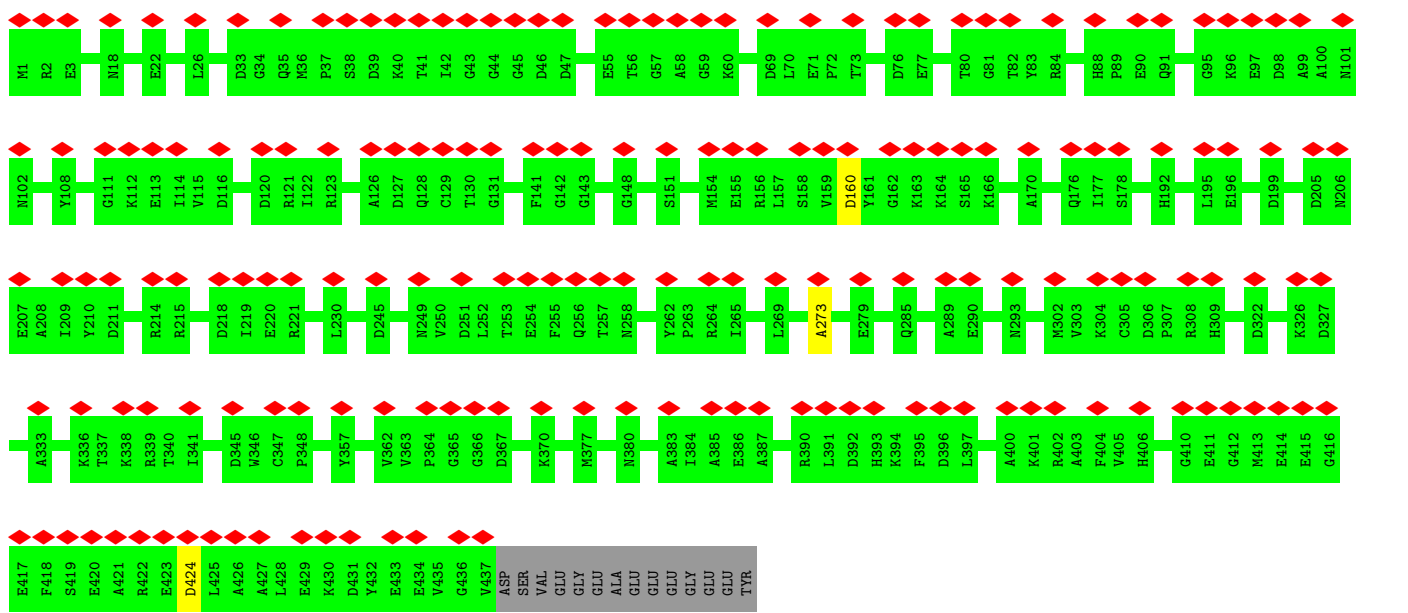
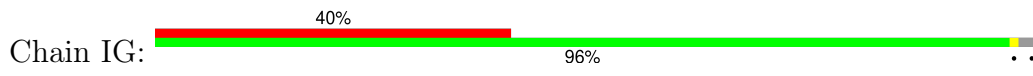
• Molecule 54: Tubulin alpha chain



• Molecule 54: Tubulin alpha chain



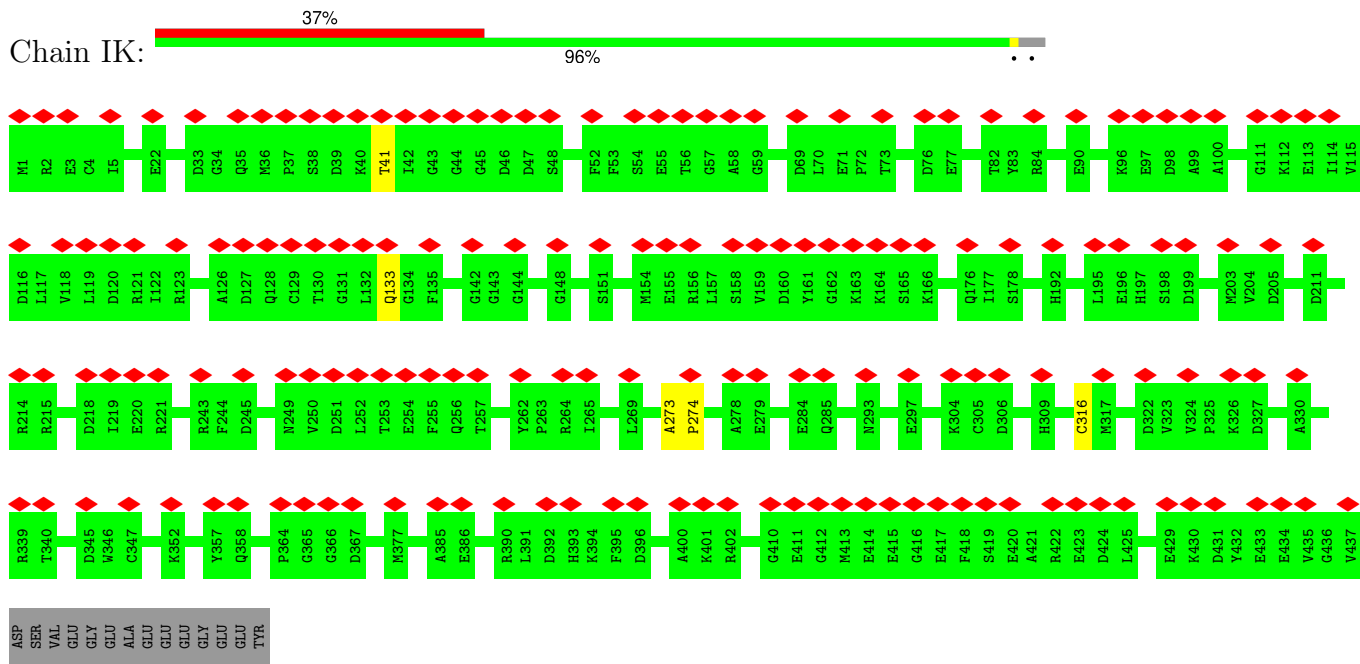
• Molecule 54: Tubulin alpha chain



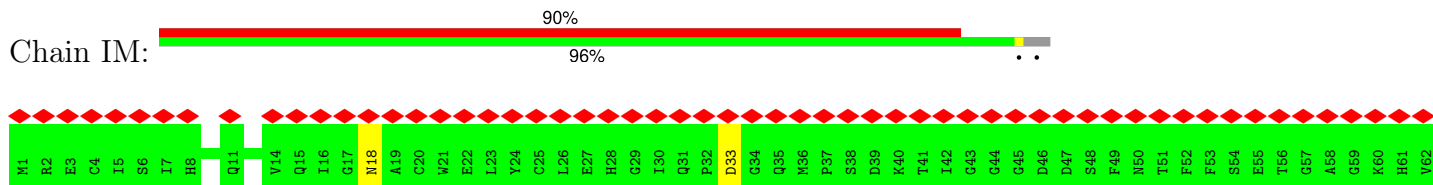
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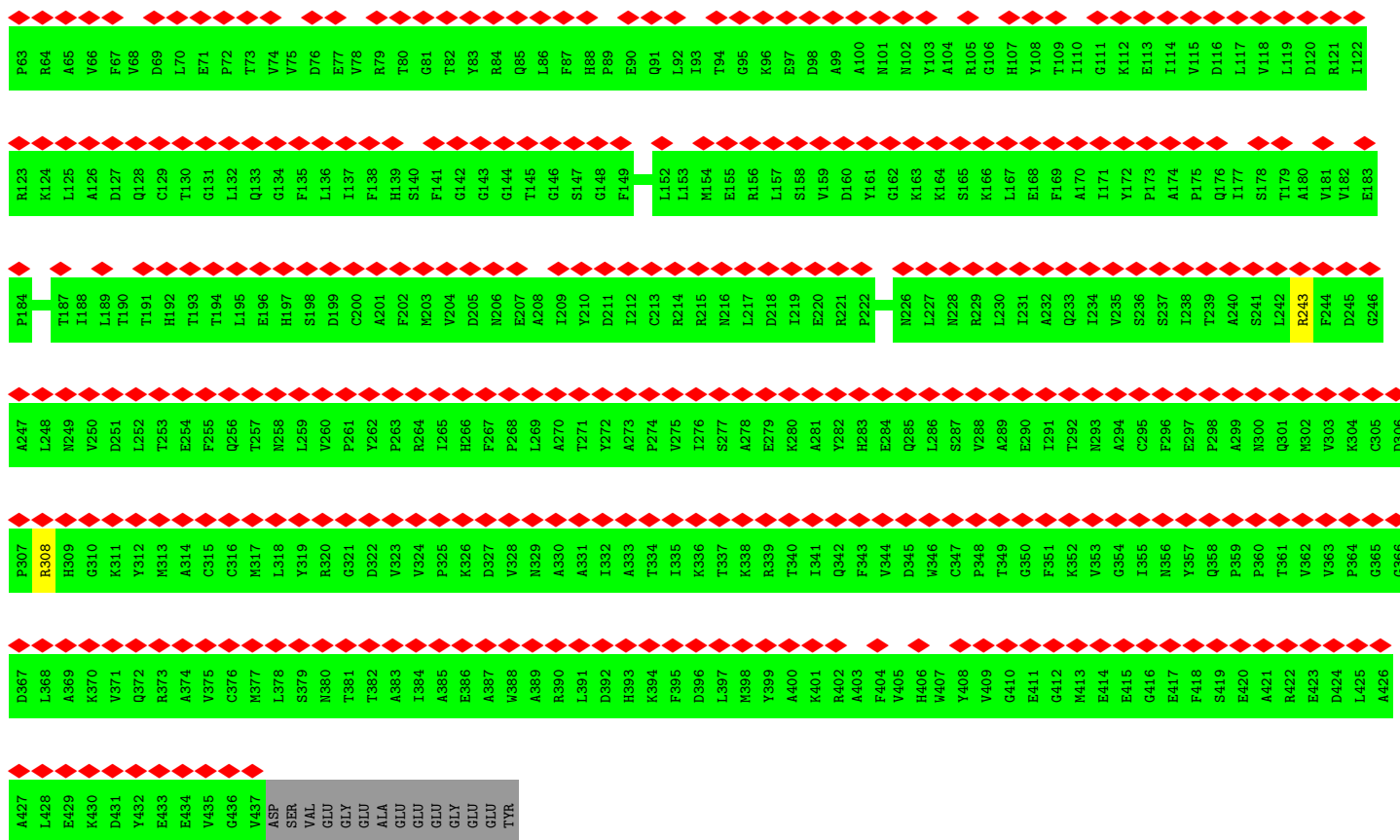


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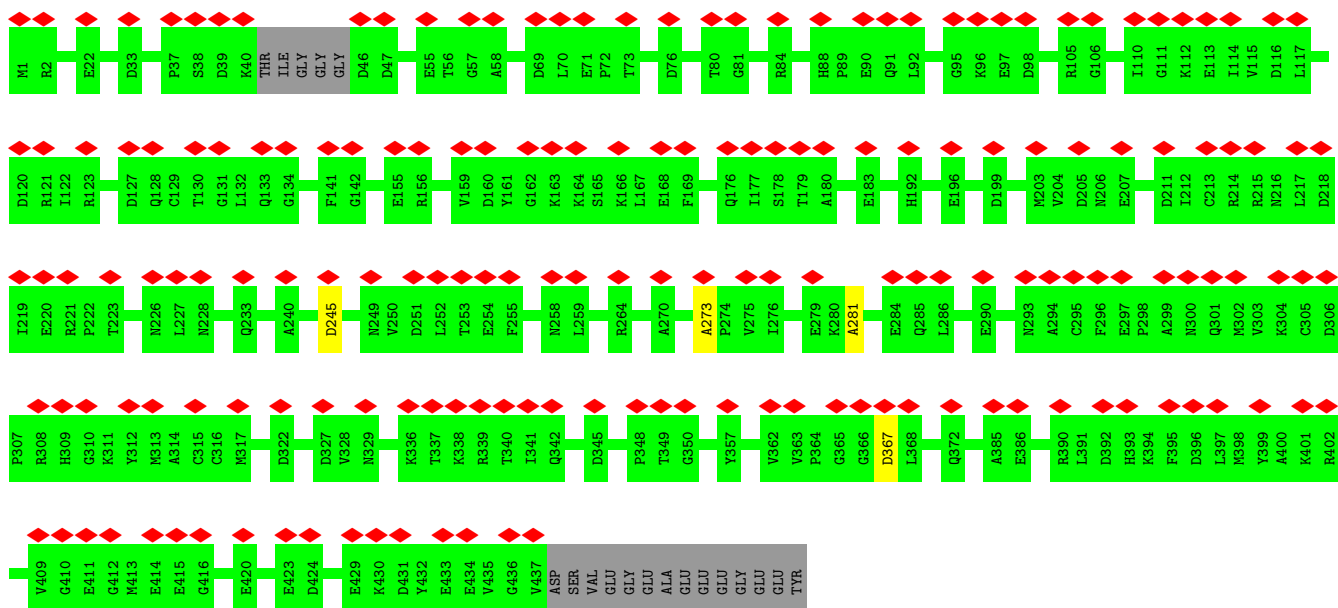
• Molecule 54: Tubulin alpha chain



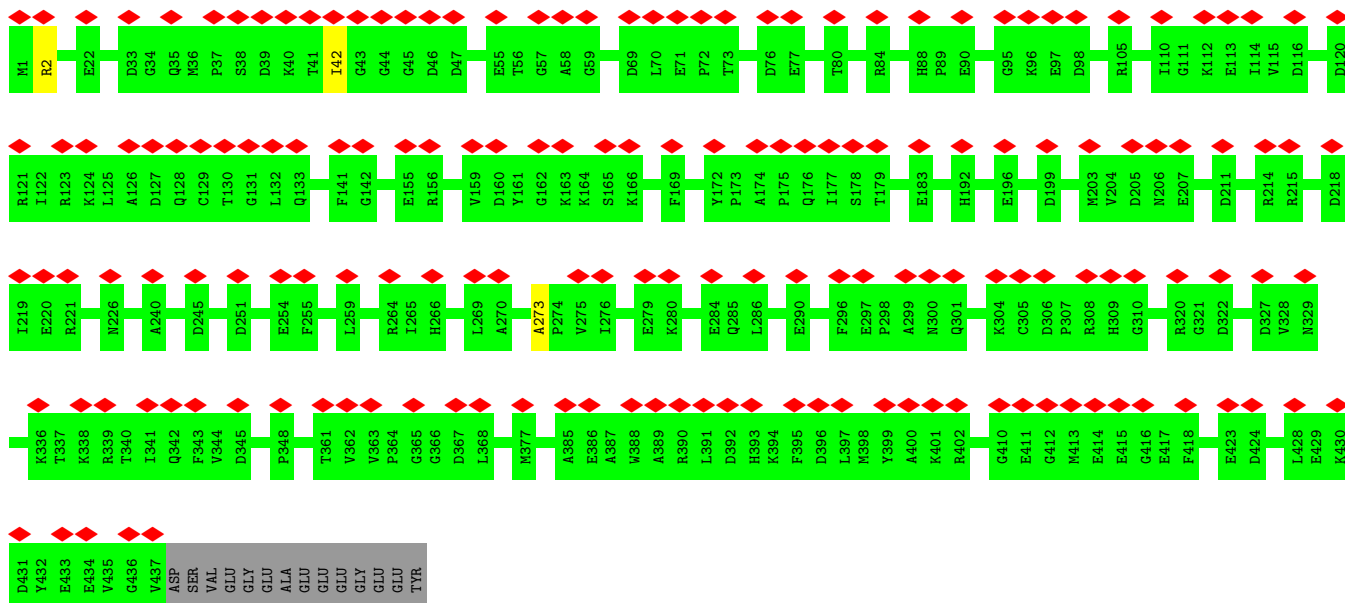


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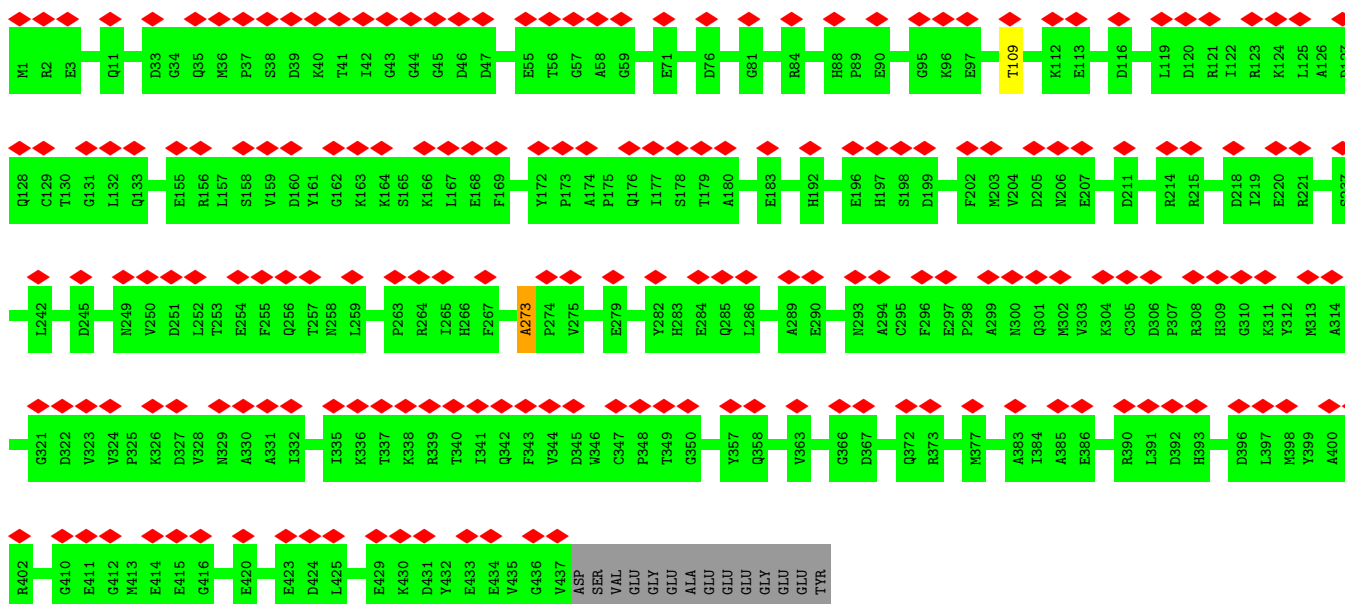
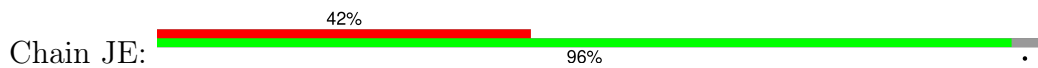
Chain JA:



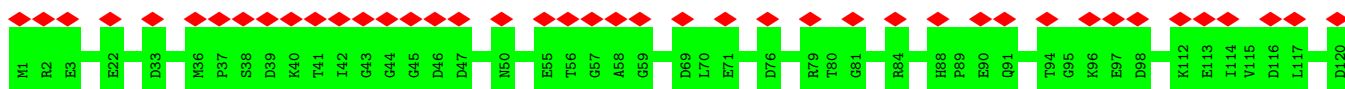
• Molecule 54: Tubulin alpha chain

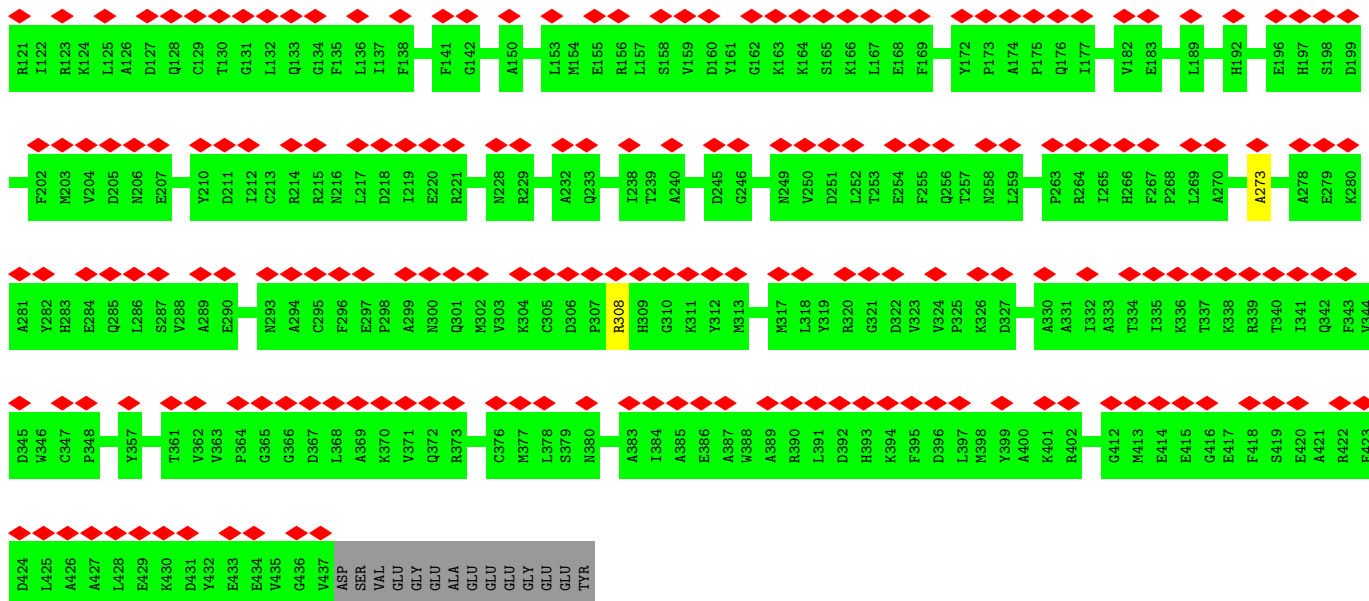


• Molecule 54: Tubulin alpha chain

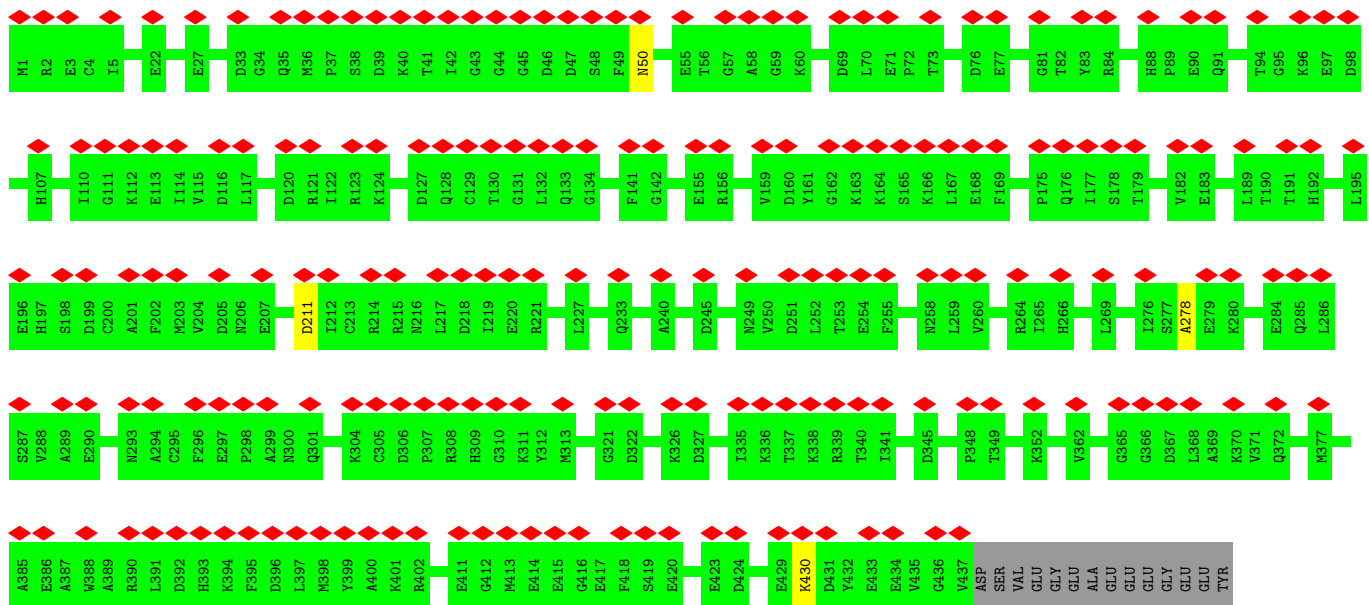
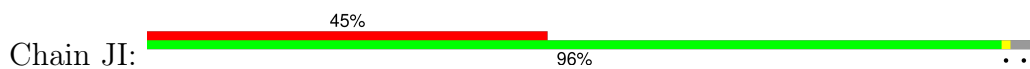


• Molecule 54: Tubulin alpha chain

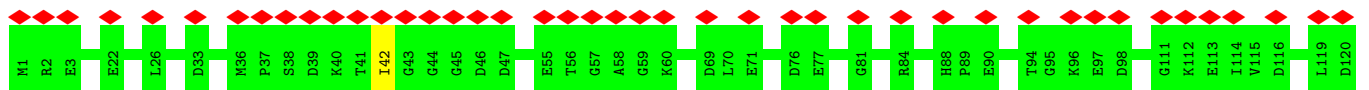


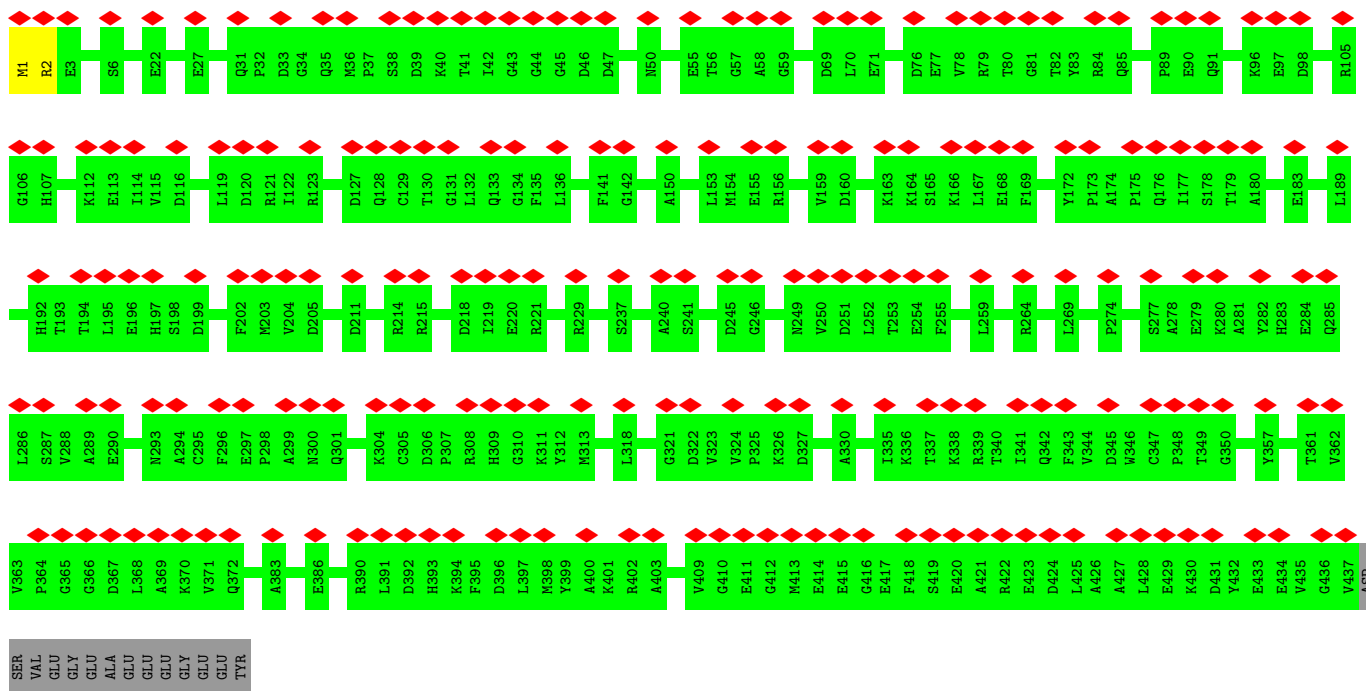


• Molecule 54: Tubulin alpha chain

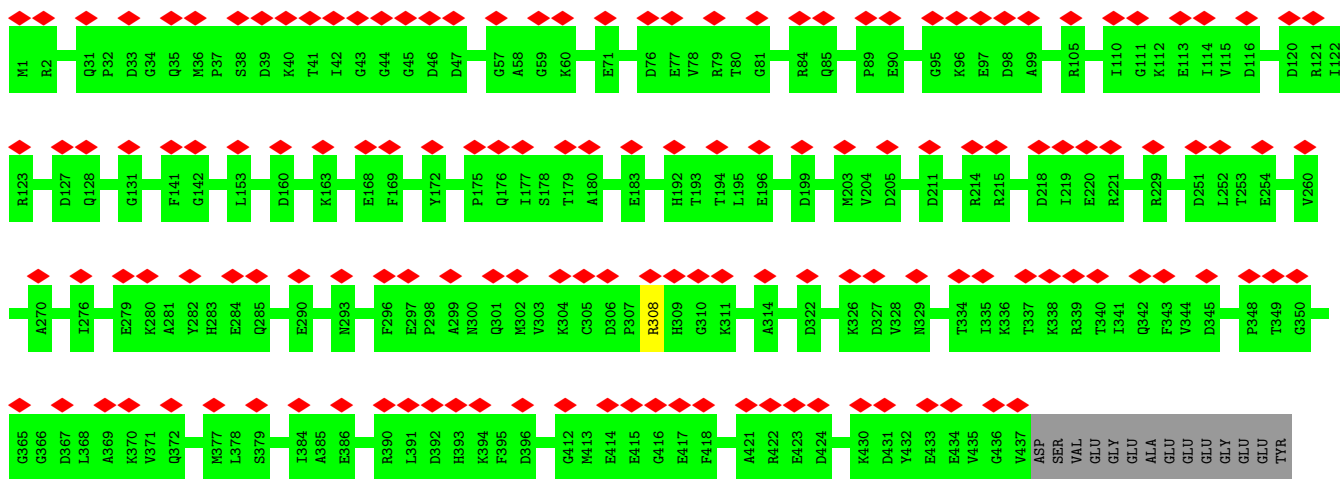


• Molecule 54: Tubulin alpha chain

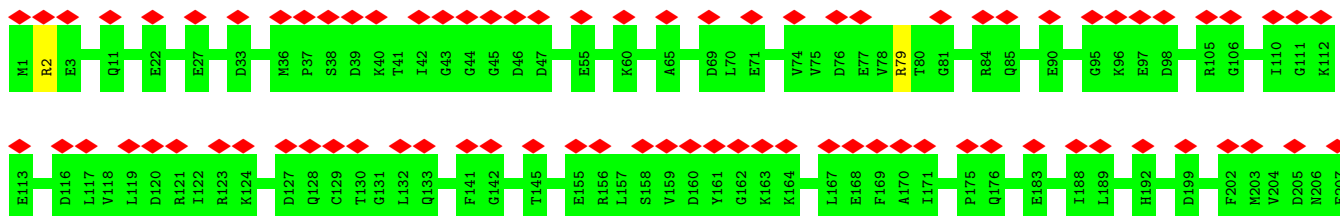


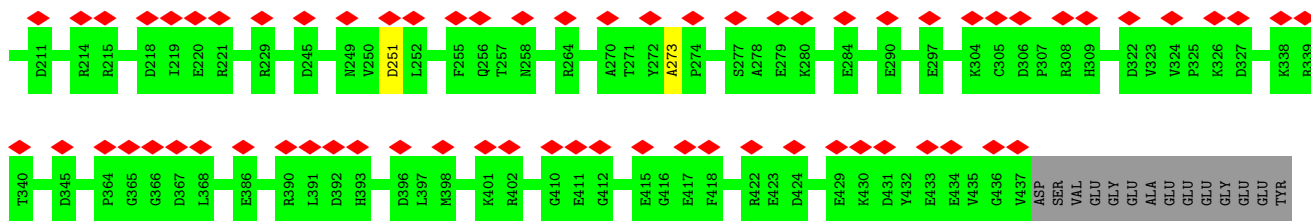


• Molecule 54: Tubulin alpha chain

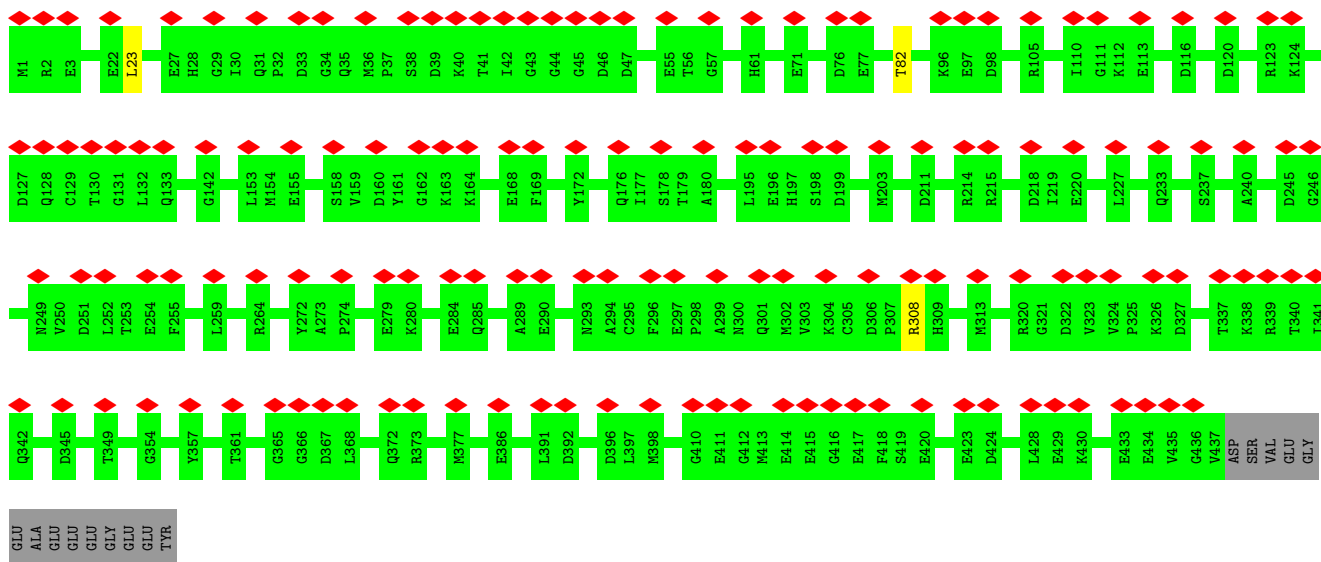


• Molecule 54: Tubulin alpha chain

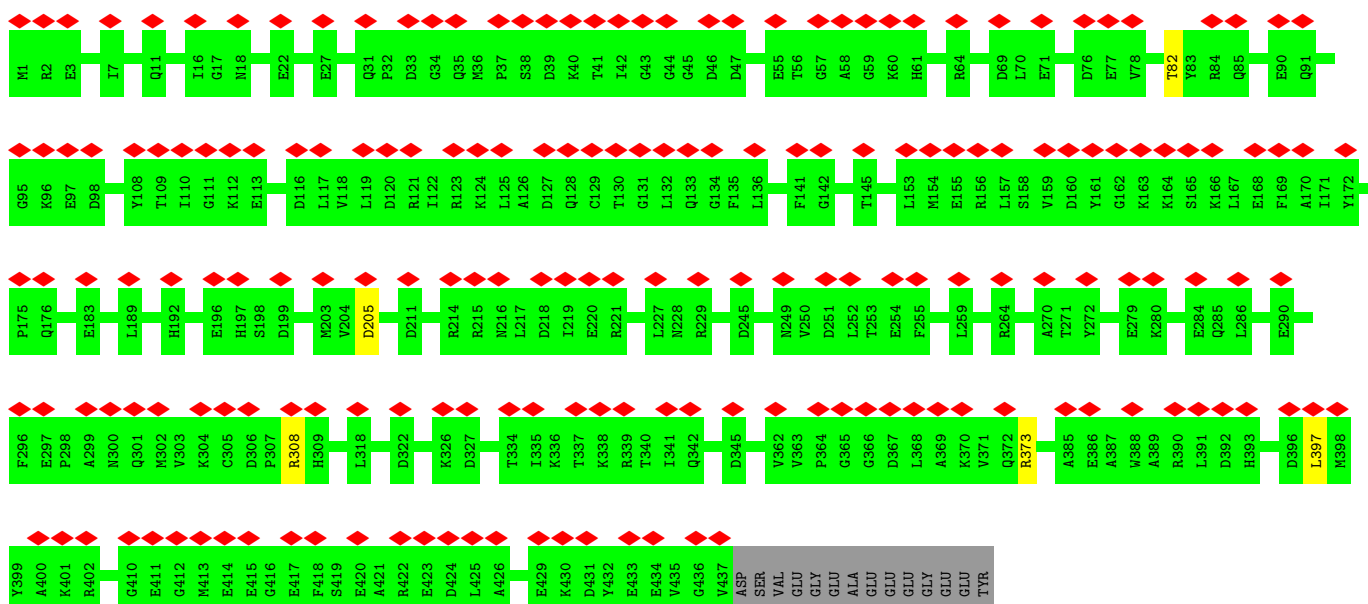




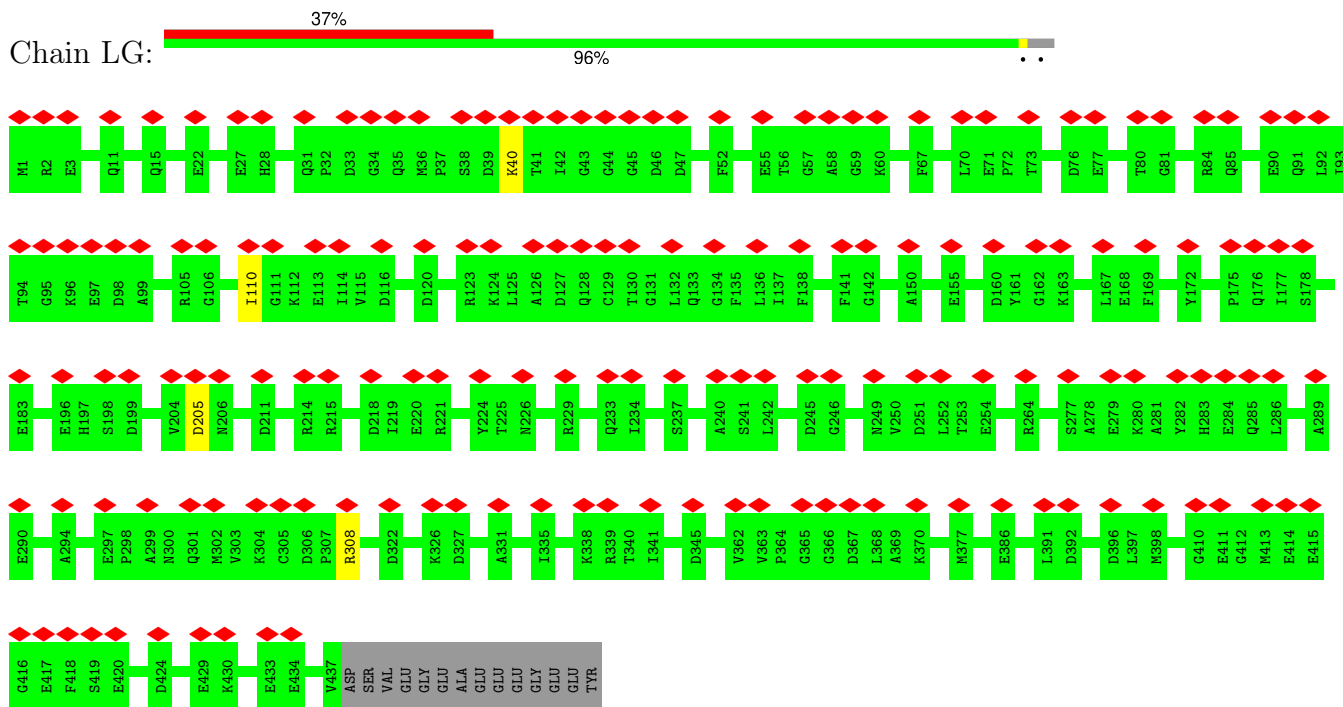
• Molecule 54: Tubulin alpha chain



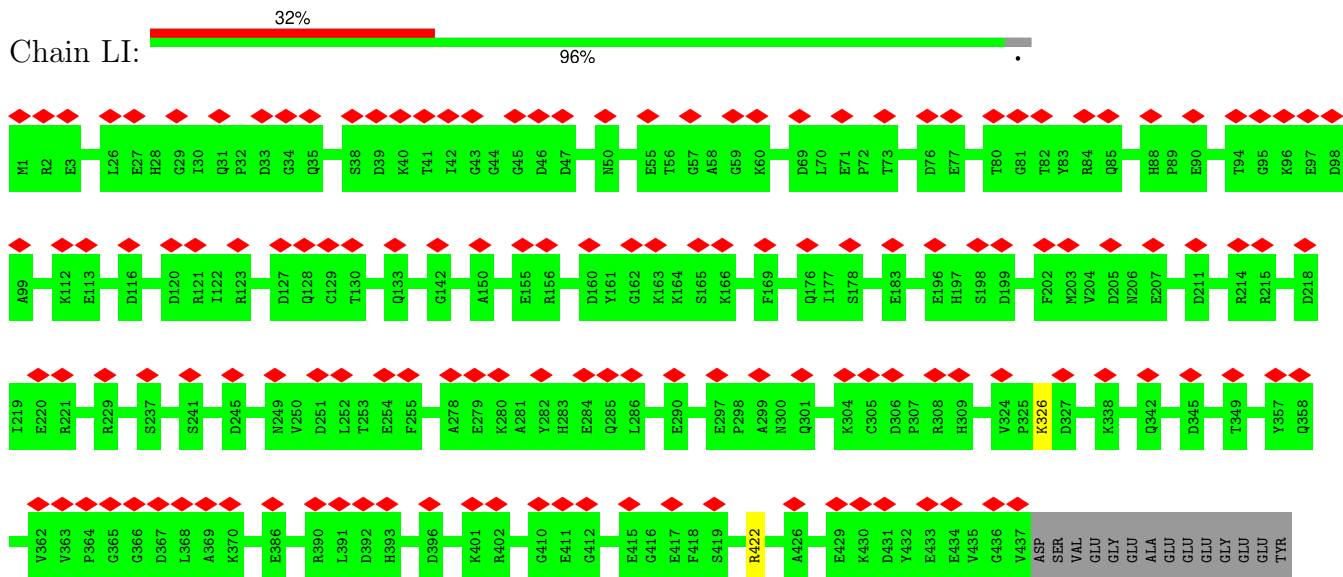
• Molecule 54: Tubulin alpha chain



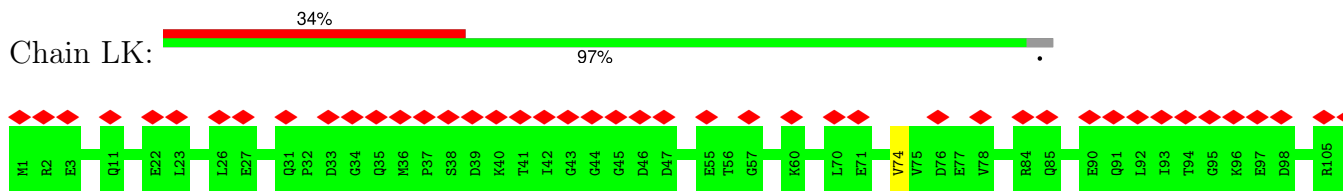
• Molecule 54: Tubulin alpha chain

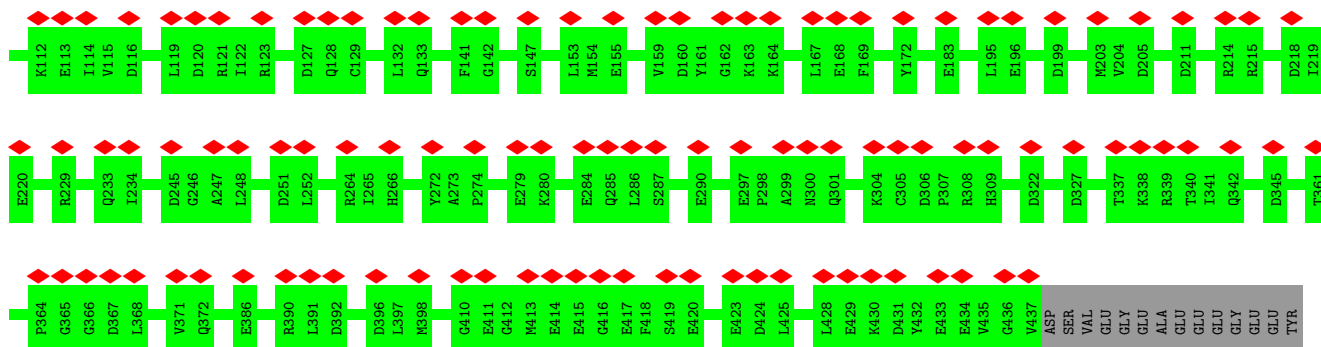


• Molecule 54: Tubulin alpha chain

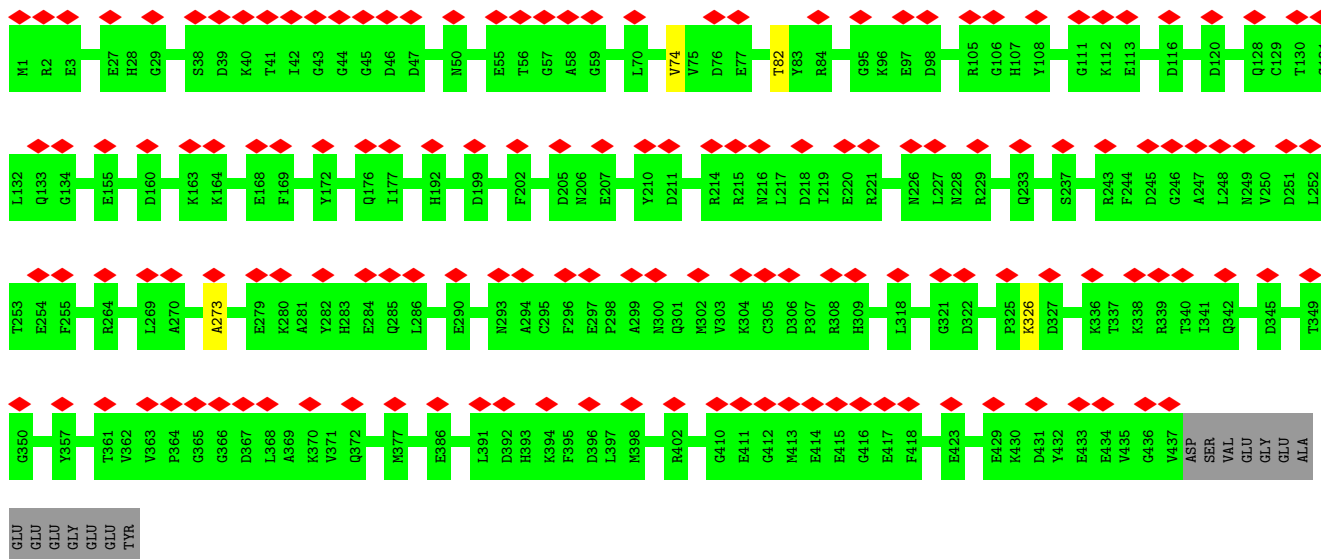


• Molecule 54: Tubulin alpha chain

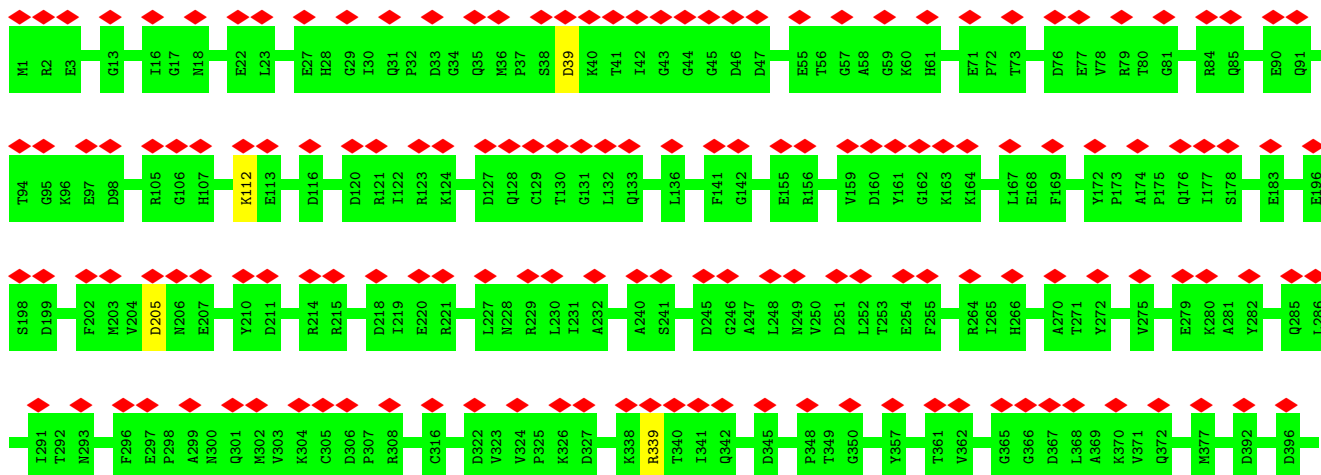
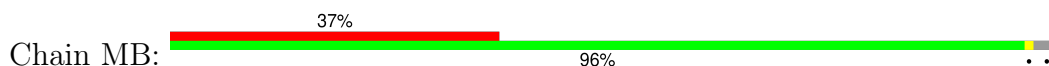


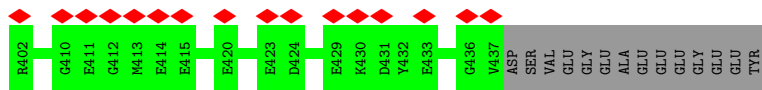


• Molecule 54: Tubulin alpha chain

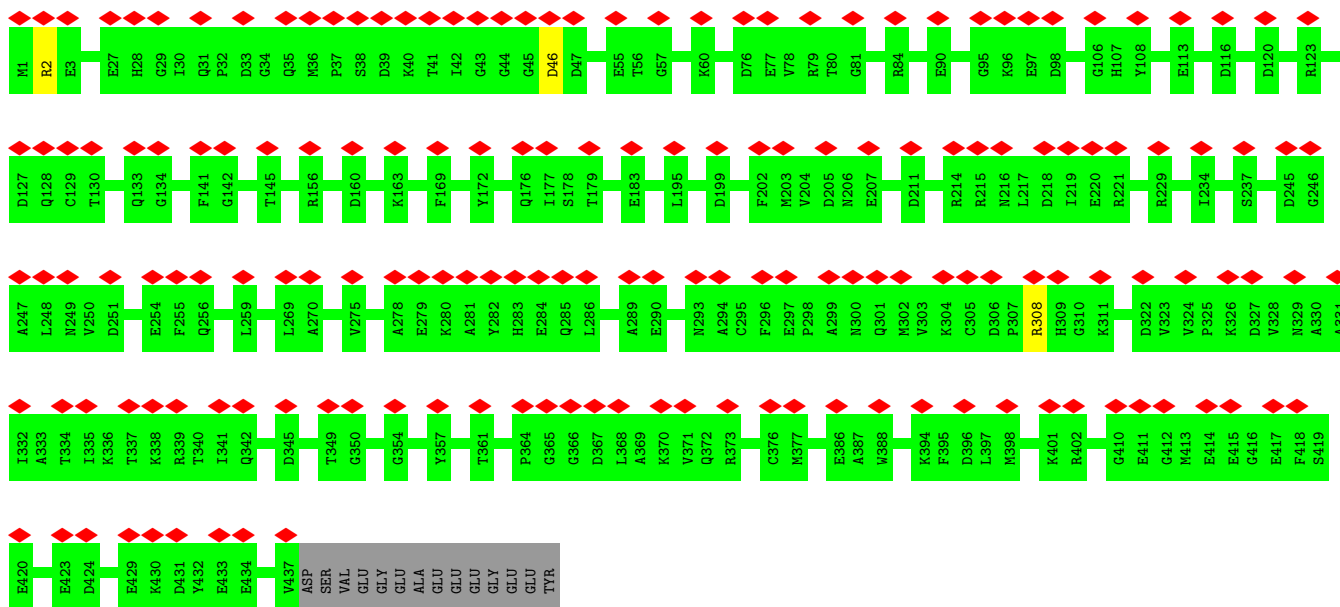
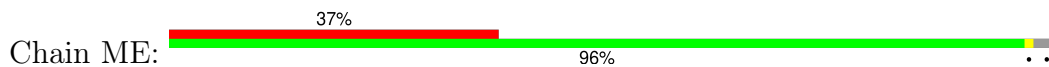


• Molecule 54: Tubulin alpha chain

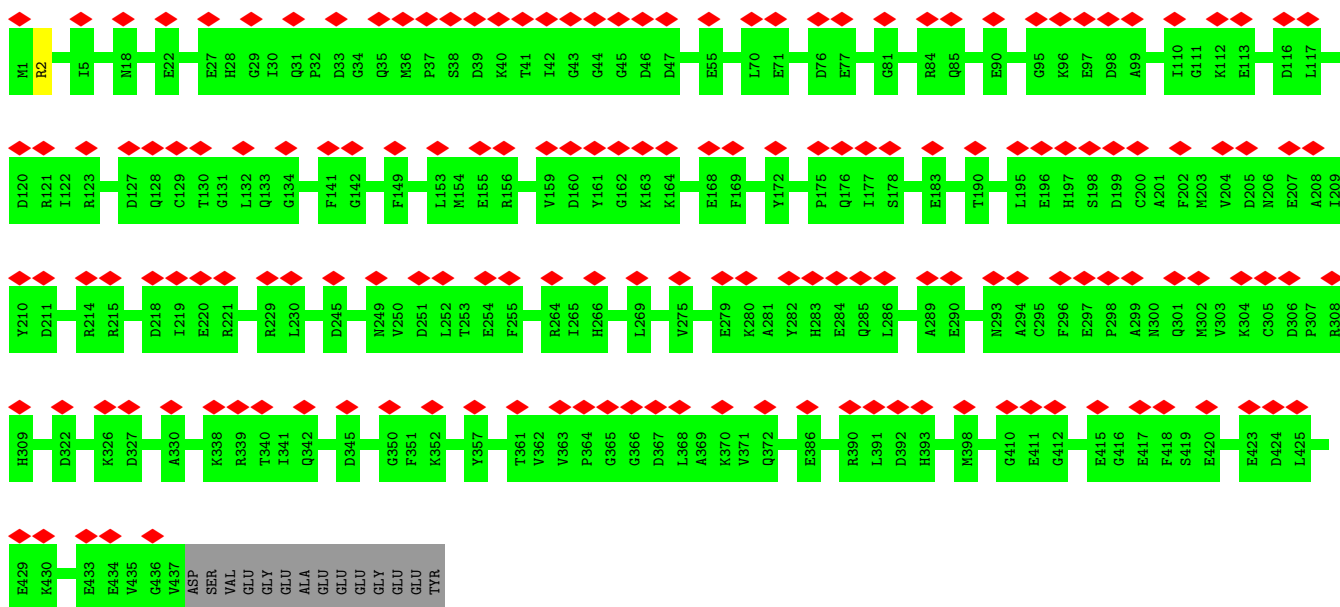
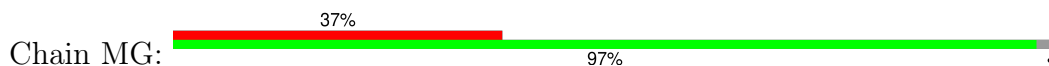




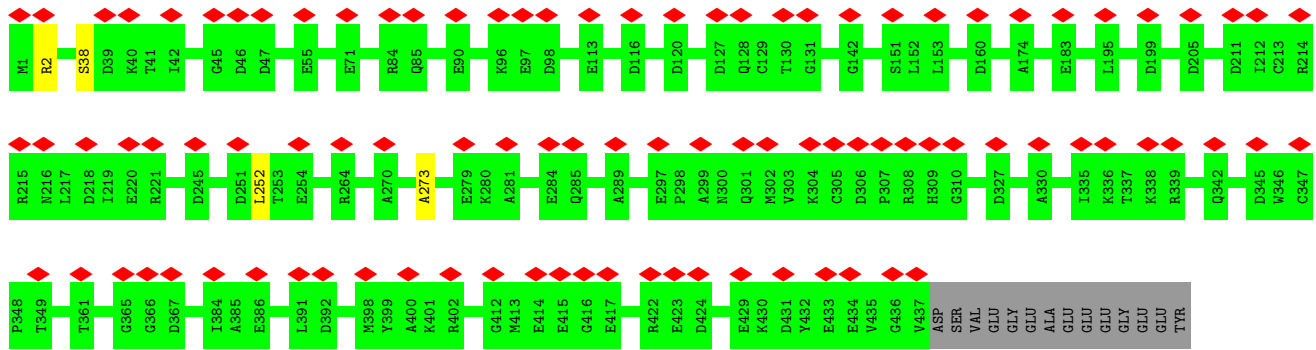
• Molecule 54: Tubulin alpha chain



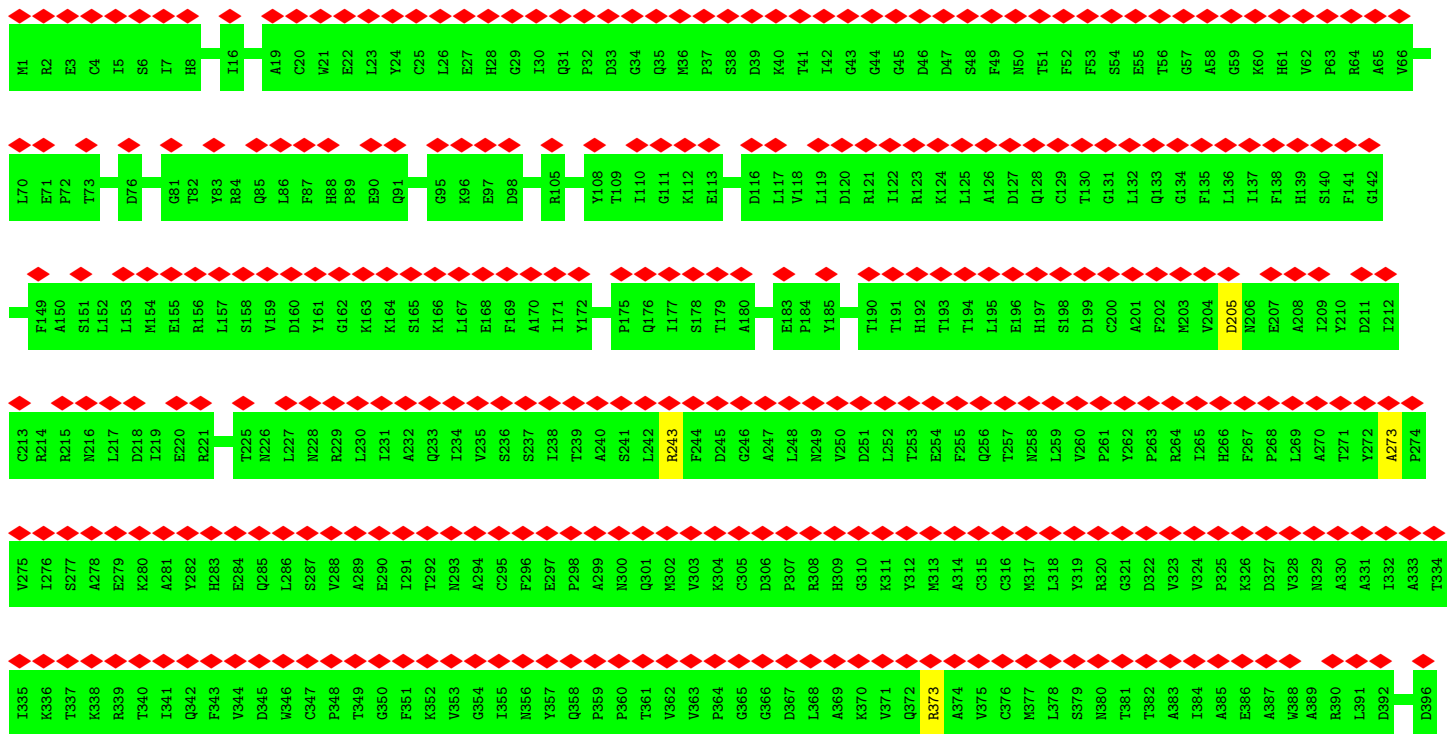
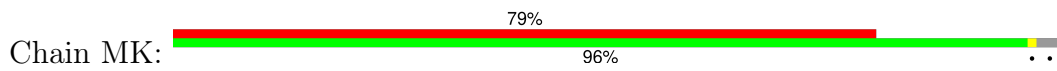
• Molecule 54: Tubulin alpha chain



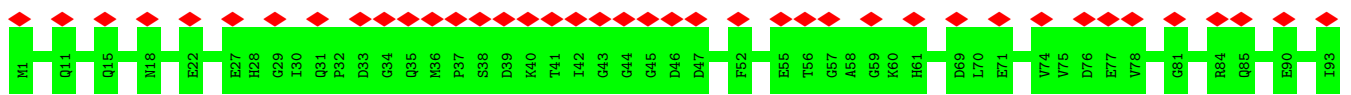
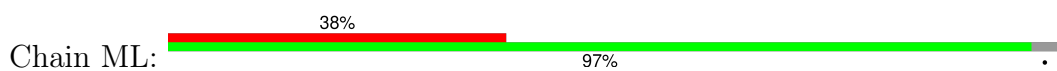
• Molecule 54: Tubulin alpha chain

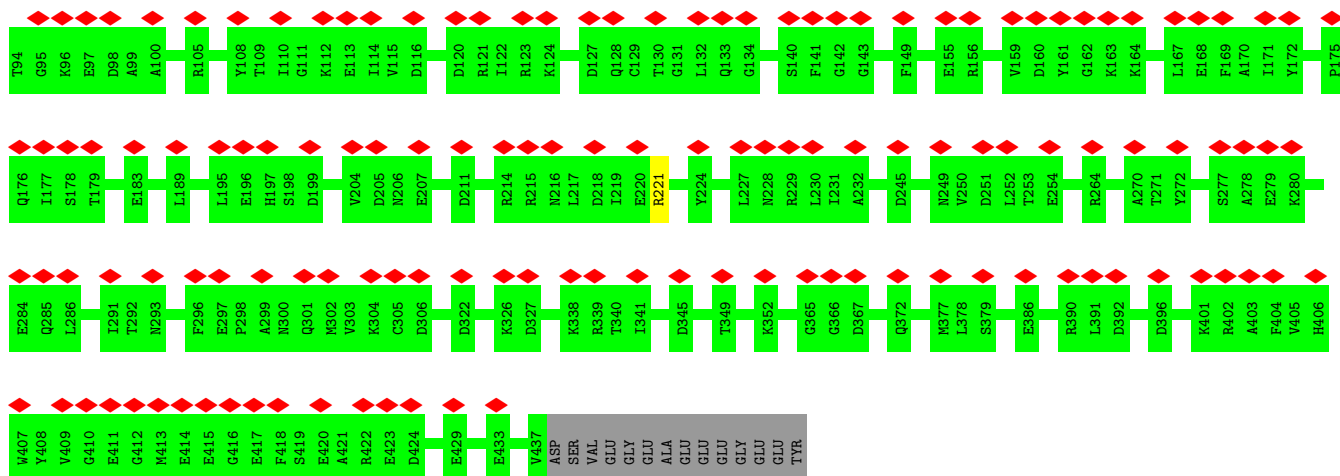


• Molecule 54: Tubulin alpha chain

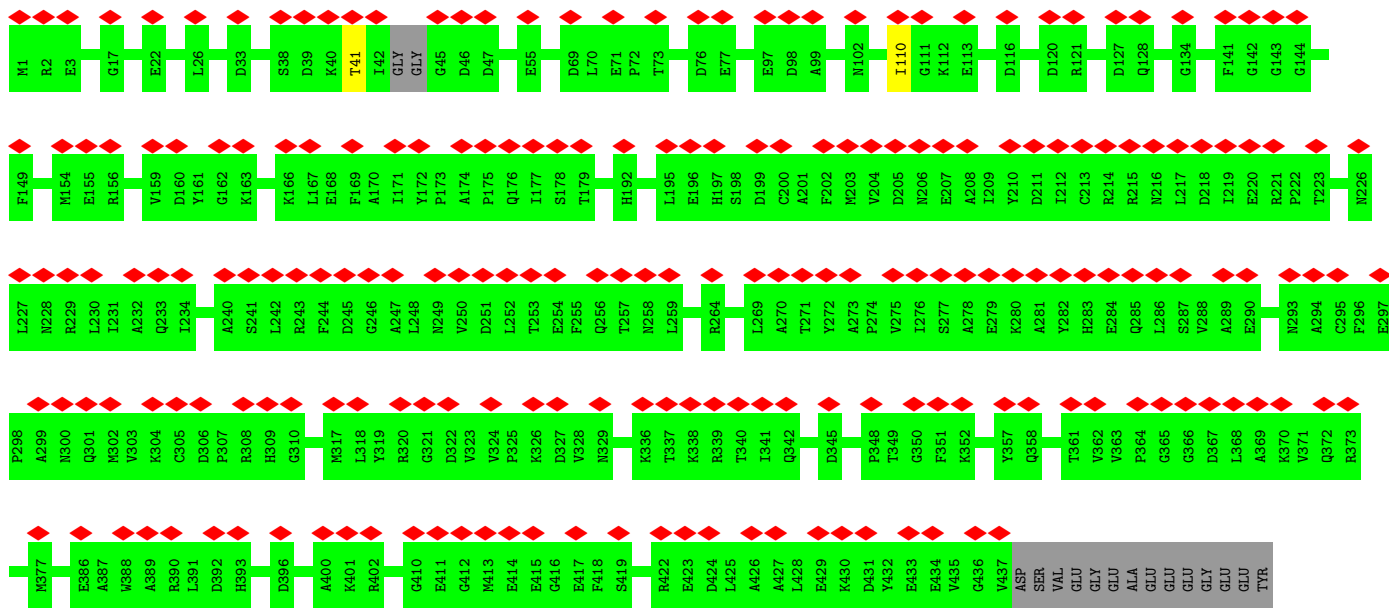


• Molecule 54: Tubulin alpha chain

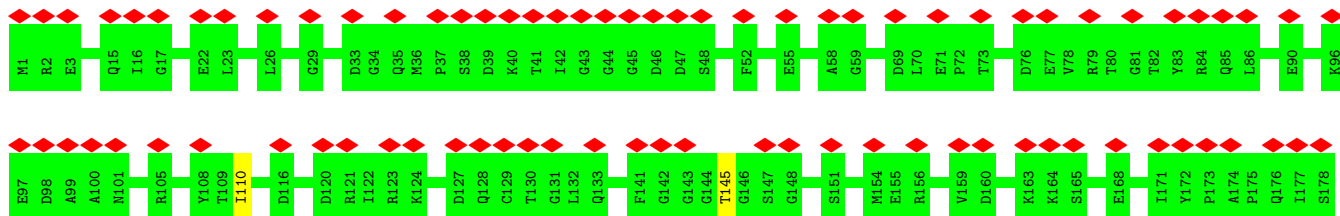


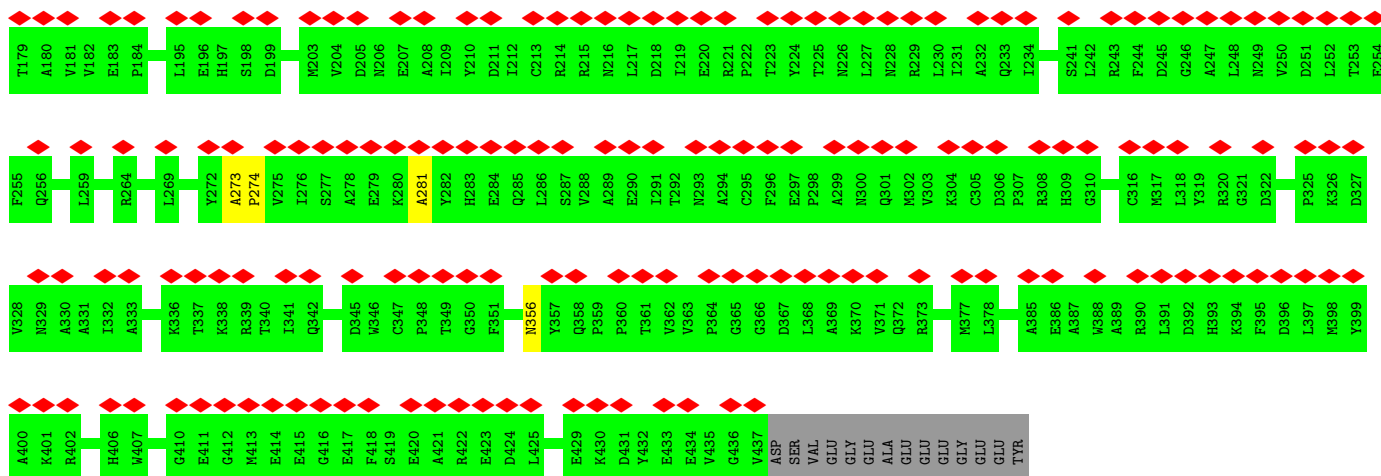


• Molecule 54: Tubulin alpha chain

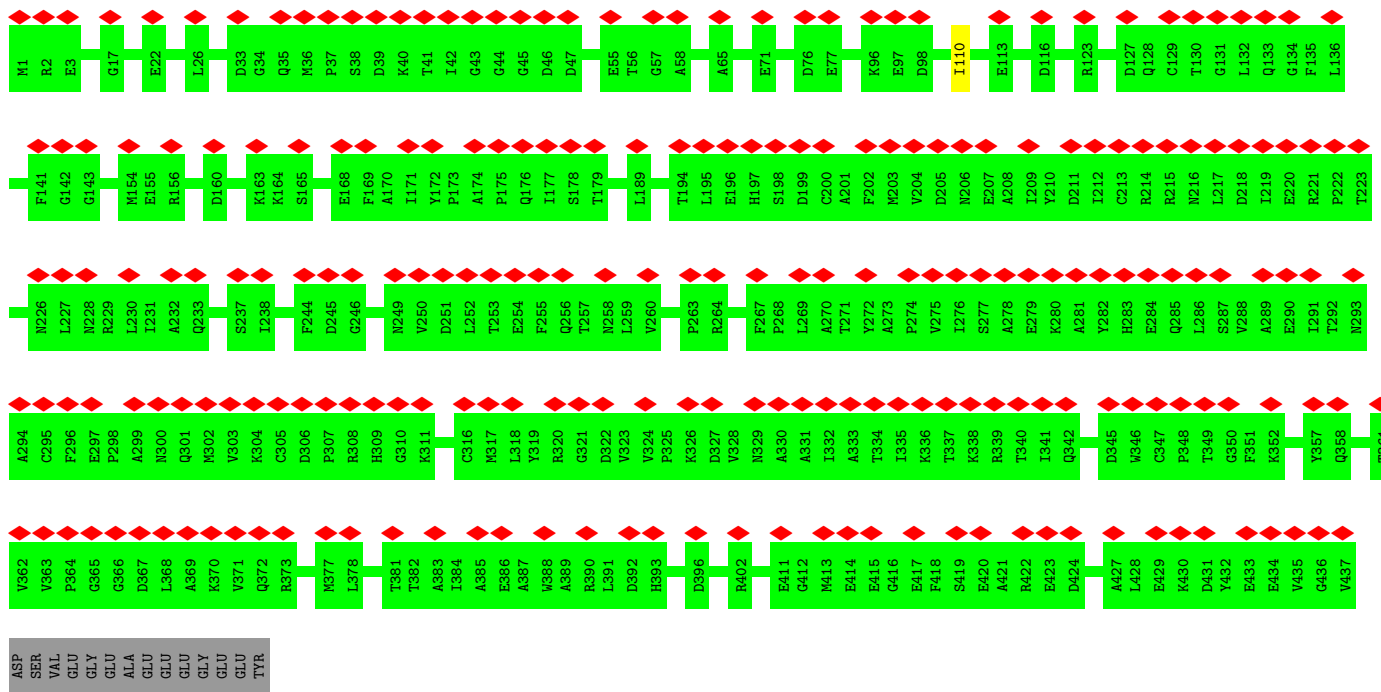


• Molecule 54: Tubulin alpha chain

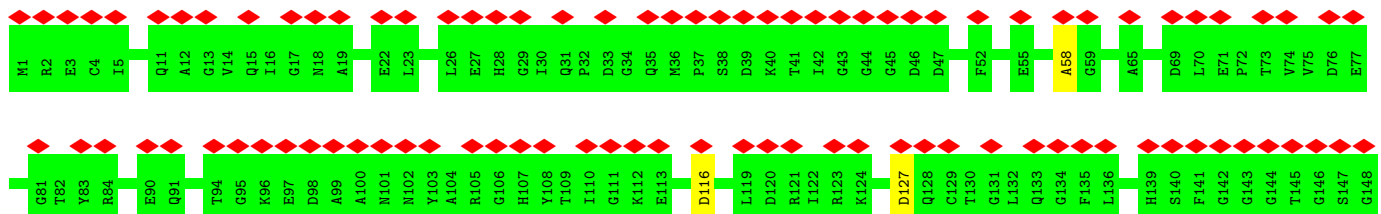
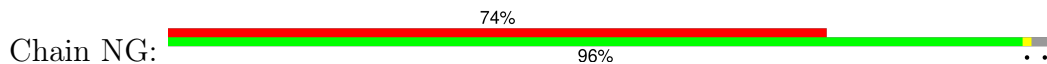




- Molecule 54: Tubulin alpha chain

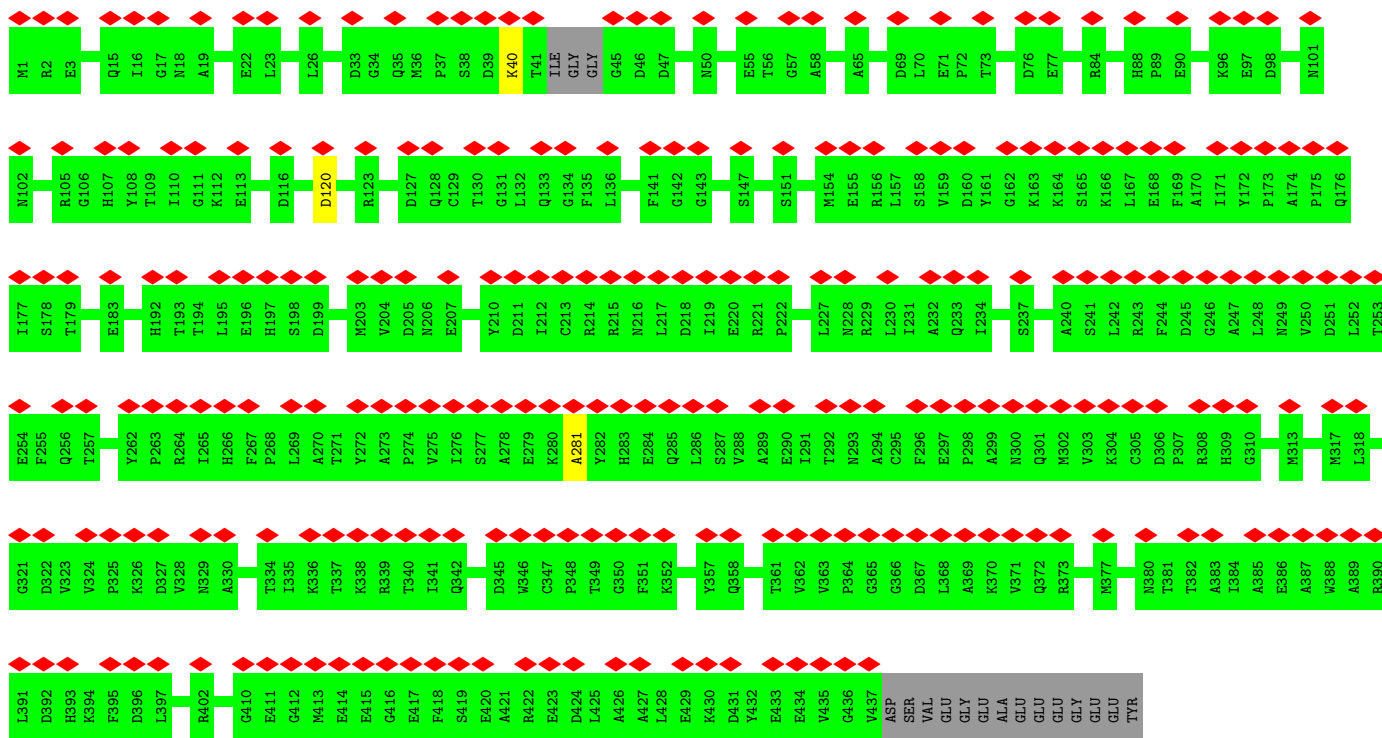


- Molecule 54: Tubulin alpha chain



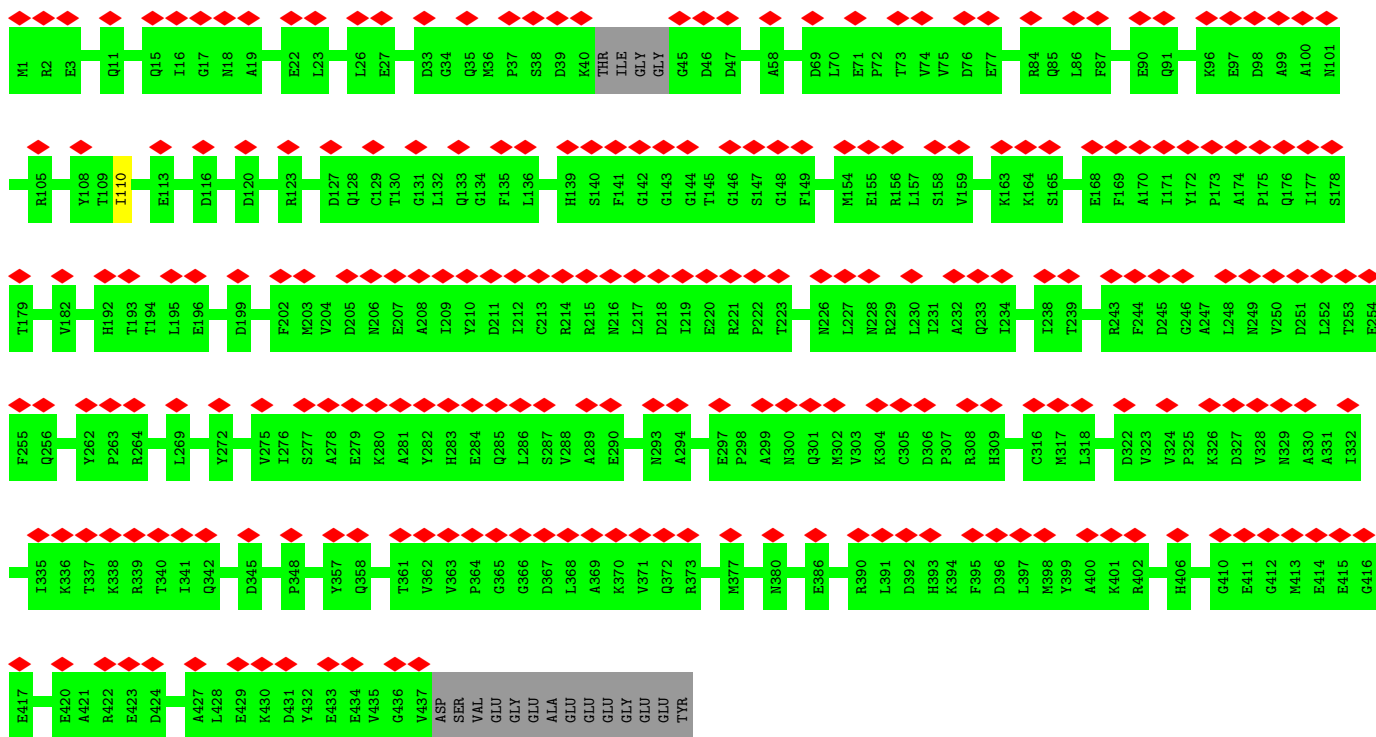


• Molecule 54: Tubulin alpha chain

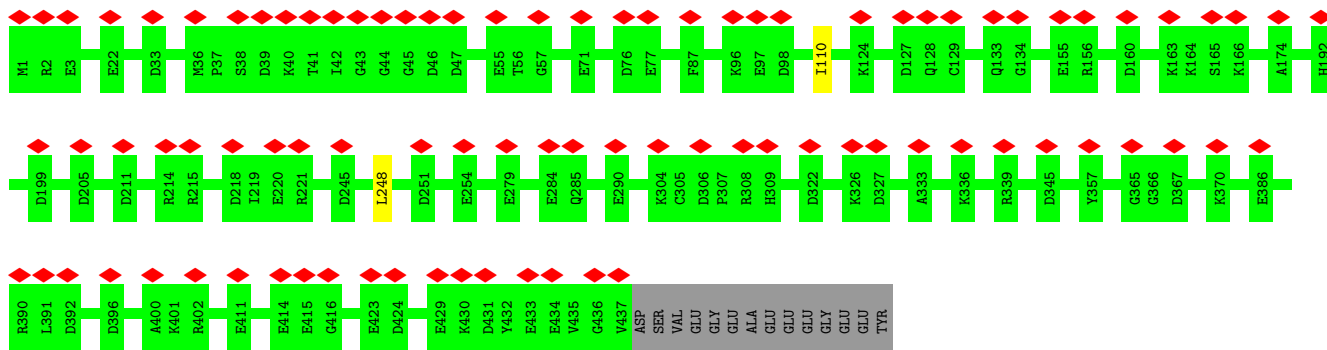


• Molecule 54: Tubulin alpha chain

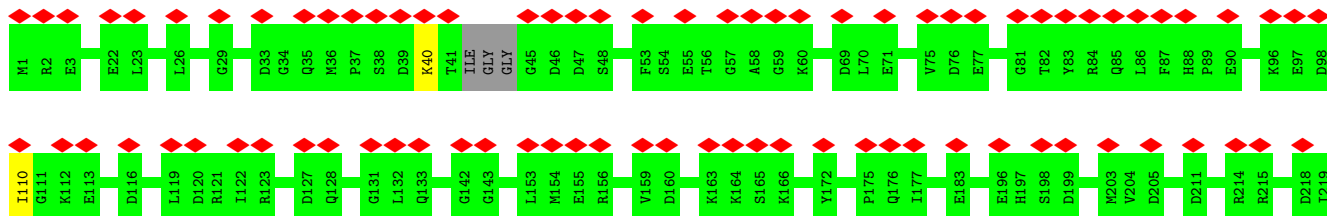


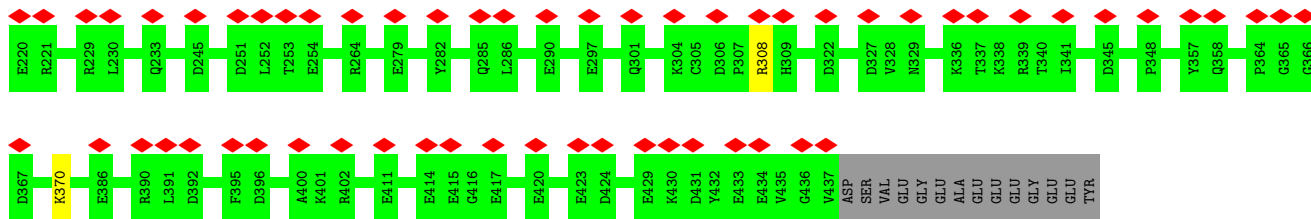


• Molecule 54: Tubulin alpha chain

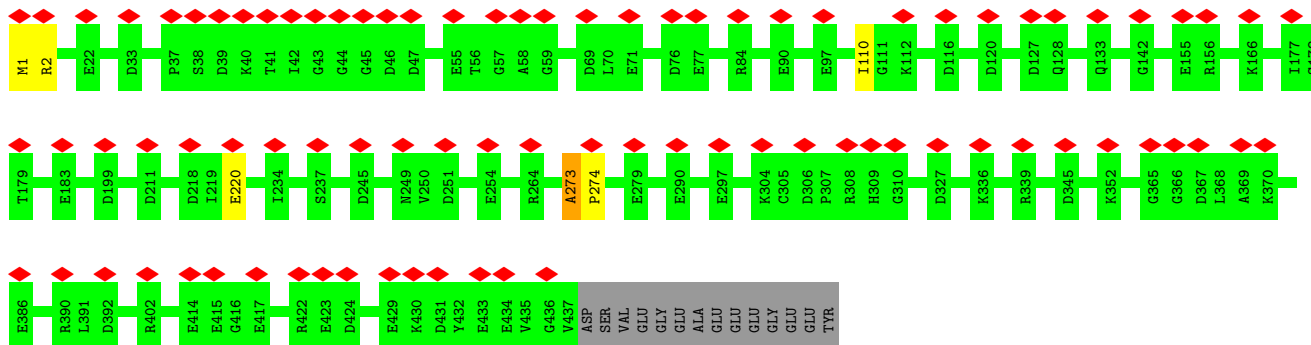


• Molecule 54: Tubulin alpha chain

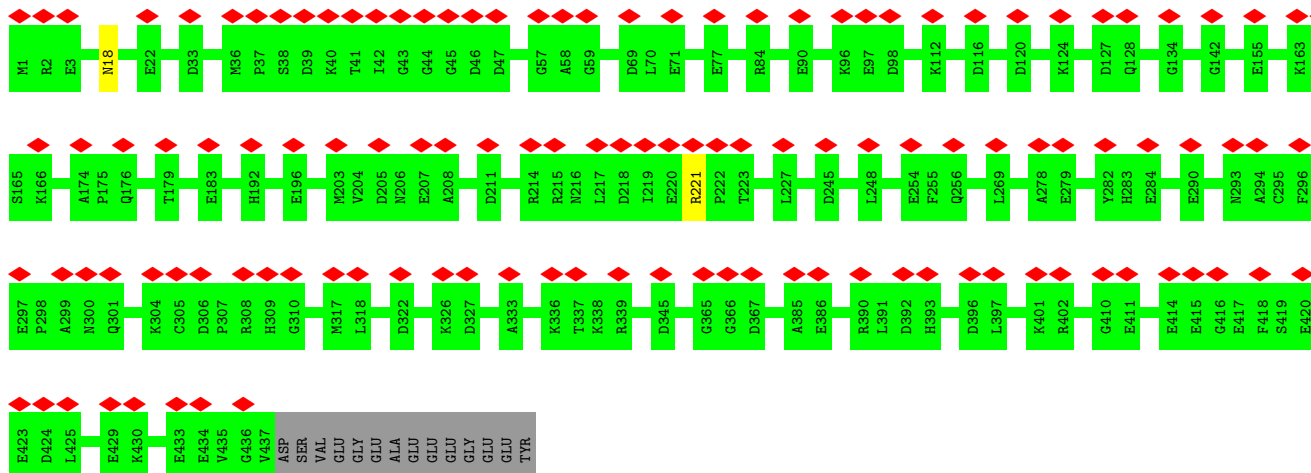




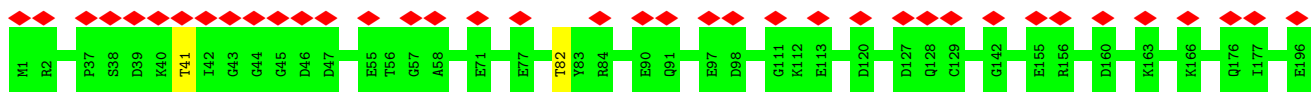
• Molecule 54: Tubulin alpha chain

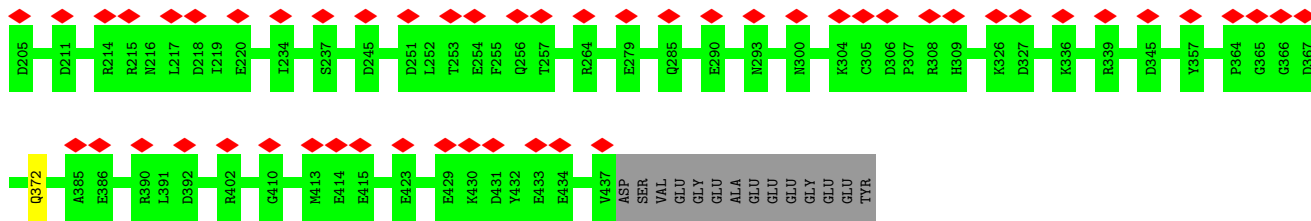


• Molecule 54: Tubulin alpha chain

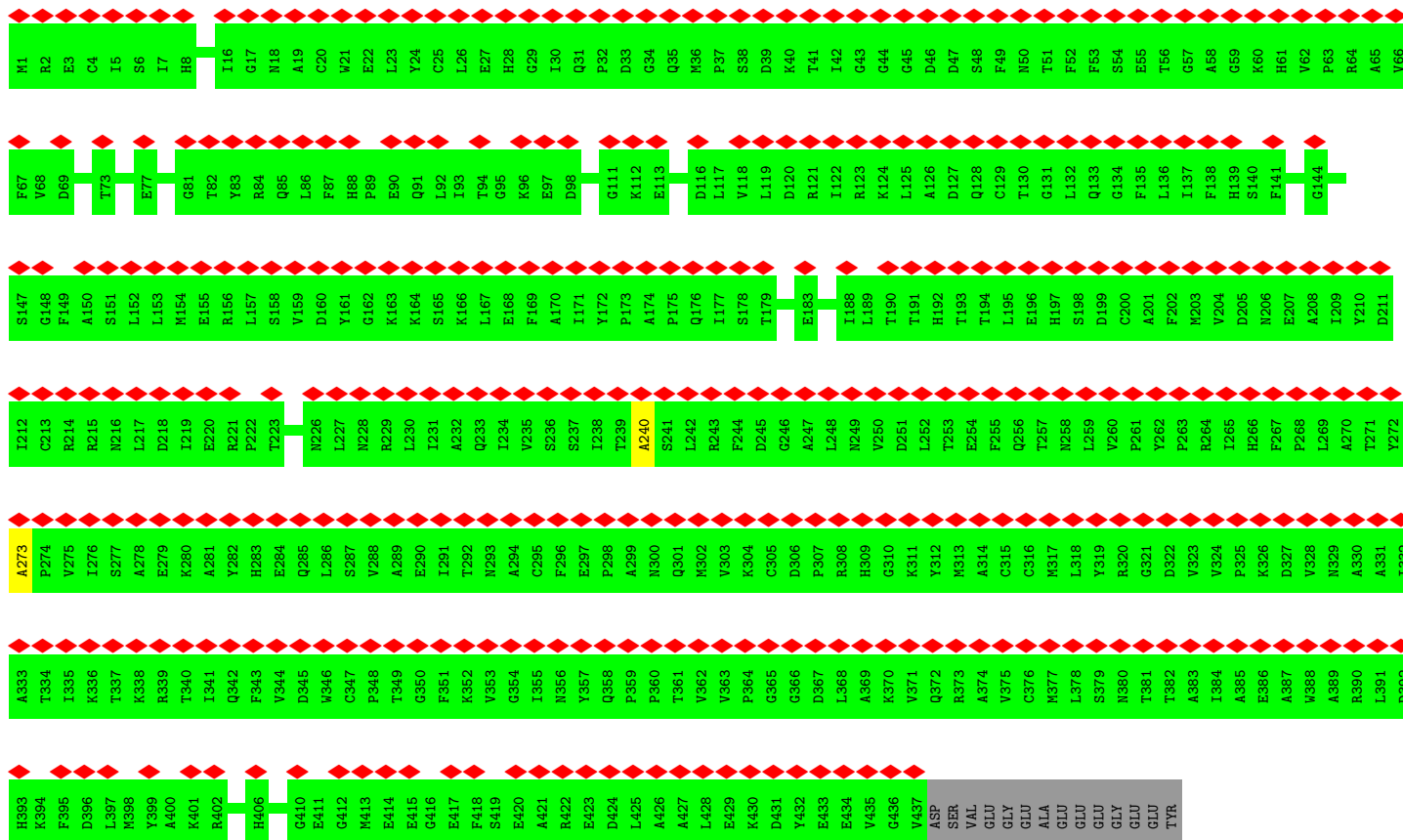
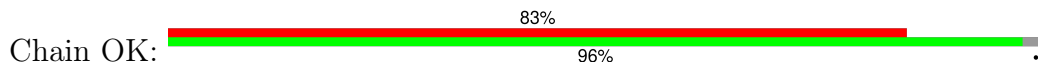


• Molecule 54: Tubulin alpha chain

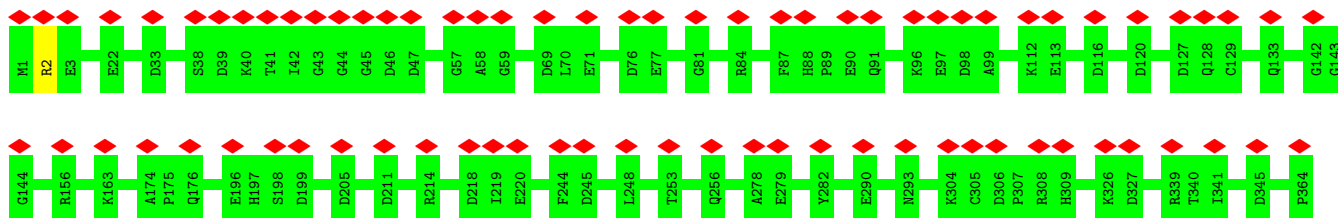


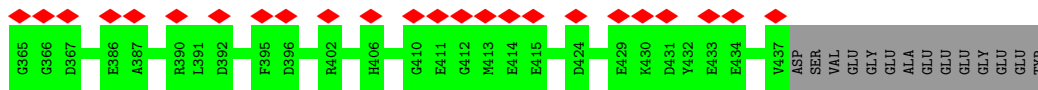


• Molecule 54: Tubulin alpha chain

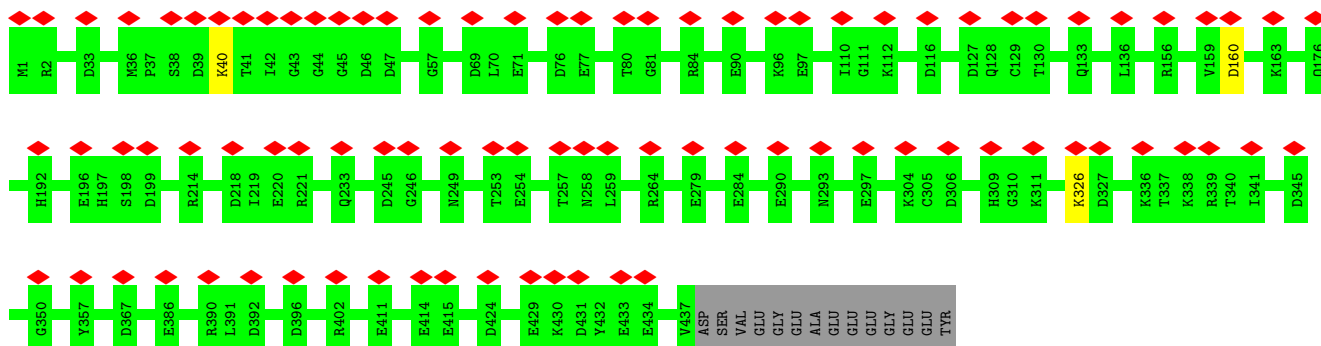


• Molecule 54: Tubulin alpha chain





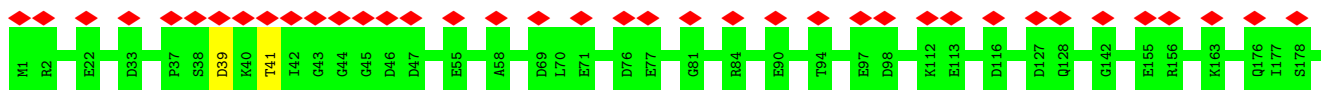
• Molecule 54: Tubulin alpha chain

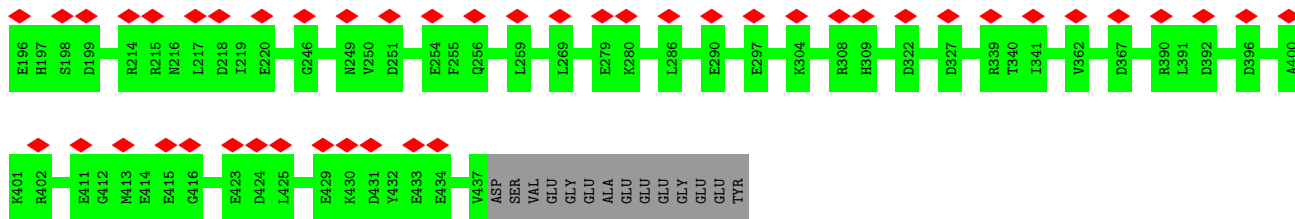


• Molecule 54: Tubulin alpha chain

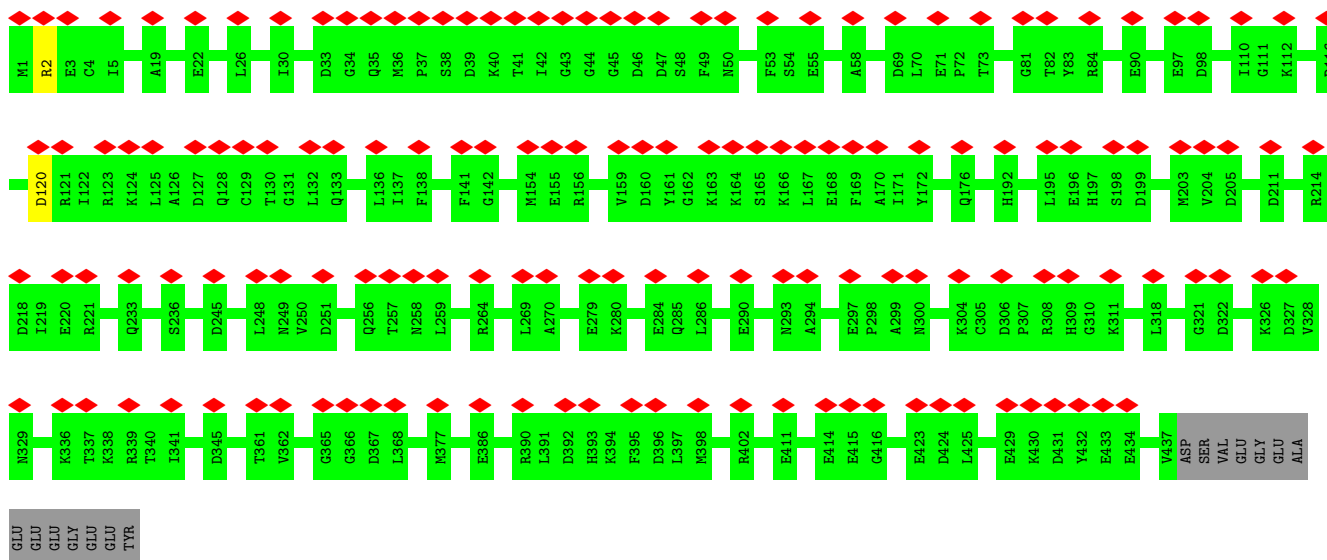


• Molecule 54: Tubulin alpha chain

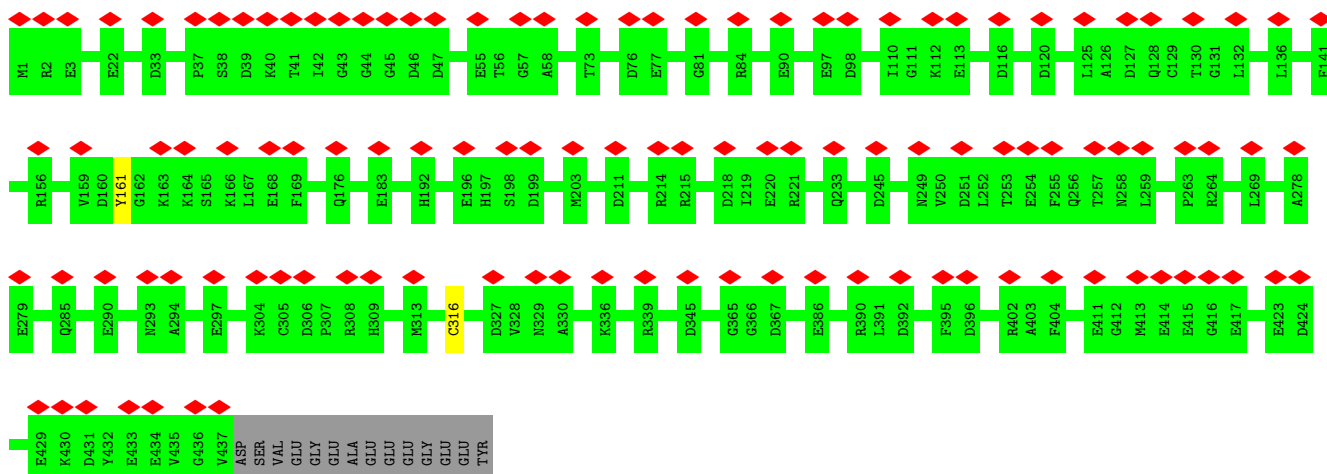




• Molecule 54: Tubulin alpha chain

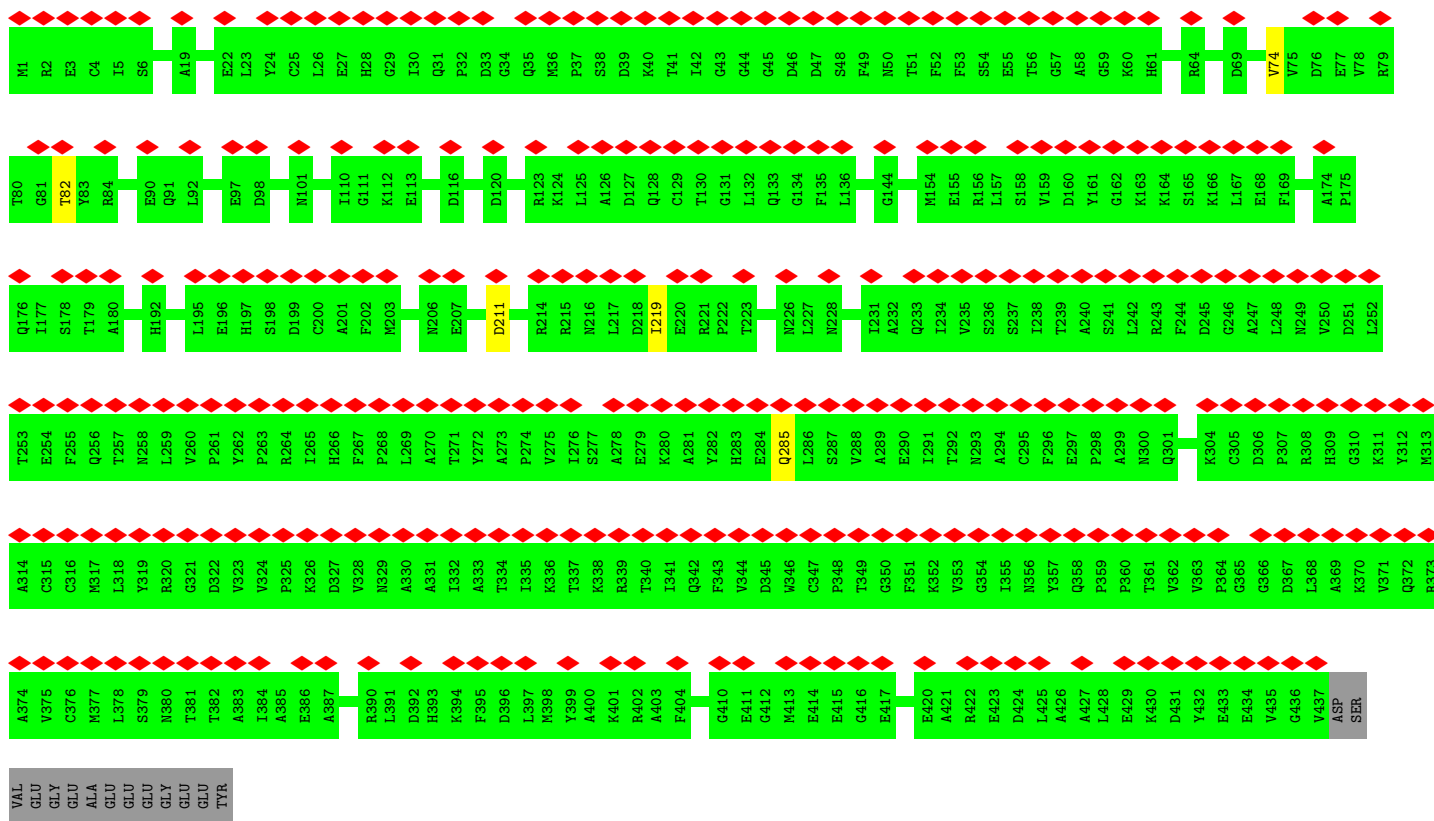


• Molecule 54: Tubulin alpha chain



• Molecule 54: Tubulin alpha chain



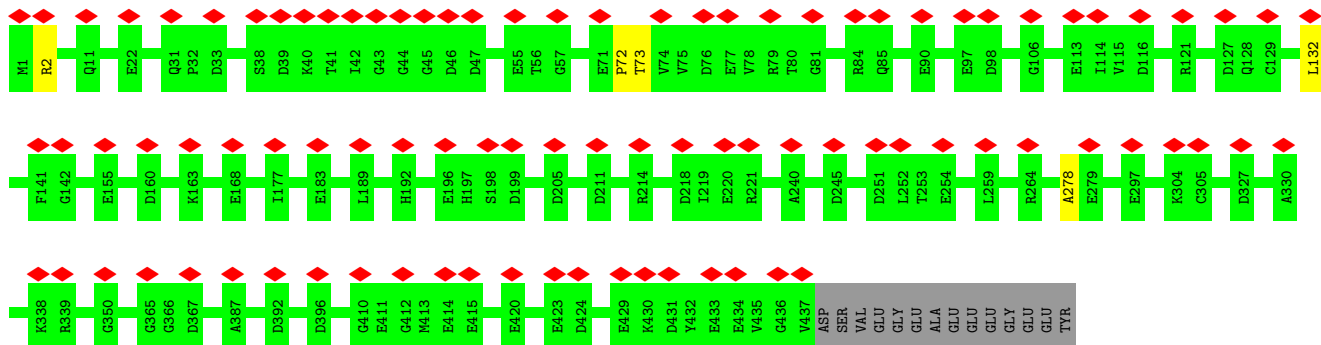


• Molecule 54: Tubulin alpha chain

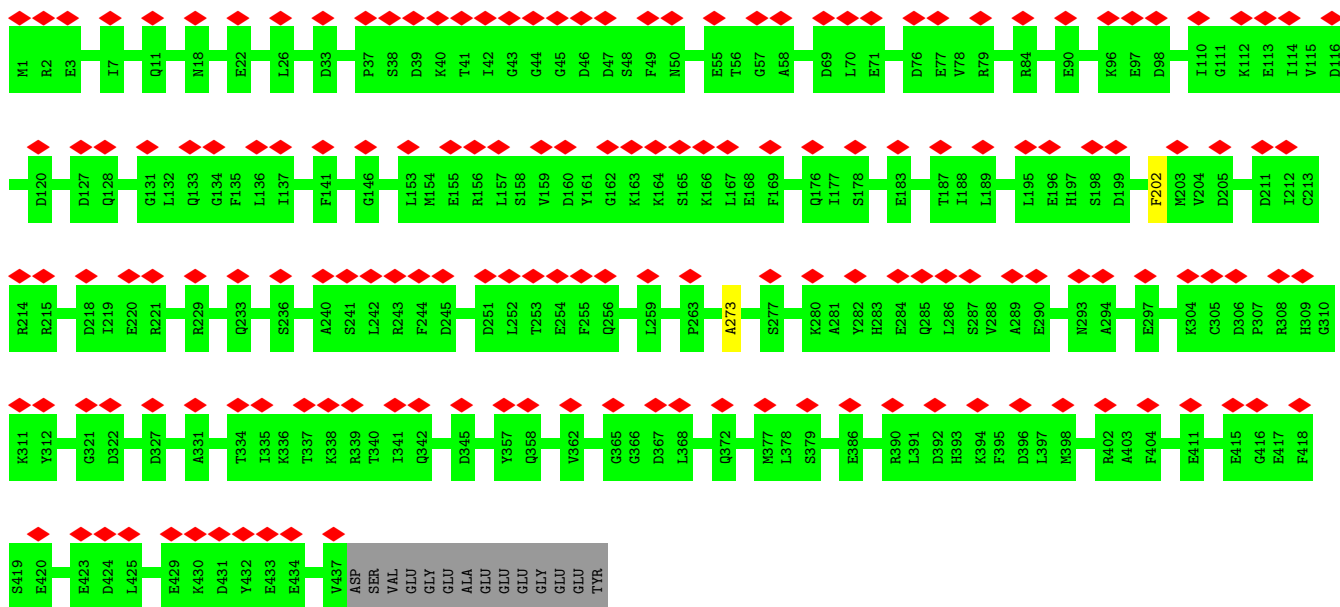
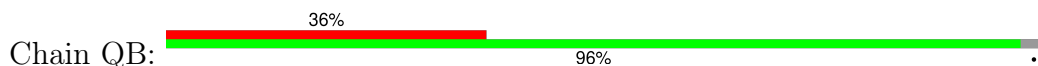


• Molecule 54: Tubulin alpha chain

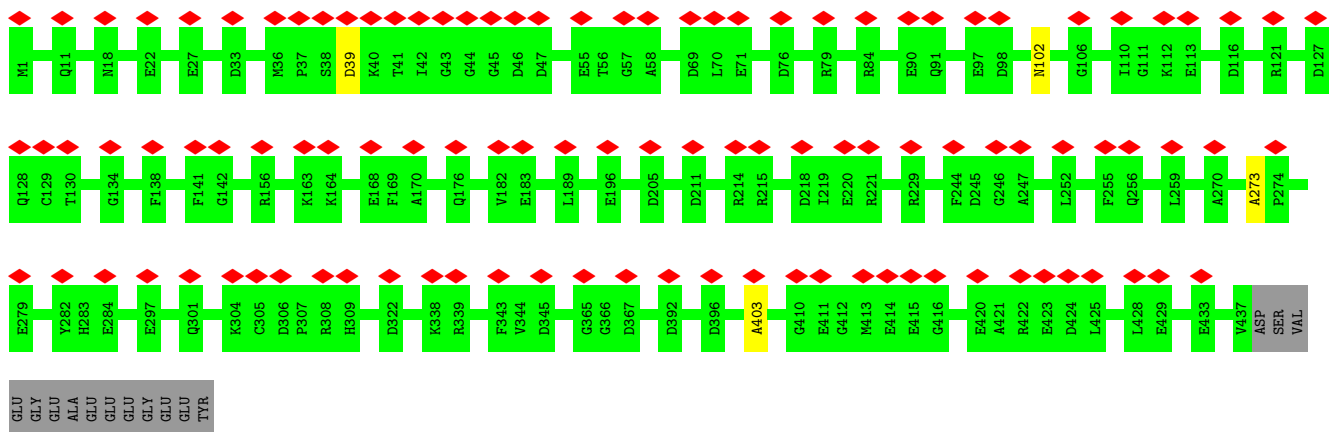




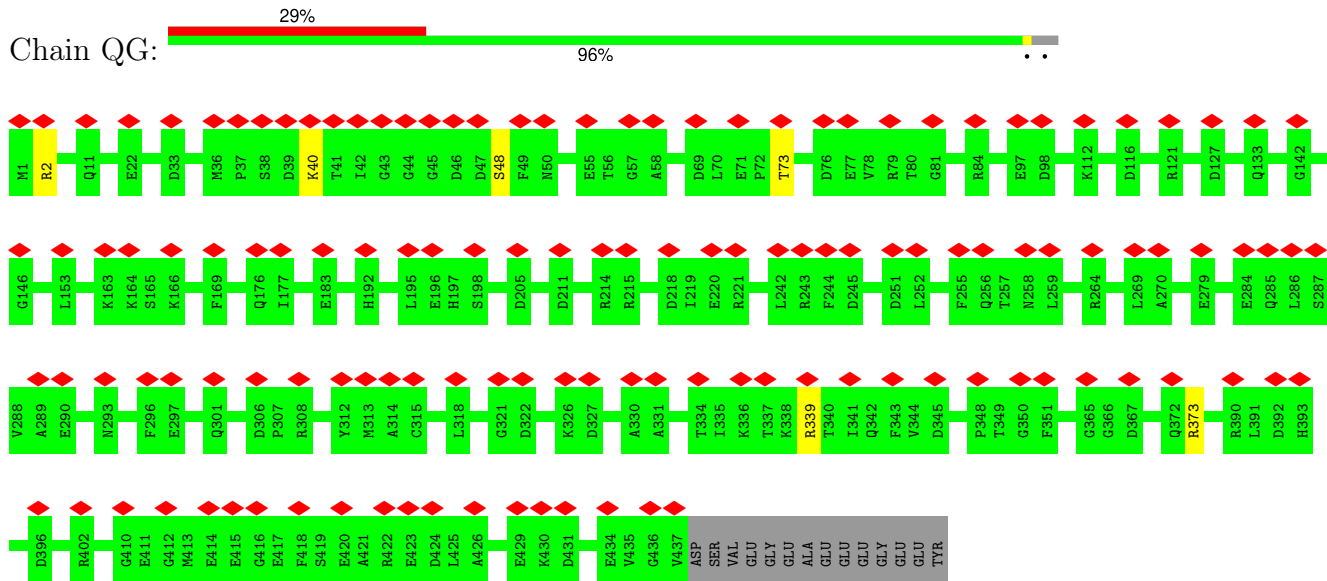
• Molecule 54: Tubulin alpha chain



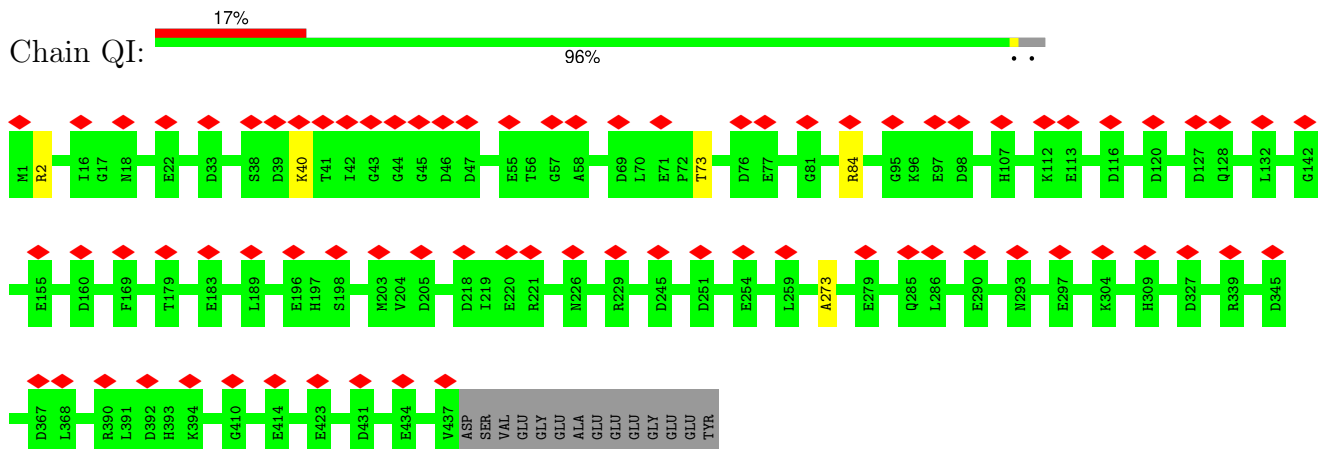
• Molecule 54: Tubulin alpha chain



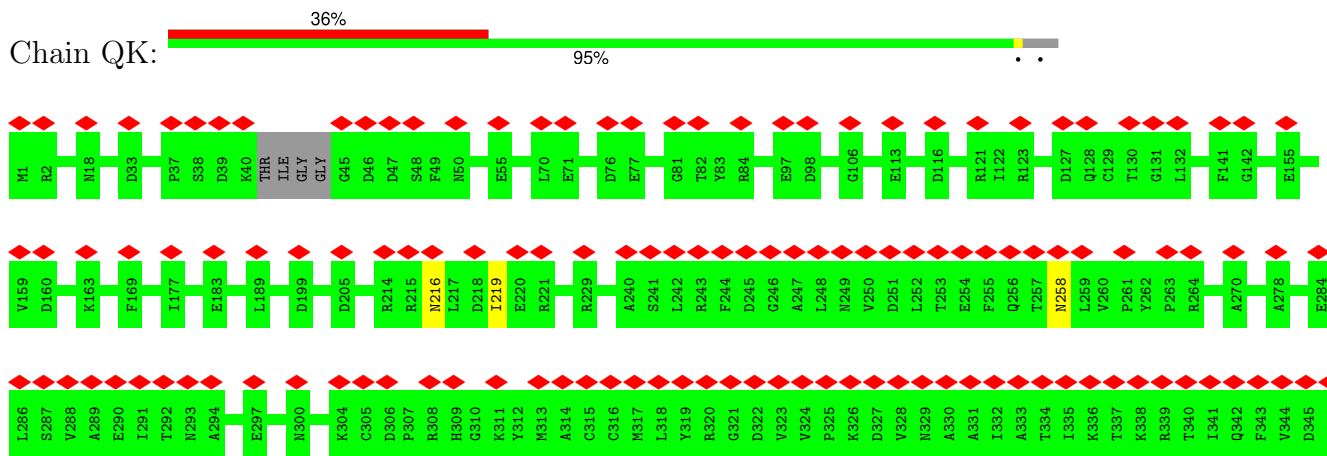
• Molecule 54: Tubulin alpha chain

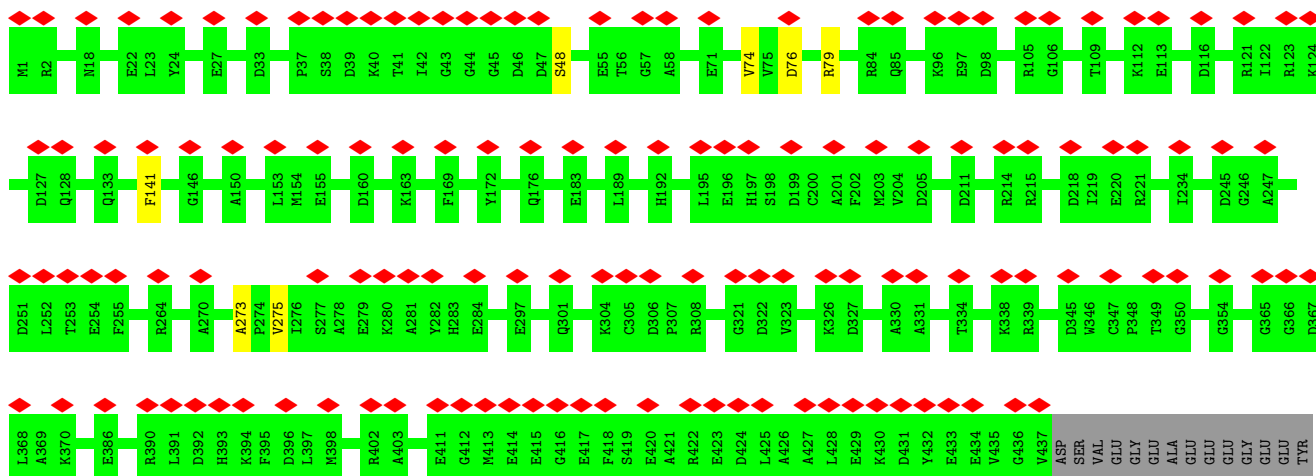


• Molecule 54: Tubulin alpha chain

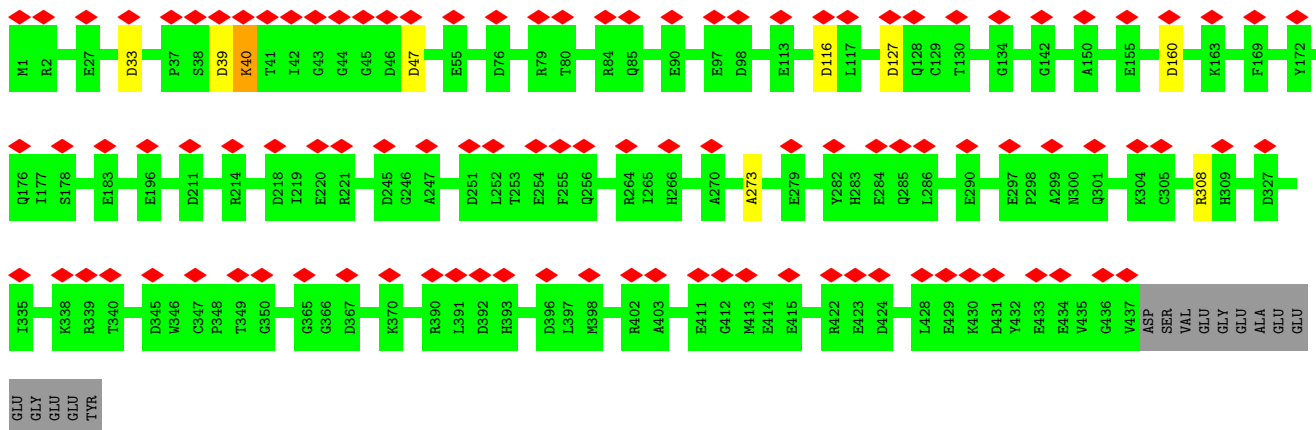


• Molecule 54: Tubulin alpha chain

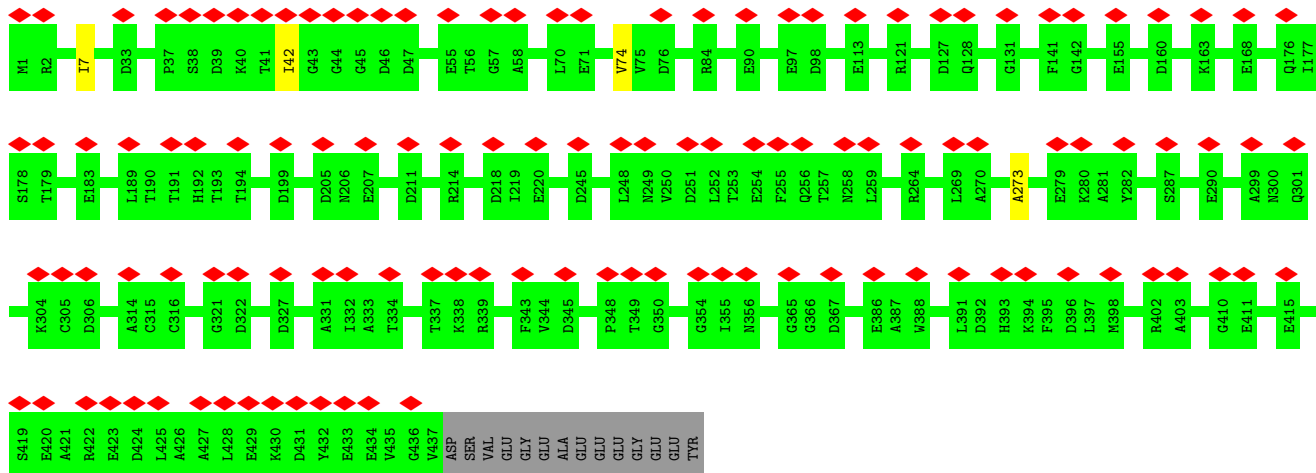




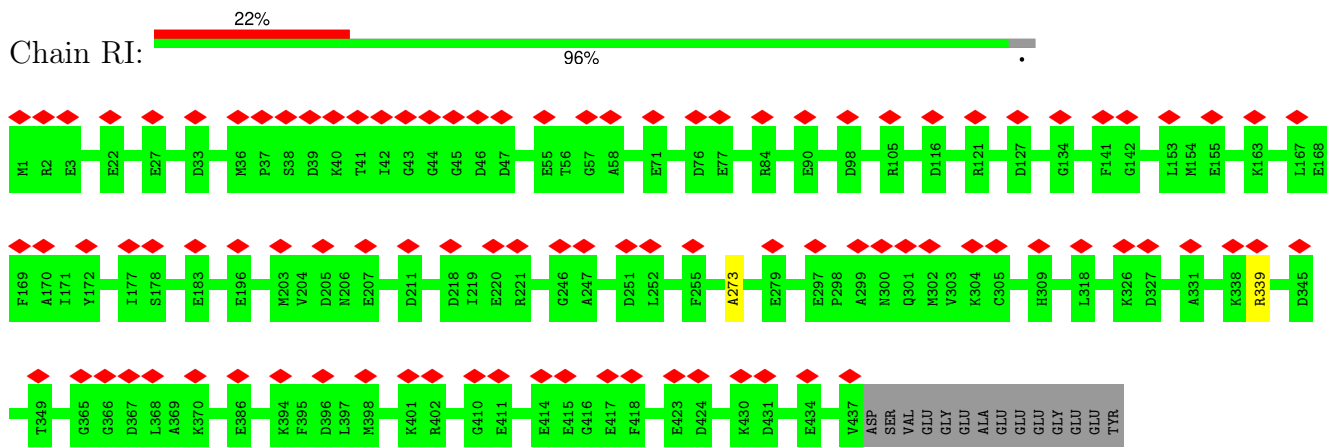
• Molecule 54: Tubulin alpha chain



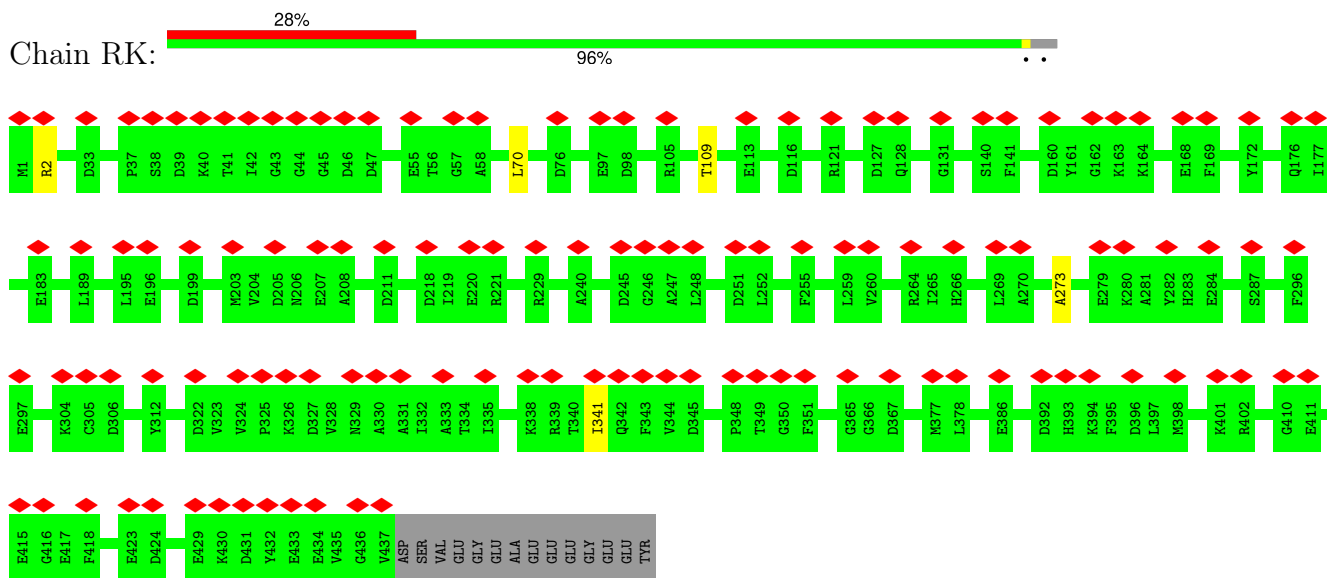
• Molecule 54: Tubulin alpha chain



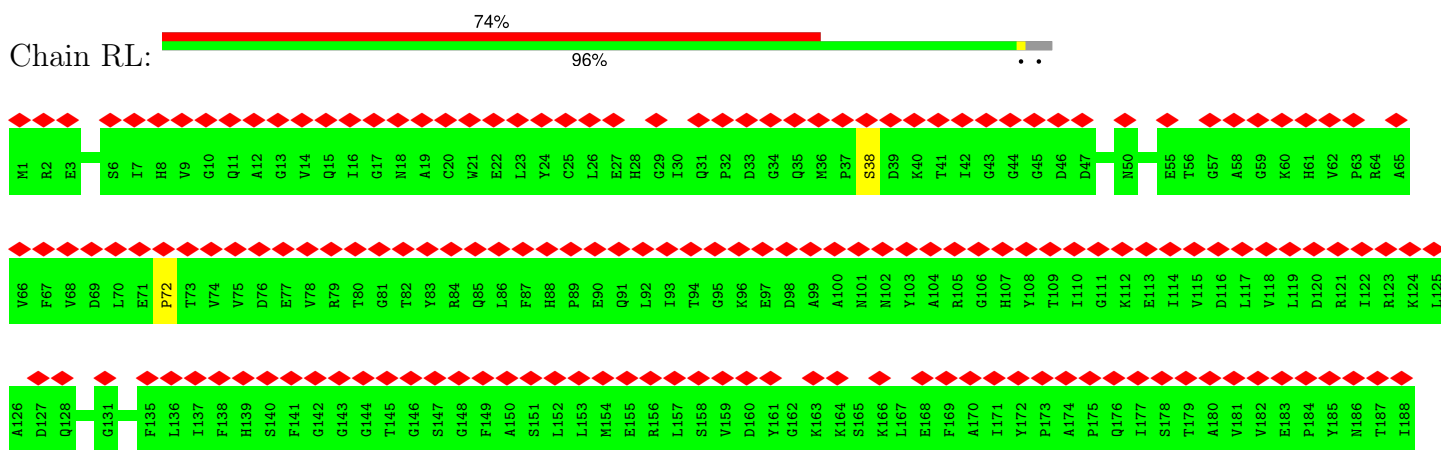
• Molecule 54: Tubulin alpha chain

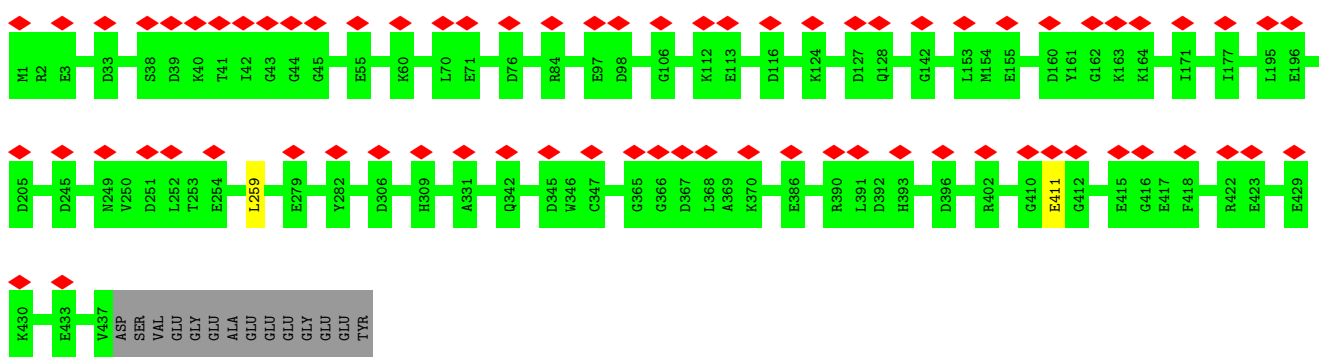


• Molecule 54: Tubulin alpha chain

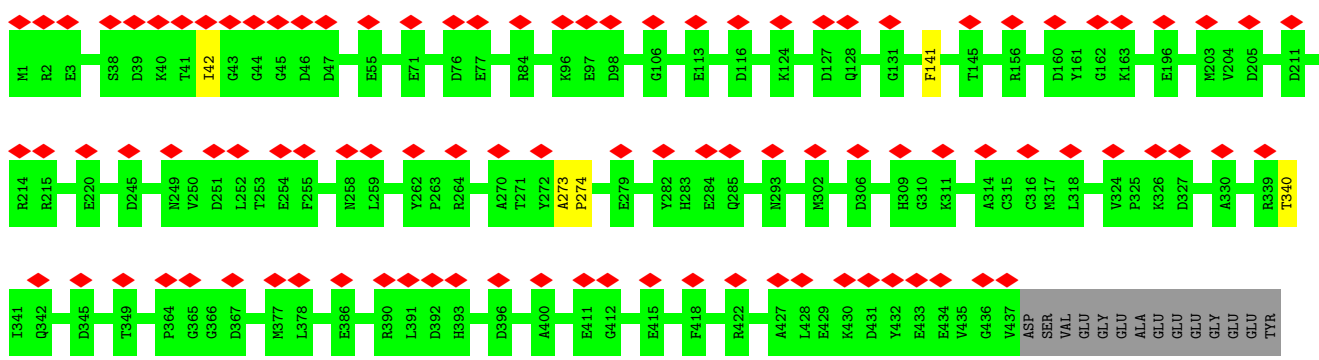


• Molecule 54: Tubulin alpha chain

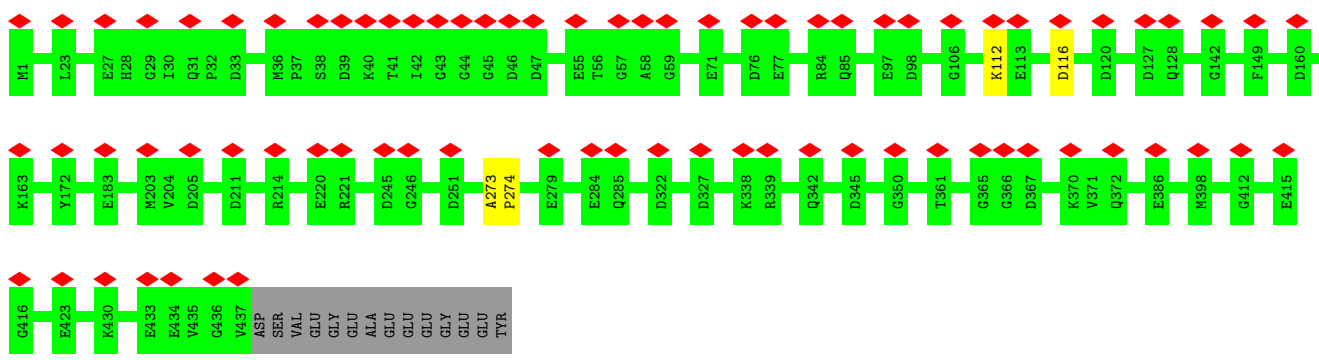




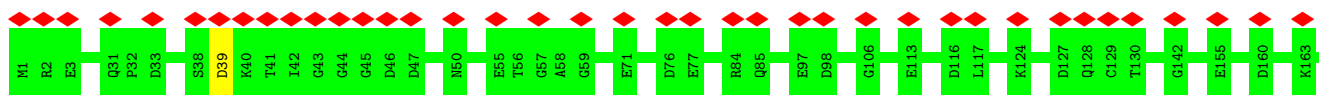
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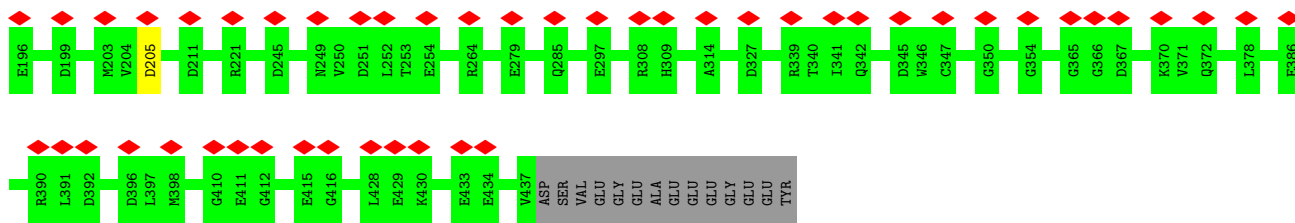


• Molecule 54: Tubulin alpha chain

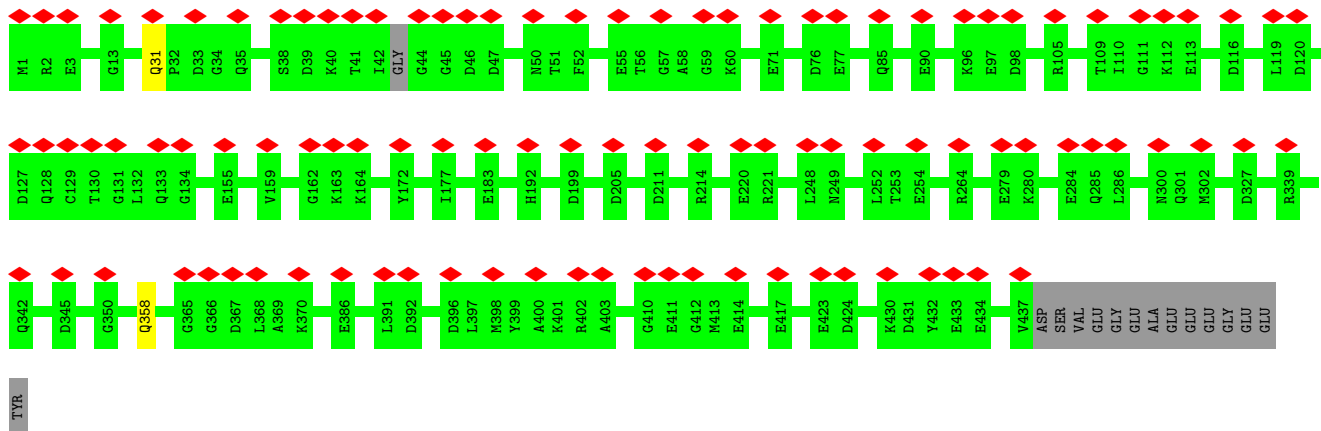


• Molecule 54: Tubulin alpha chain

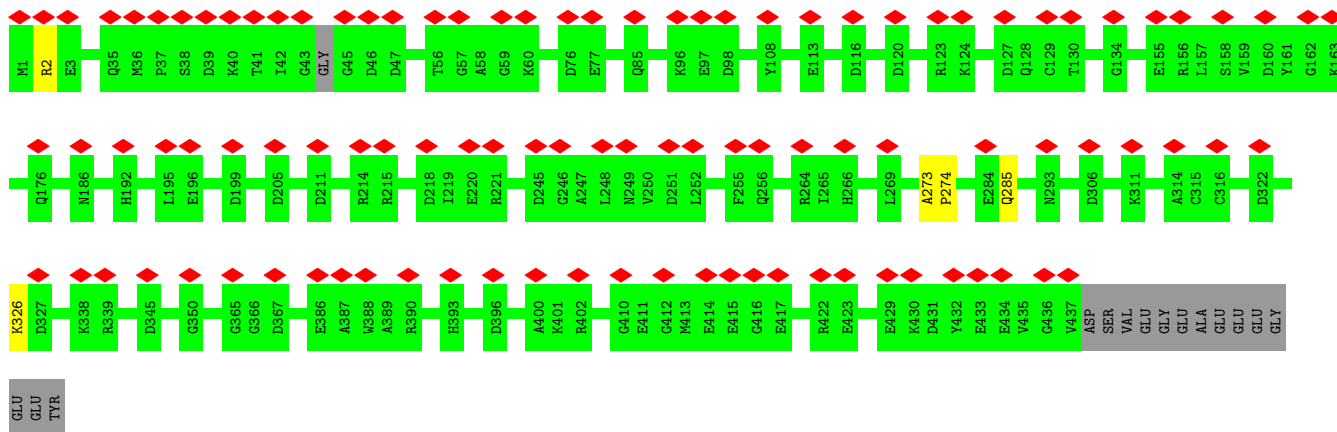




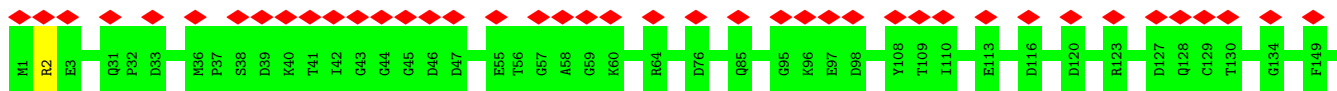
• Molecule 54: Tubulin alpha chain

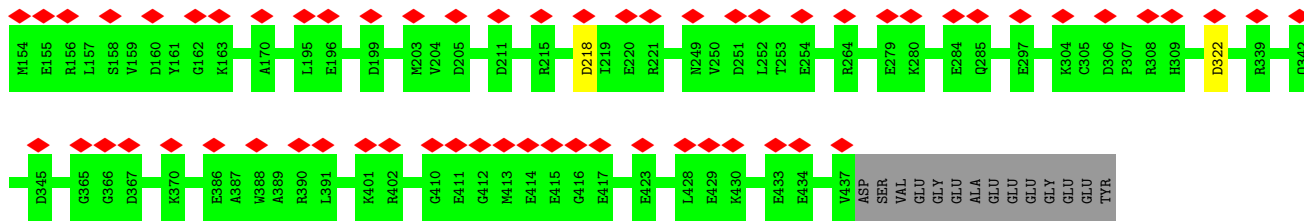


• Molecule 54: Tubulin alpha chain

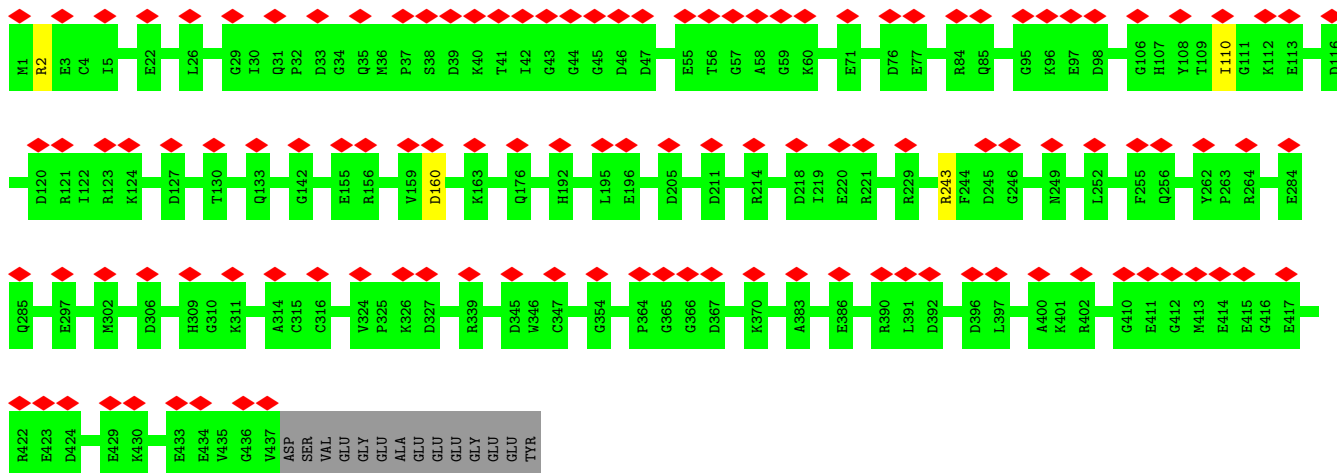


• Molecule 54: Tubulin alpha chain

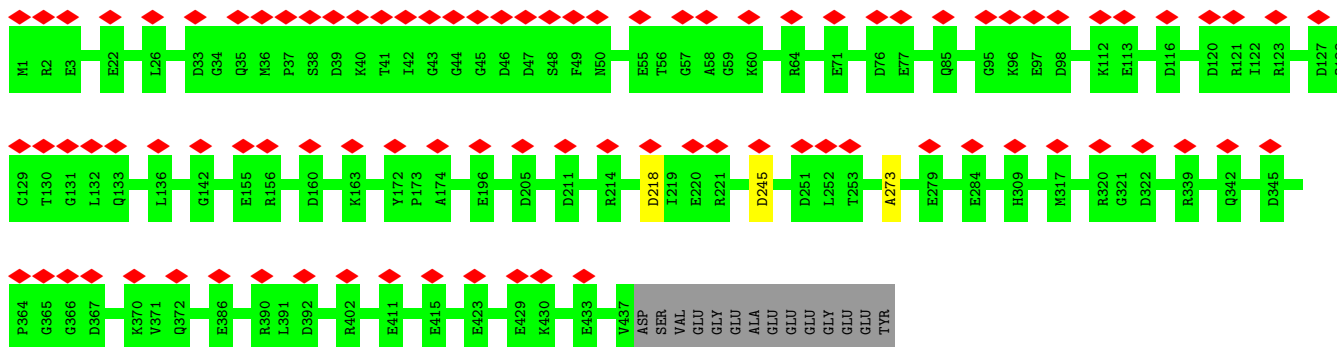




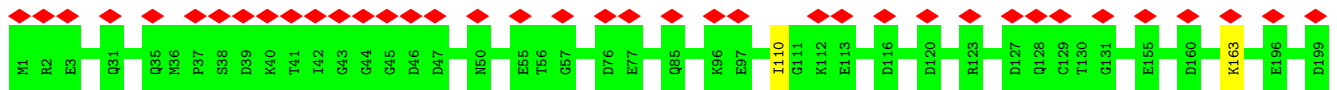
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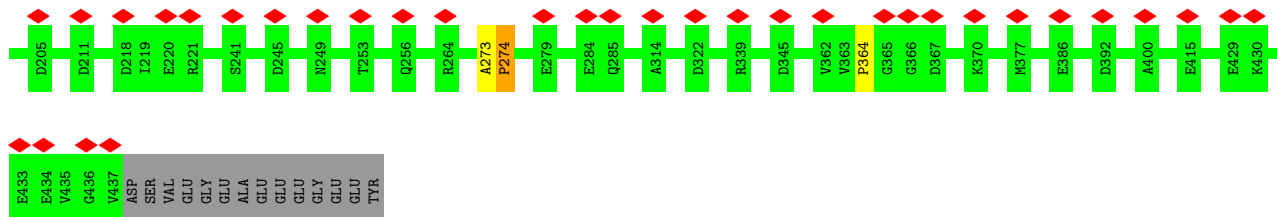


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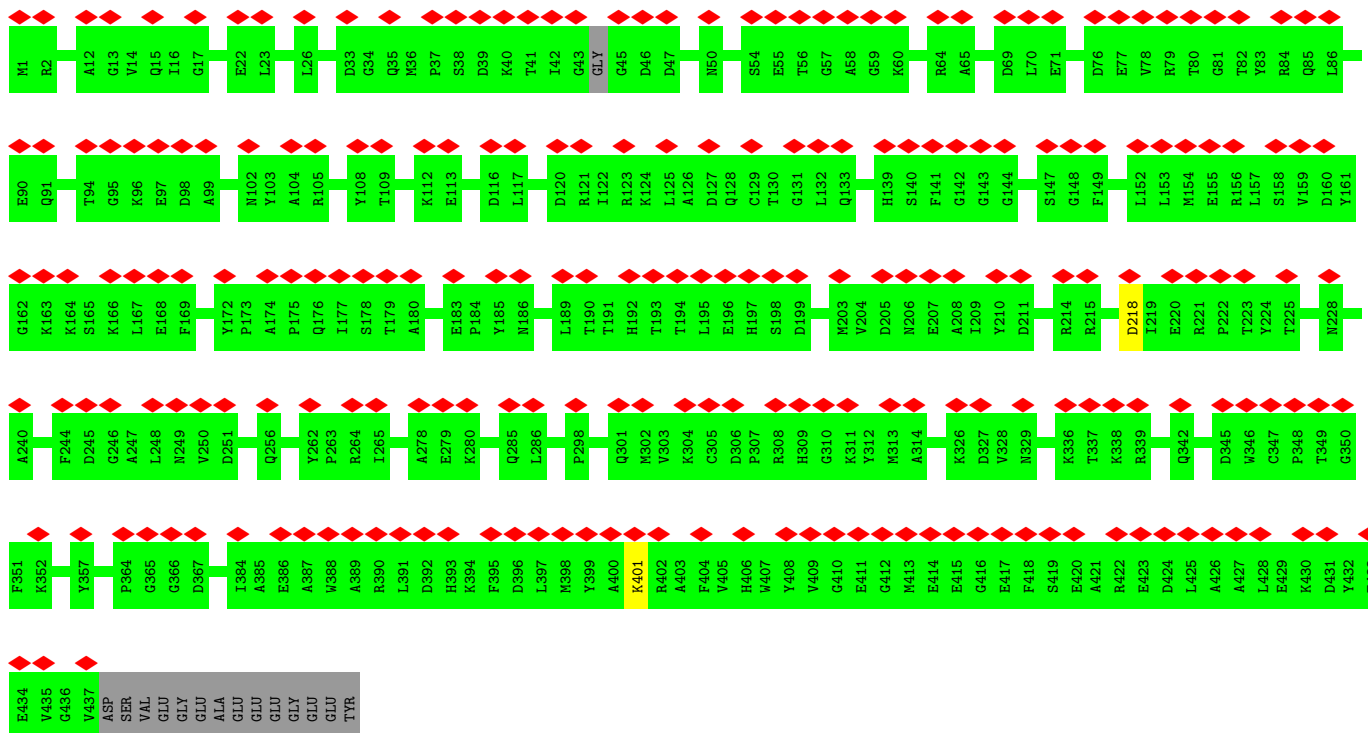


• Molecule 54: Tubulin alpha chain

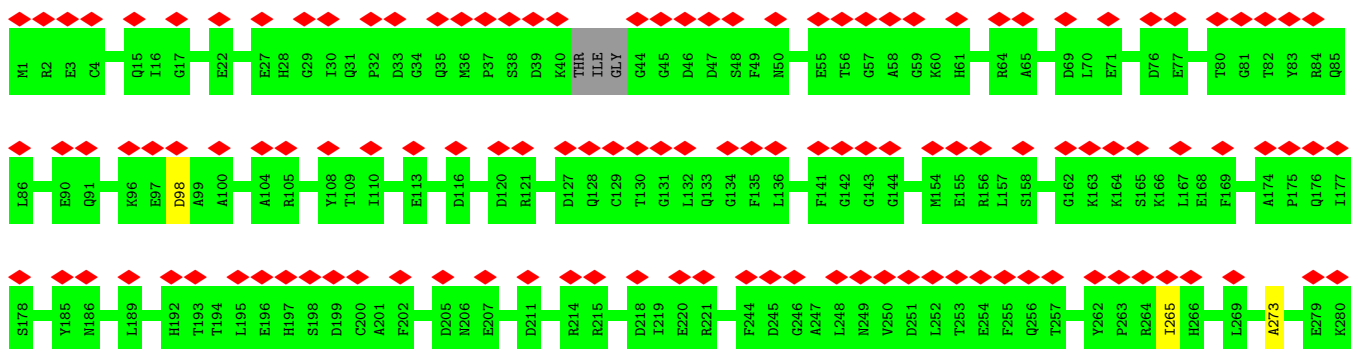


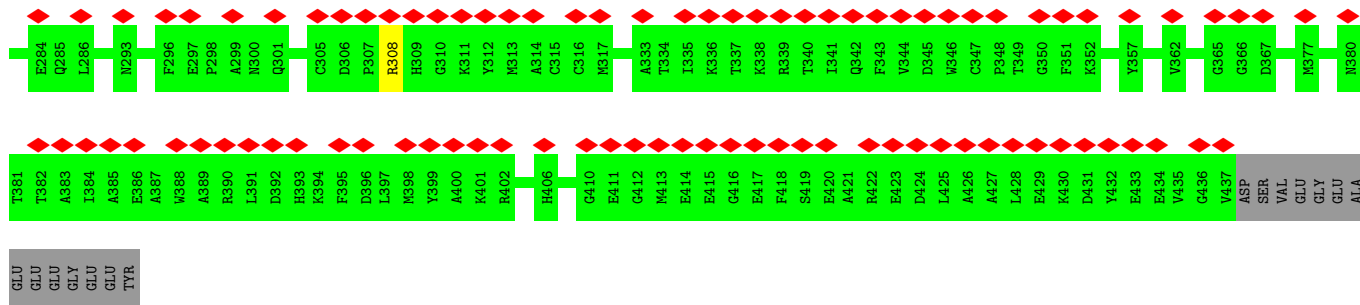


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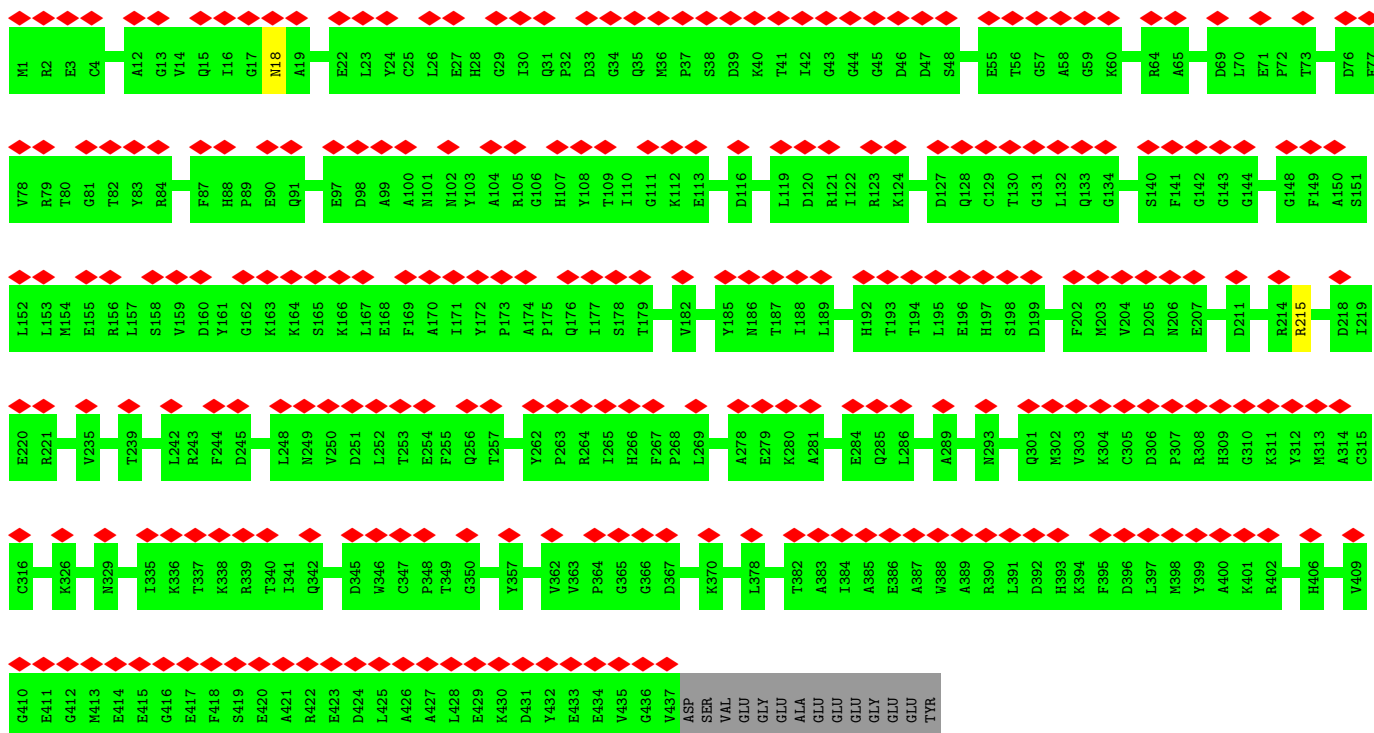


• Molecule 54: Tubulin alpha chain

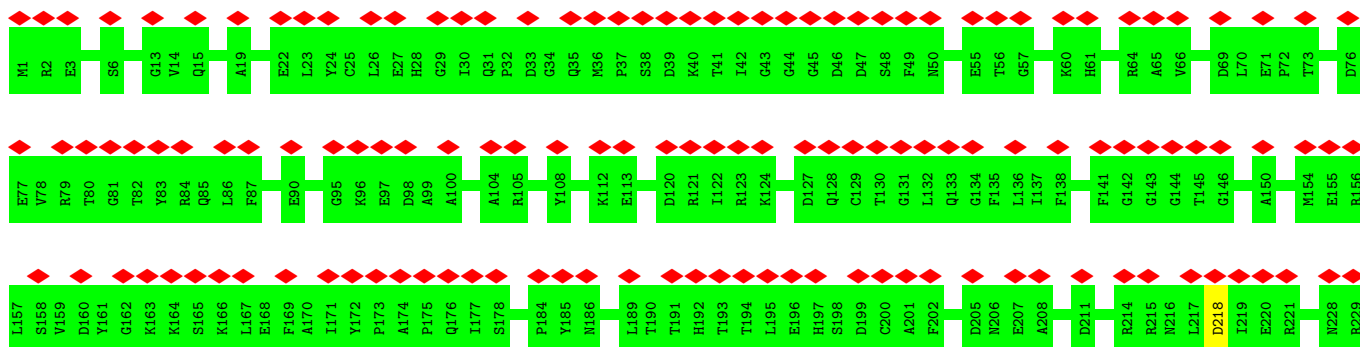


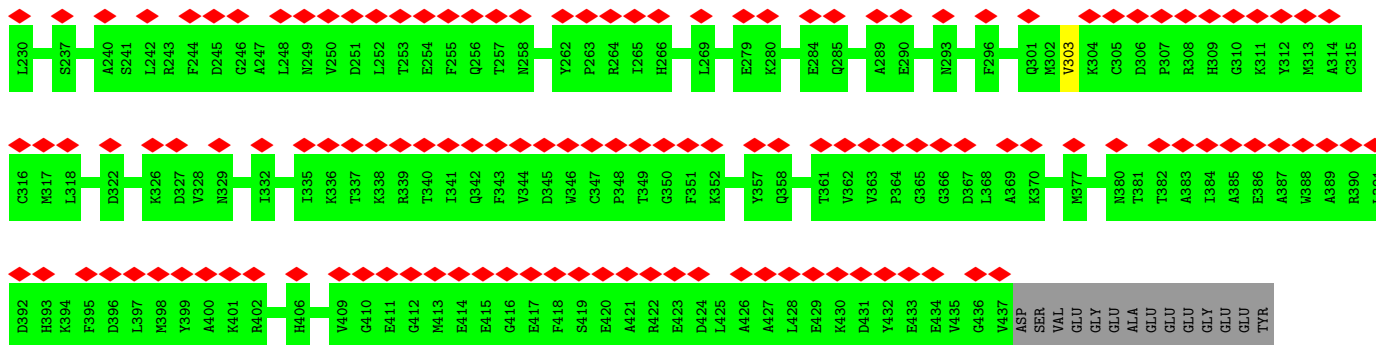


• Molecule 54: Tubulin alpha chain

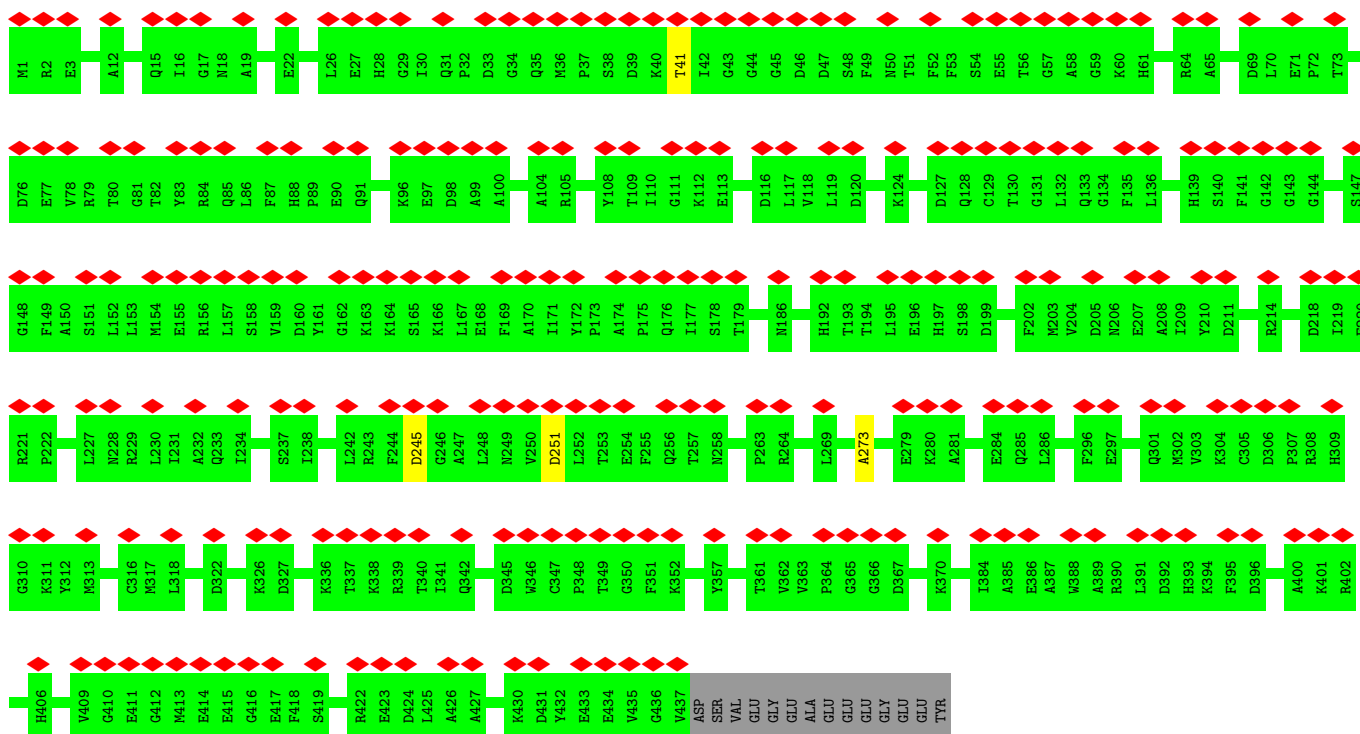


• Molecule 54: Tubulin alpha chain

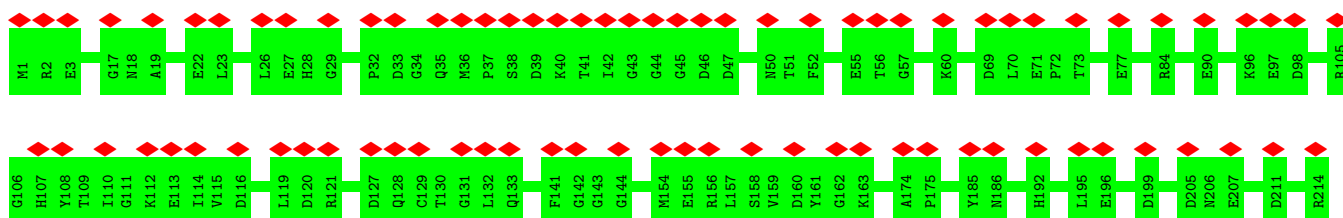


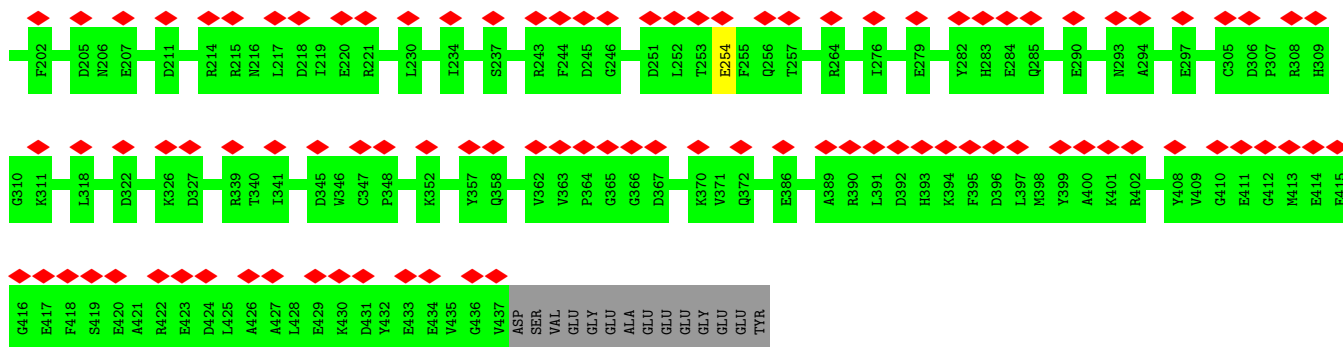


• Molecule 54: Tubulin alpha chain

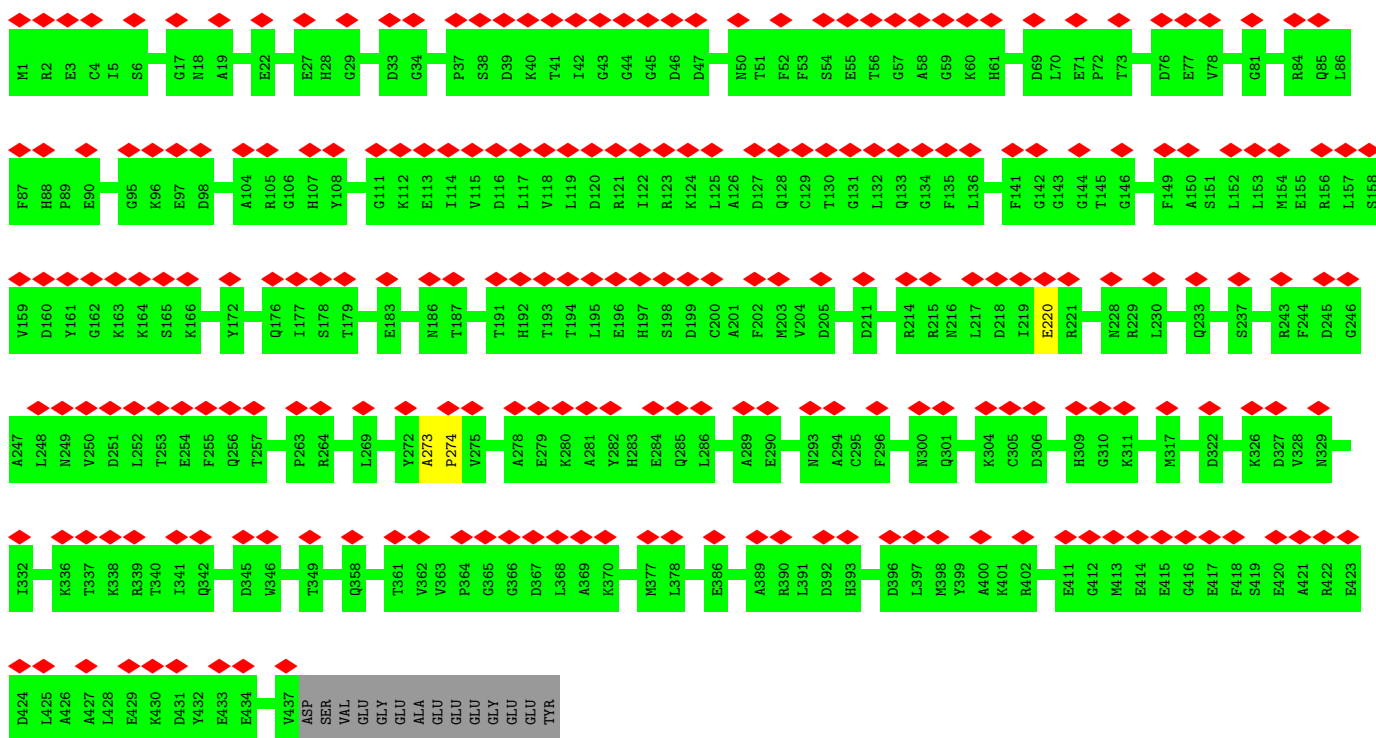


• Molecule 54: Tubulin alpha chain

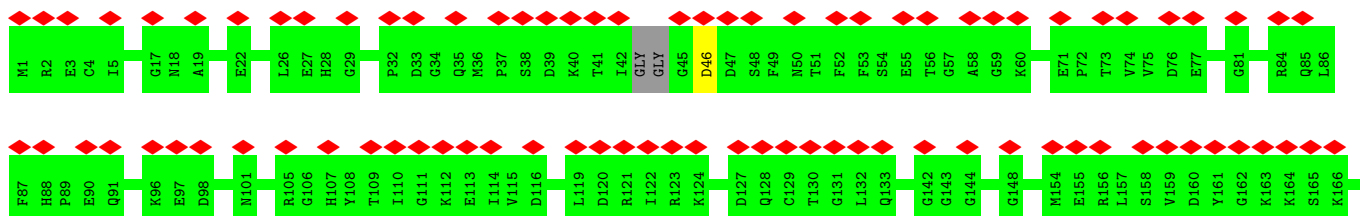


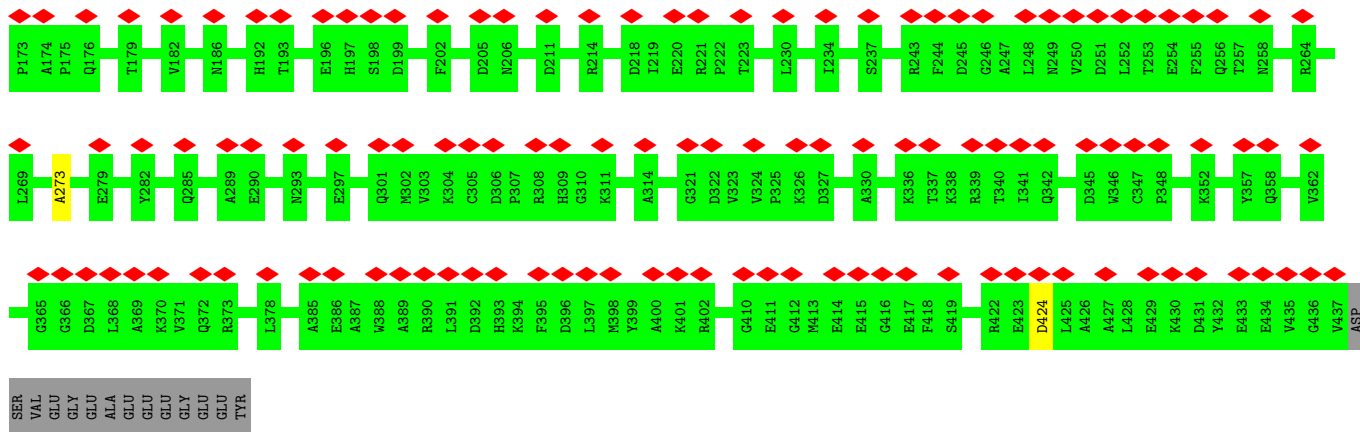


• Molecule 54: Tubulin alpha chain



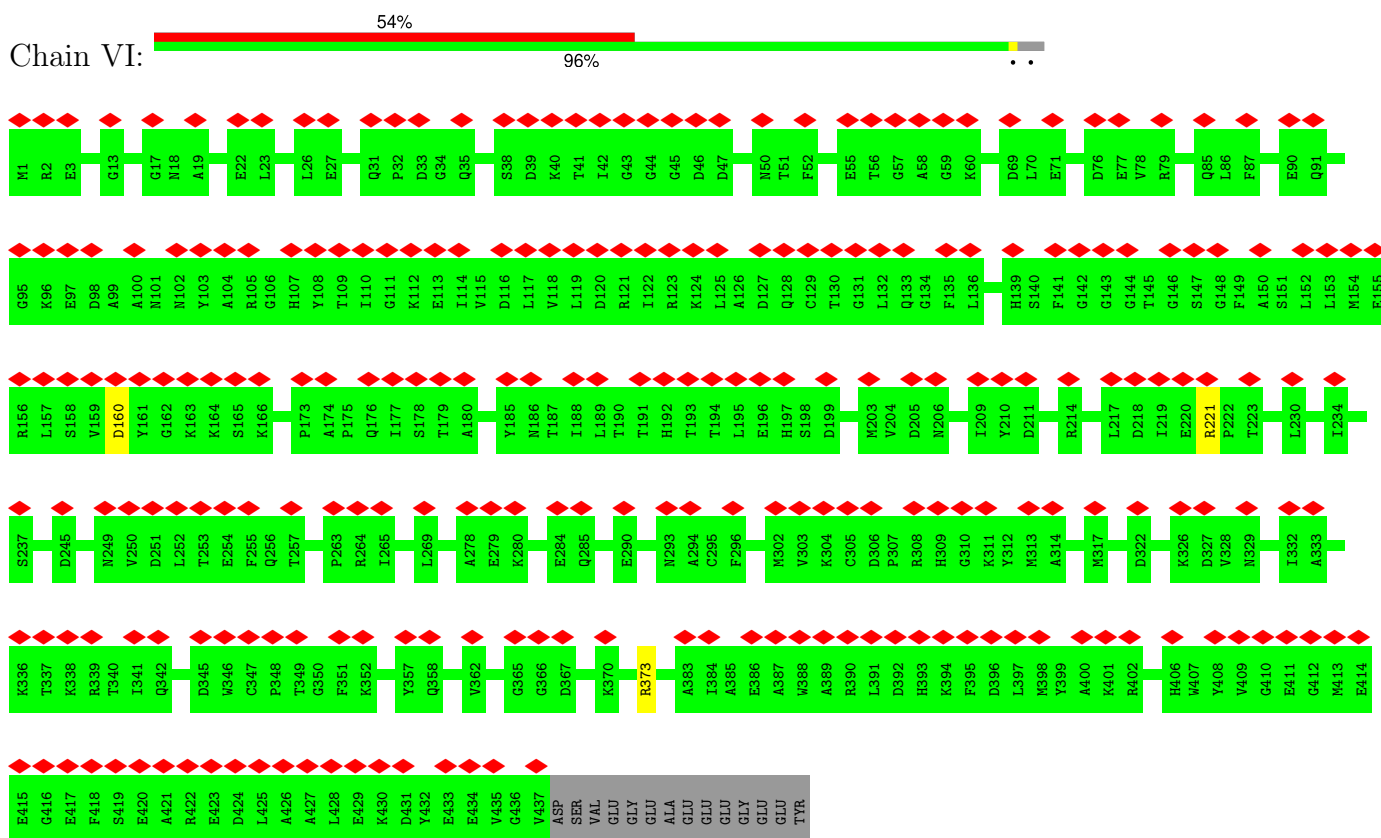
• Molecule 54: Tubulin alpha chain





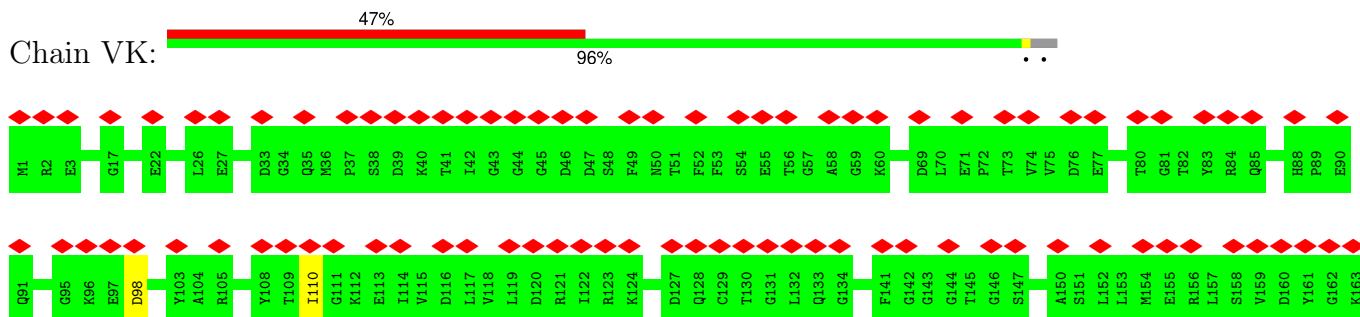
• Molecule 54: Tubulin alpha chain

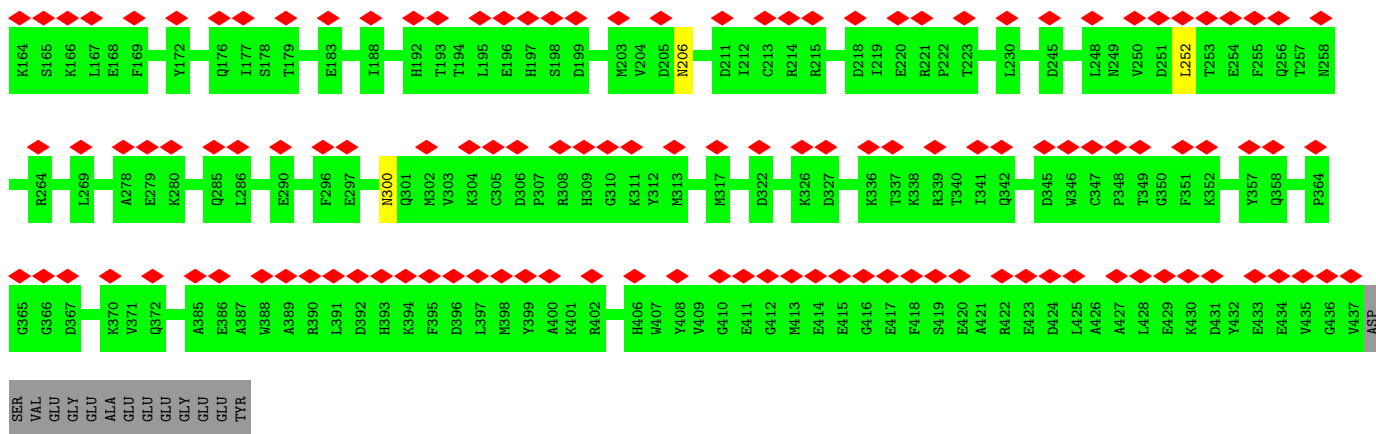
Chain VI:



• Molecule 54: Tubulin alpha chain

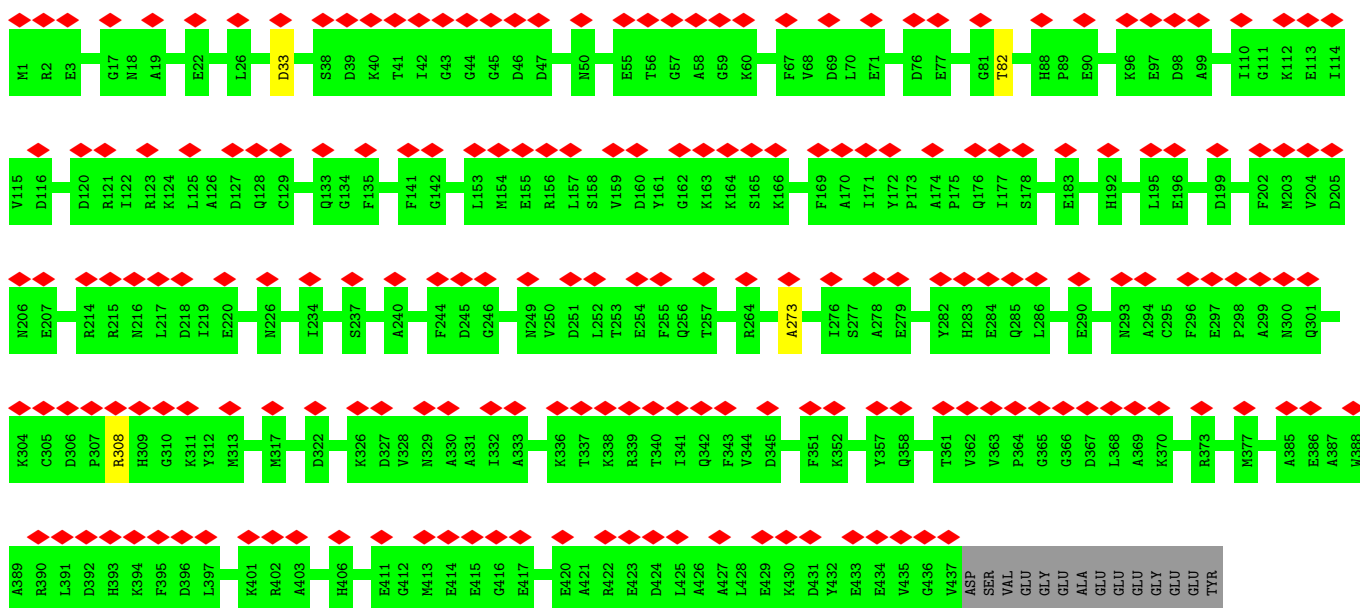
Chain VK:





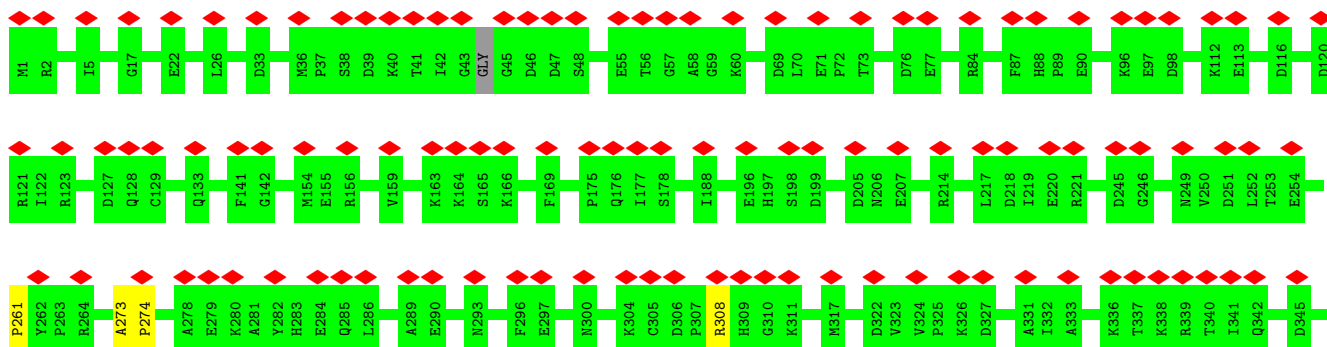
• Molecule 54: Tubulin alpha chain

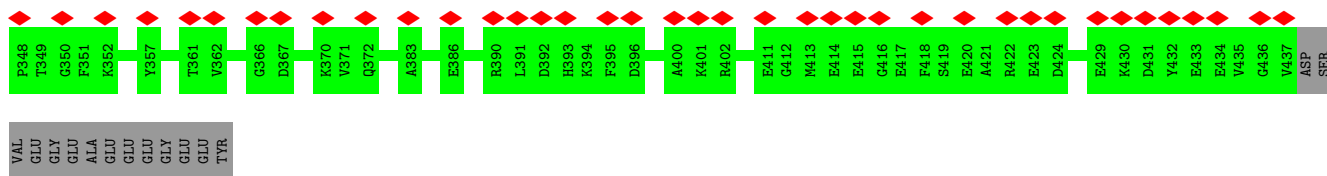
Chain WA:



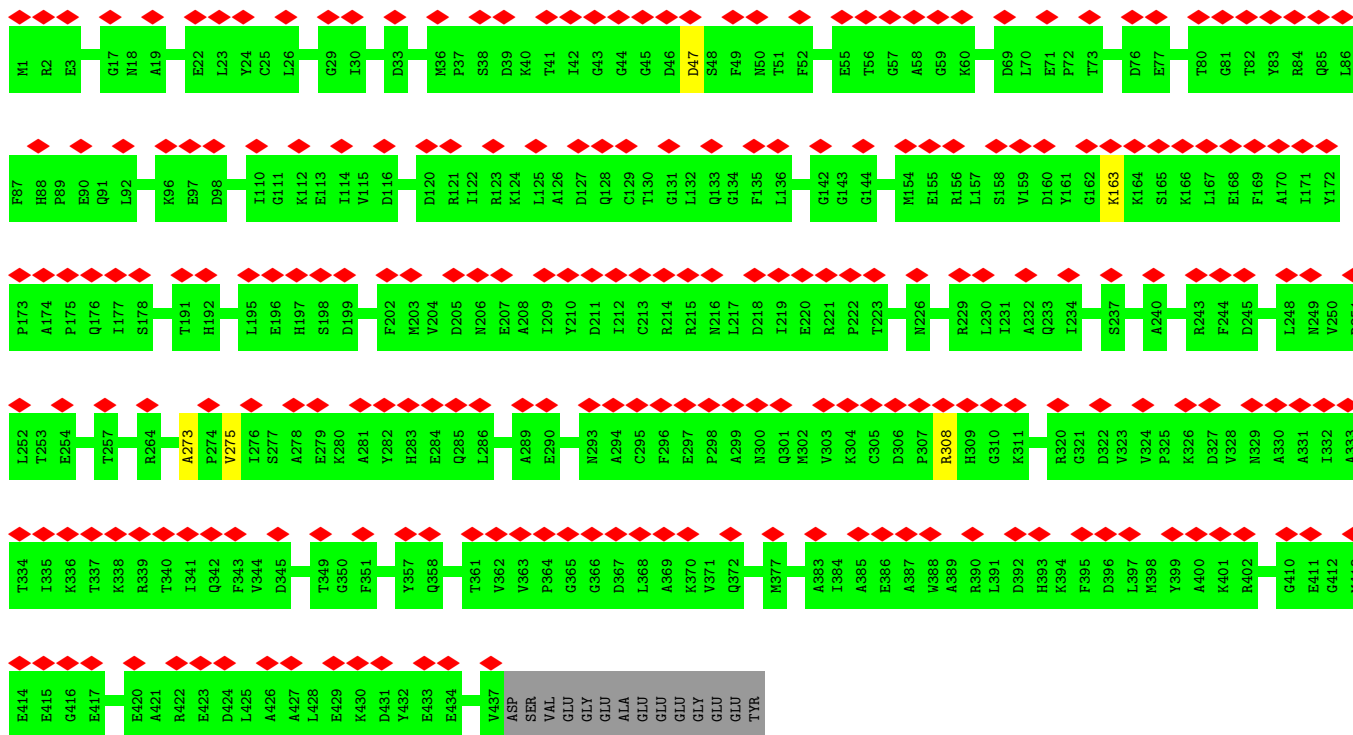
• Molecule 54: Tubulin alpha chain

Chain WB:

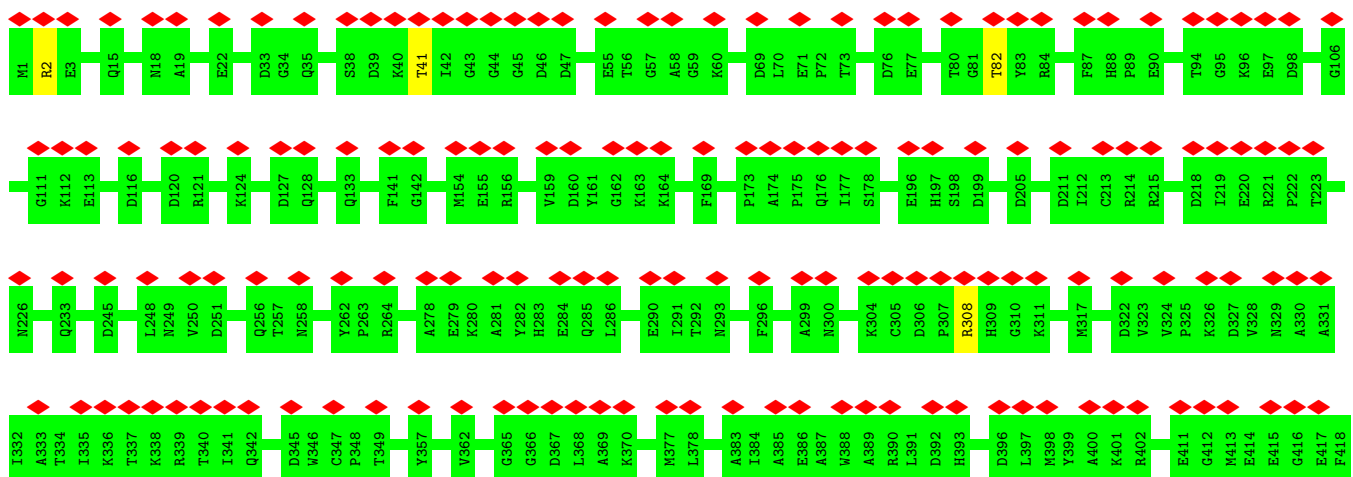
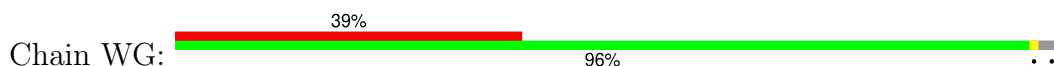


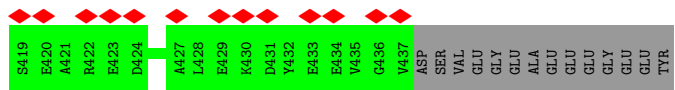


• Molecule 54: Tubulin alpha chain

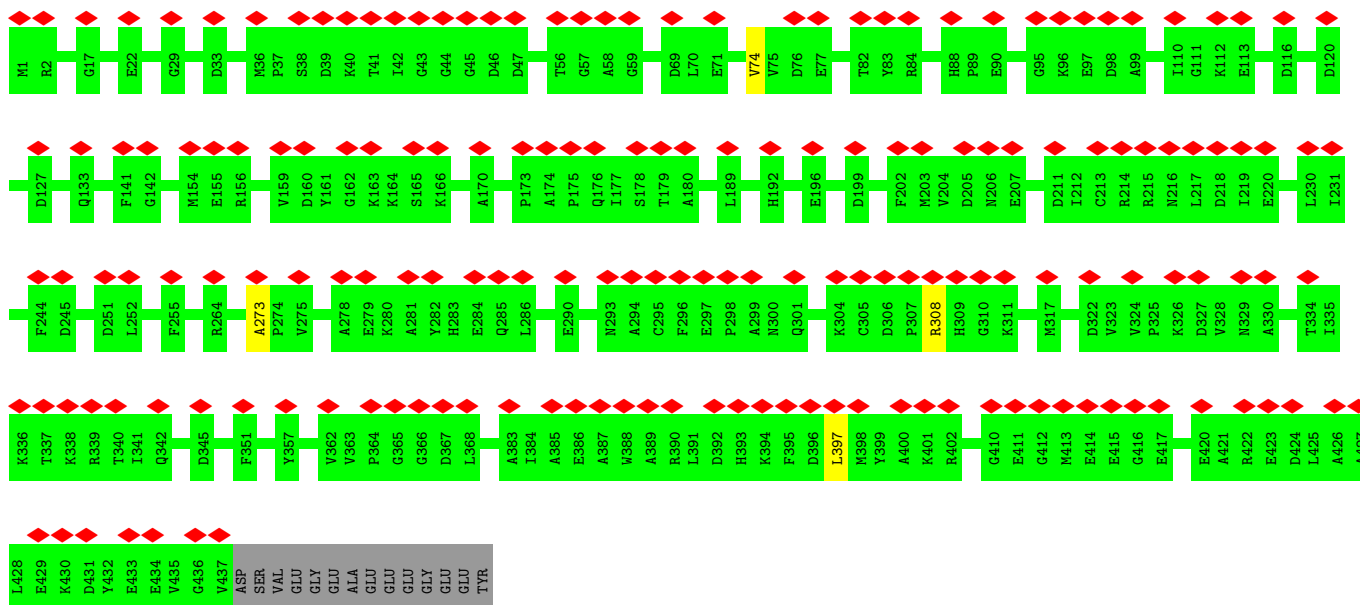
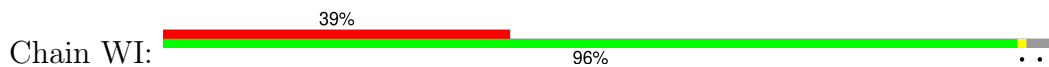


• Molecule 54: Tubulin alpha chain

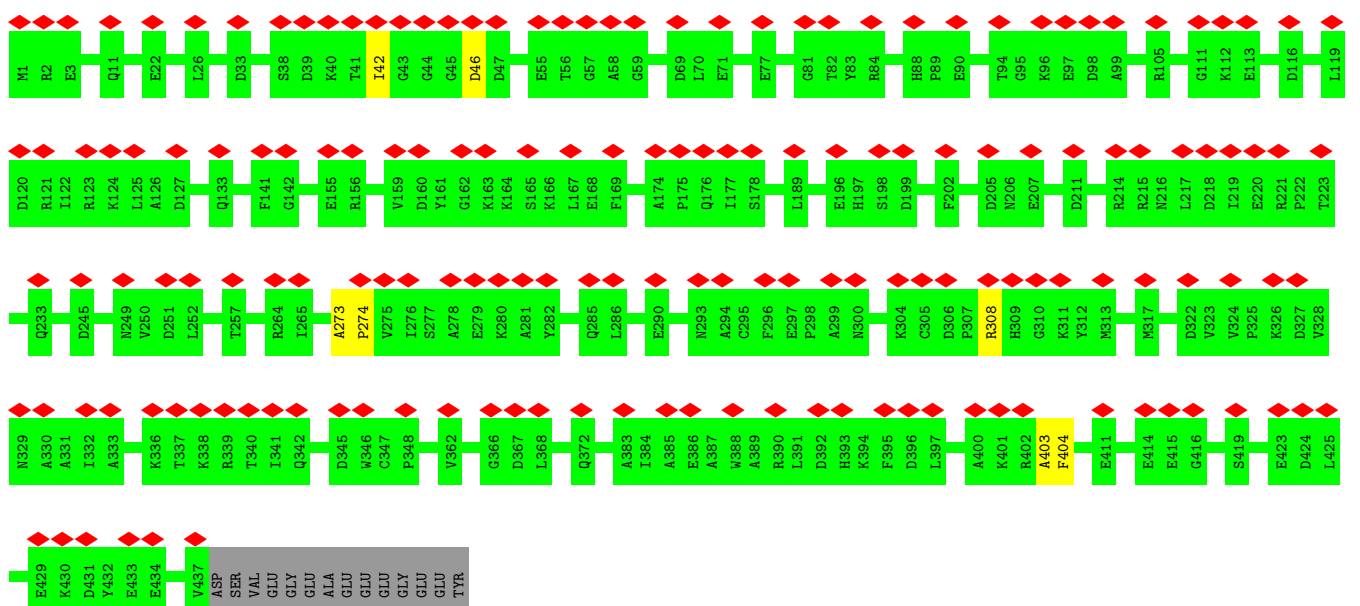
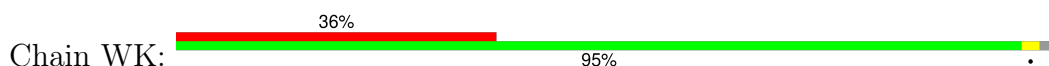




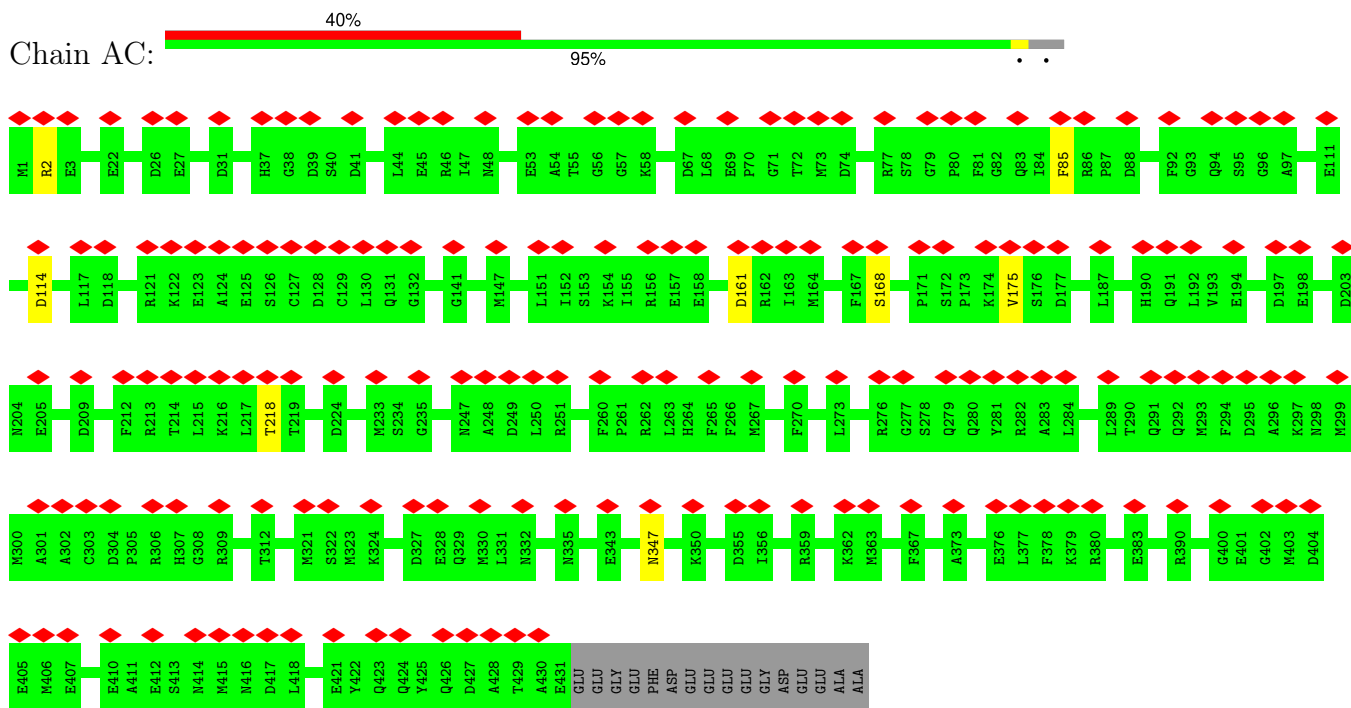
• Molecule 54: Tubulin alpha chain



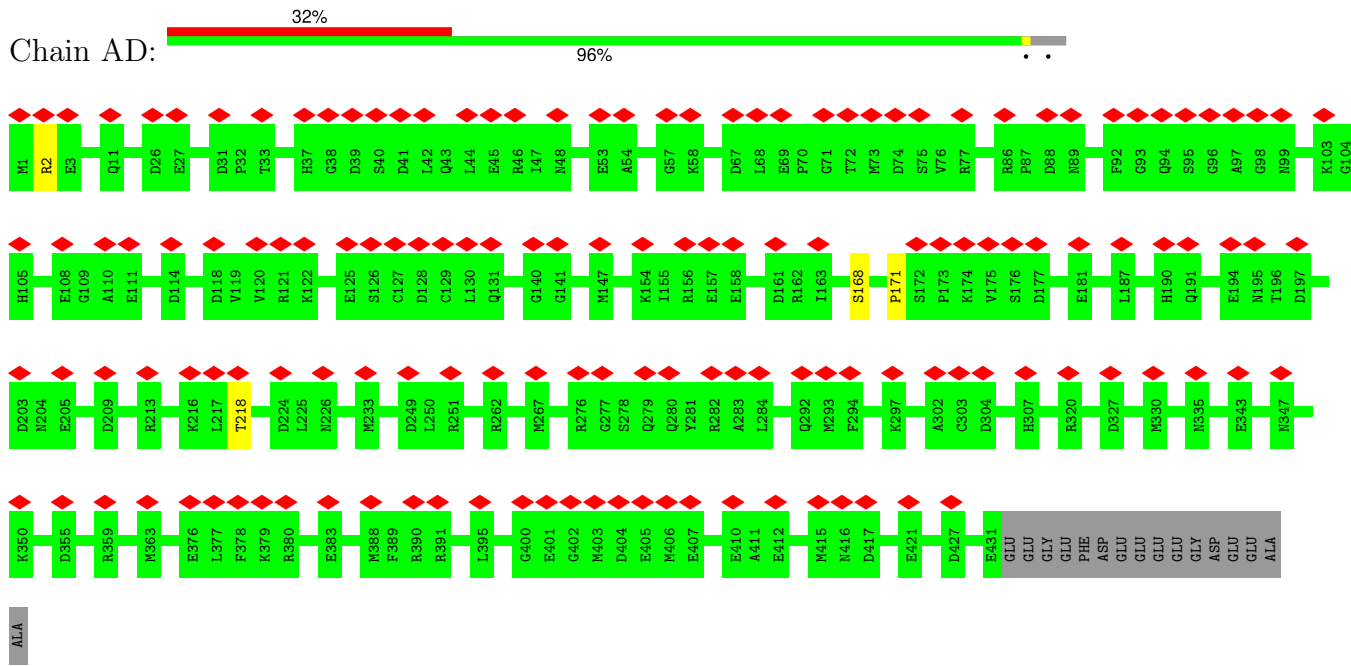
• Molecule 54: Tubulin alpha chain



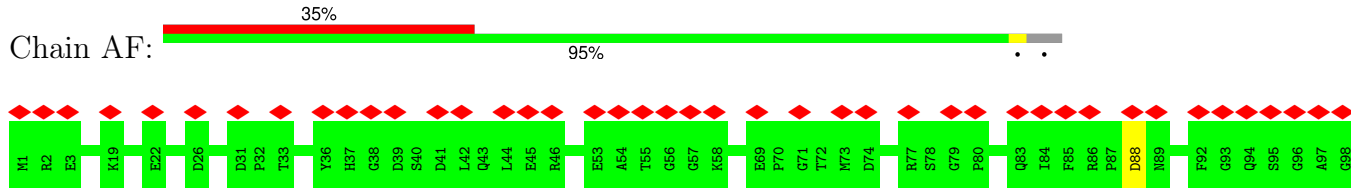
• Molecule 55: Tubulin beta chain

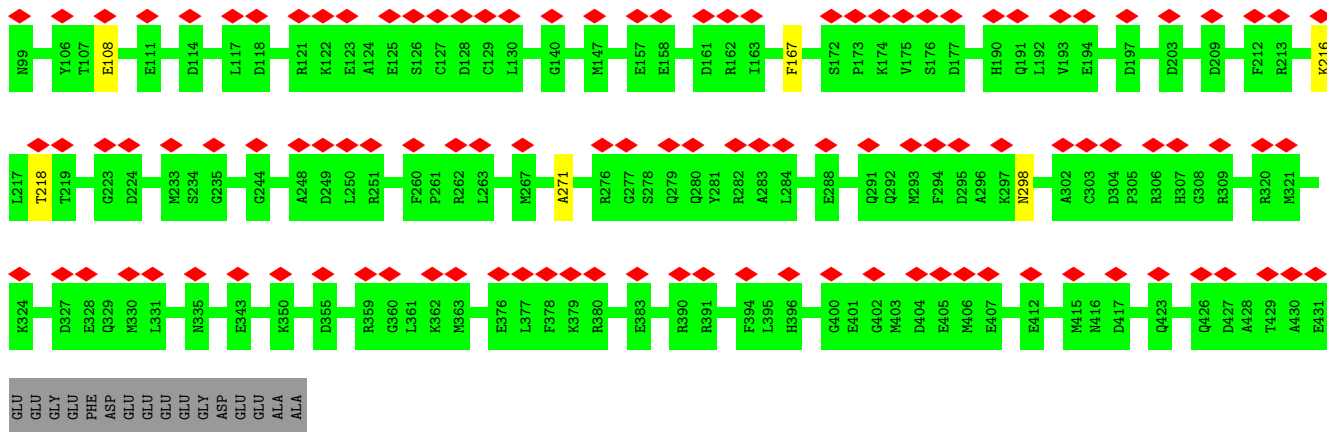


• Molecule 55: Tubulin beta chain

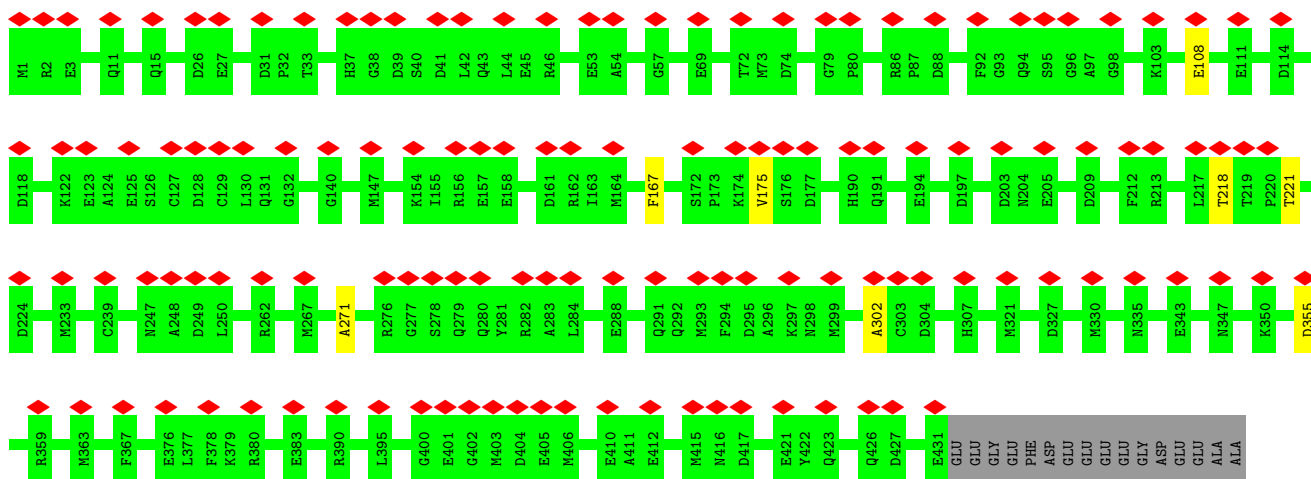


• Molecule 55: Tubulin beta chain

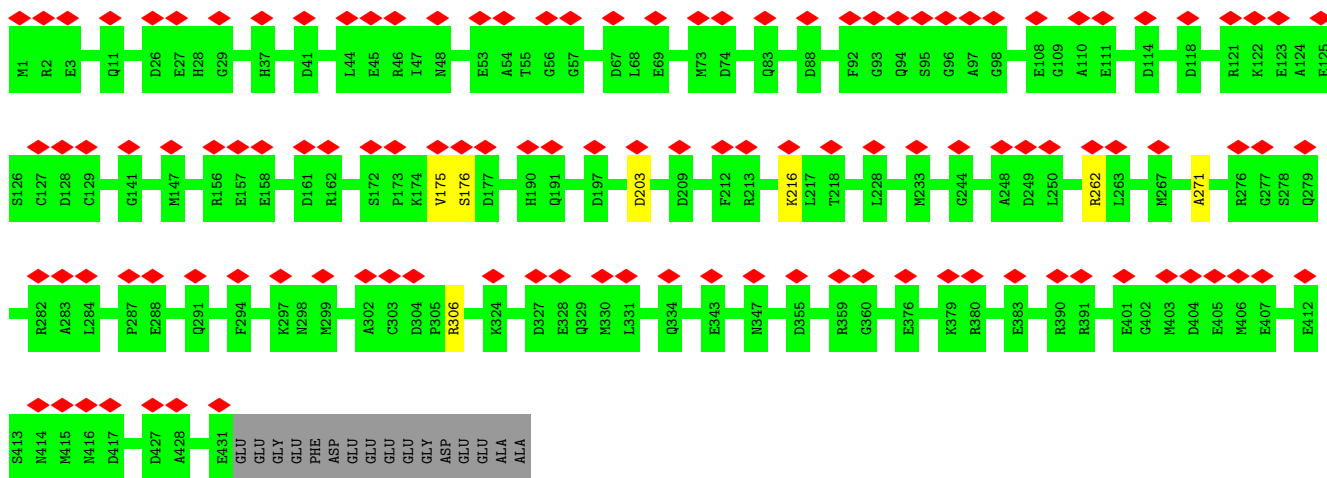




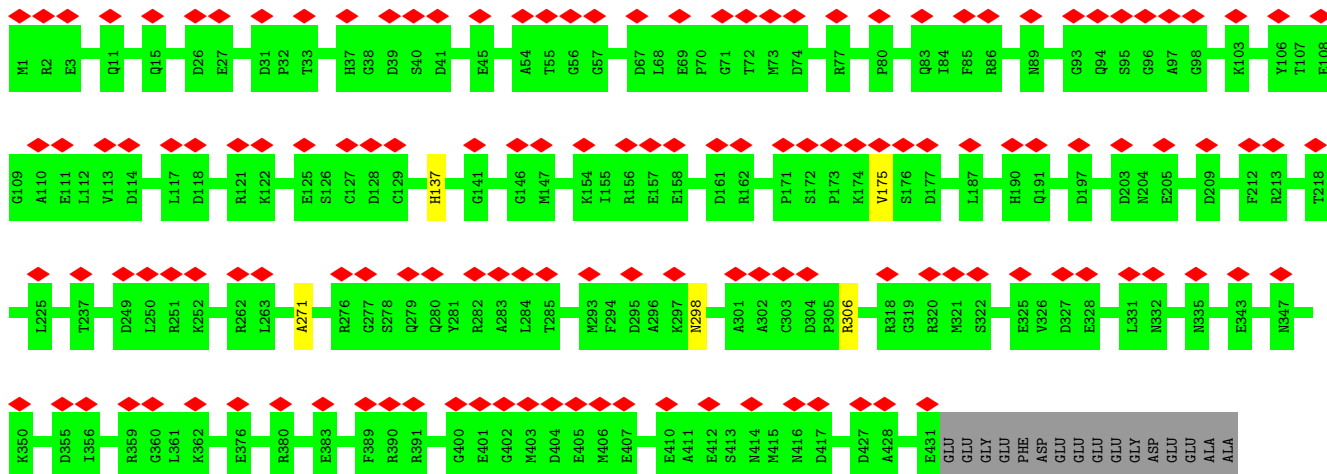
• Molecule 55: Tubulin beta chain



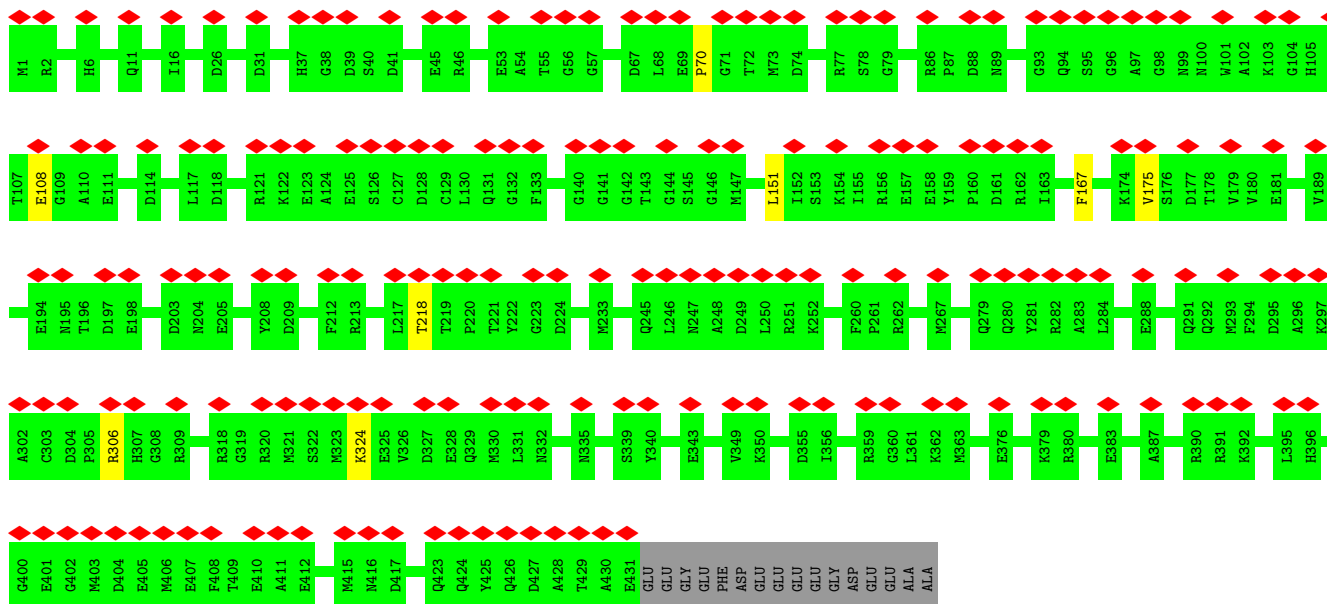
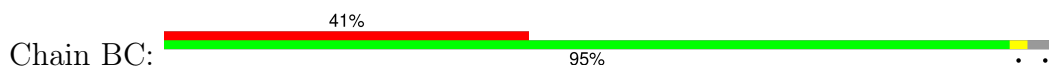
• Molecule 55: Tubulin beta chain



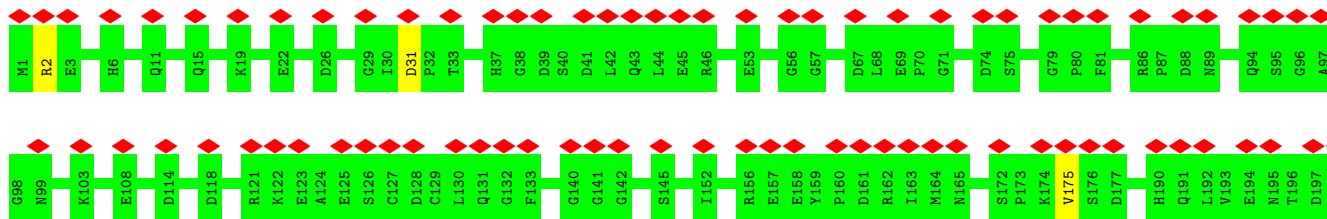
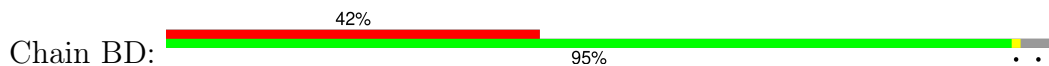
• Molecule 55: Tubulin beta chain

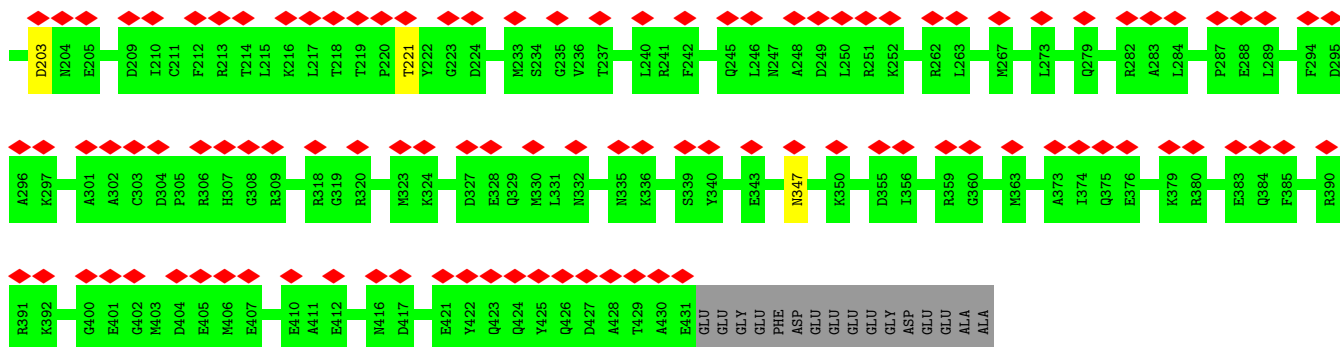


• Molecule 55: Tubulin beta chain

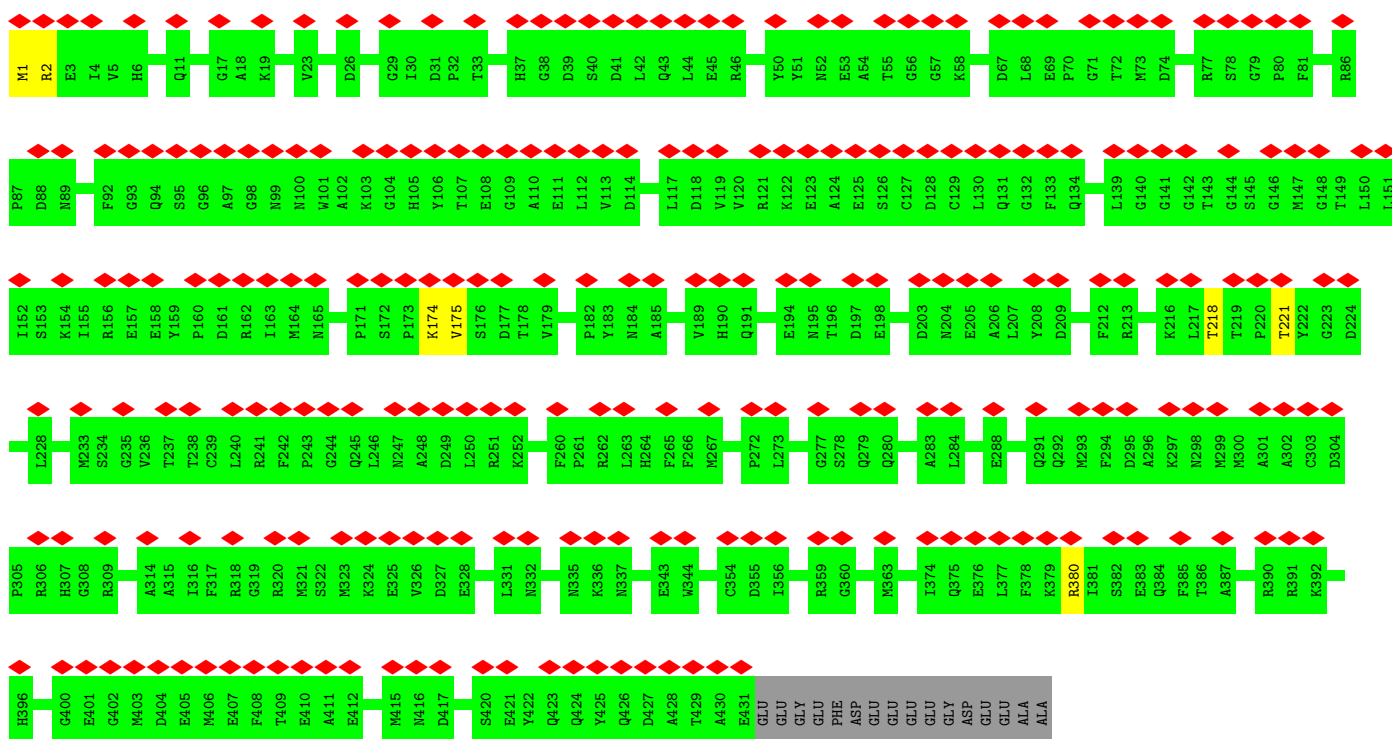


• Molecule 55: Tubulin beta chain

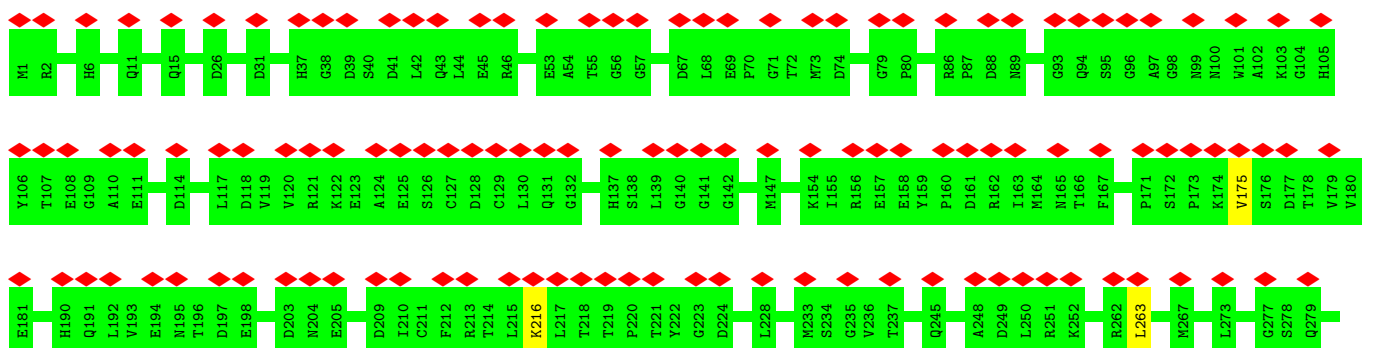


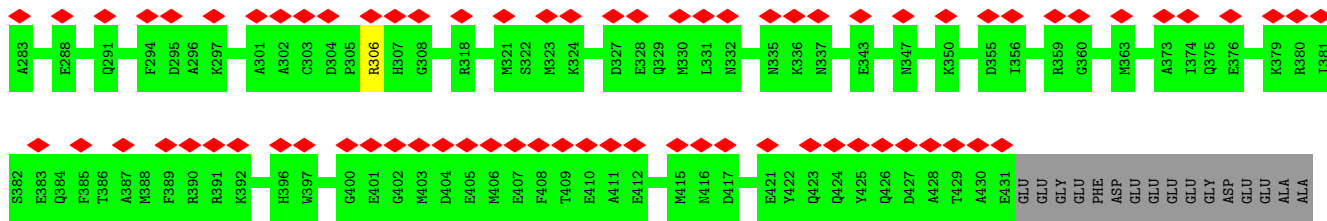


• Molecule 55: Tubulin beta chain

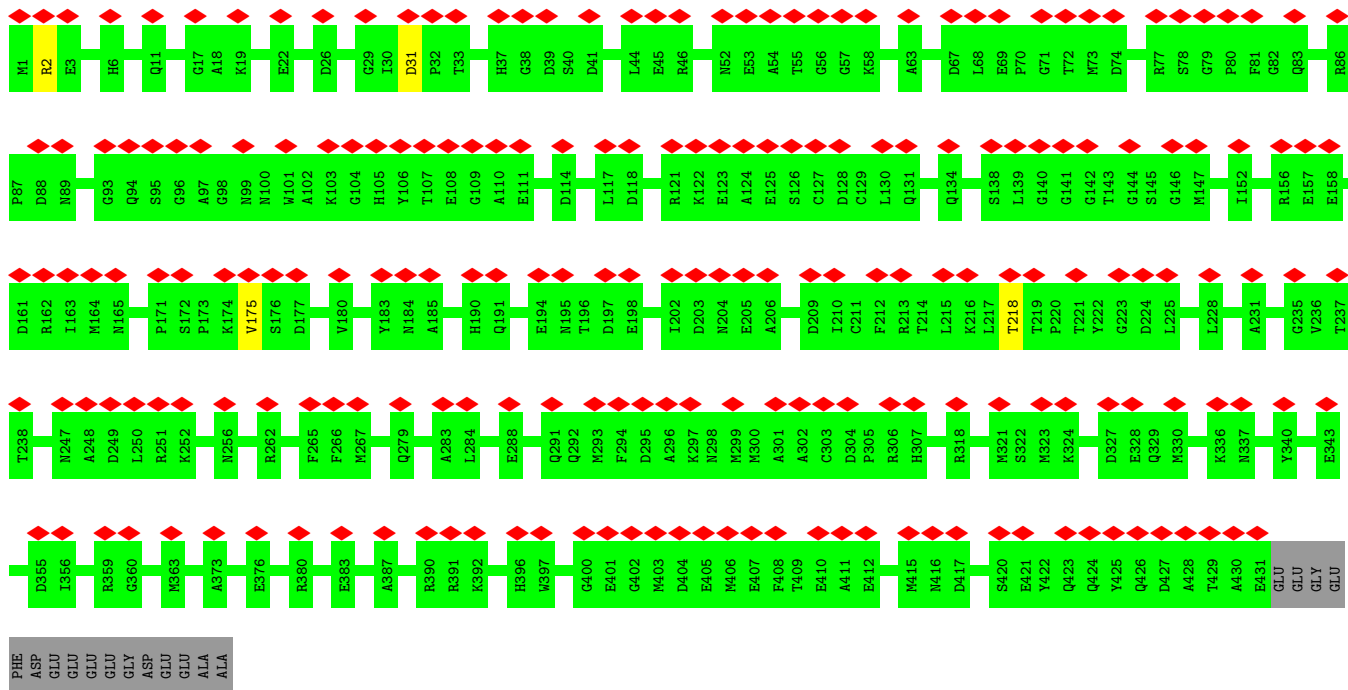


• Molecule 55: Tubulin beta chain

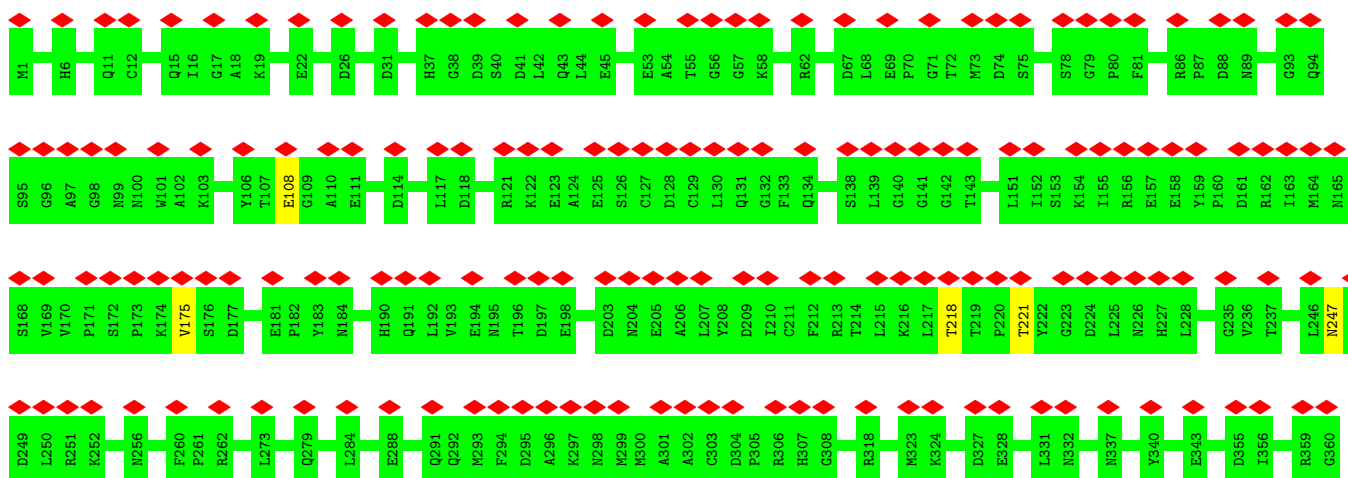




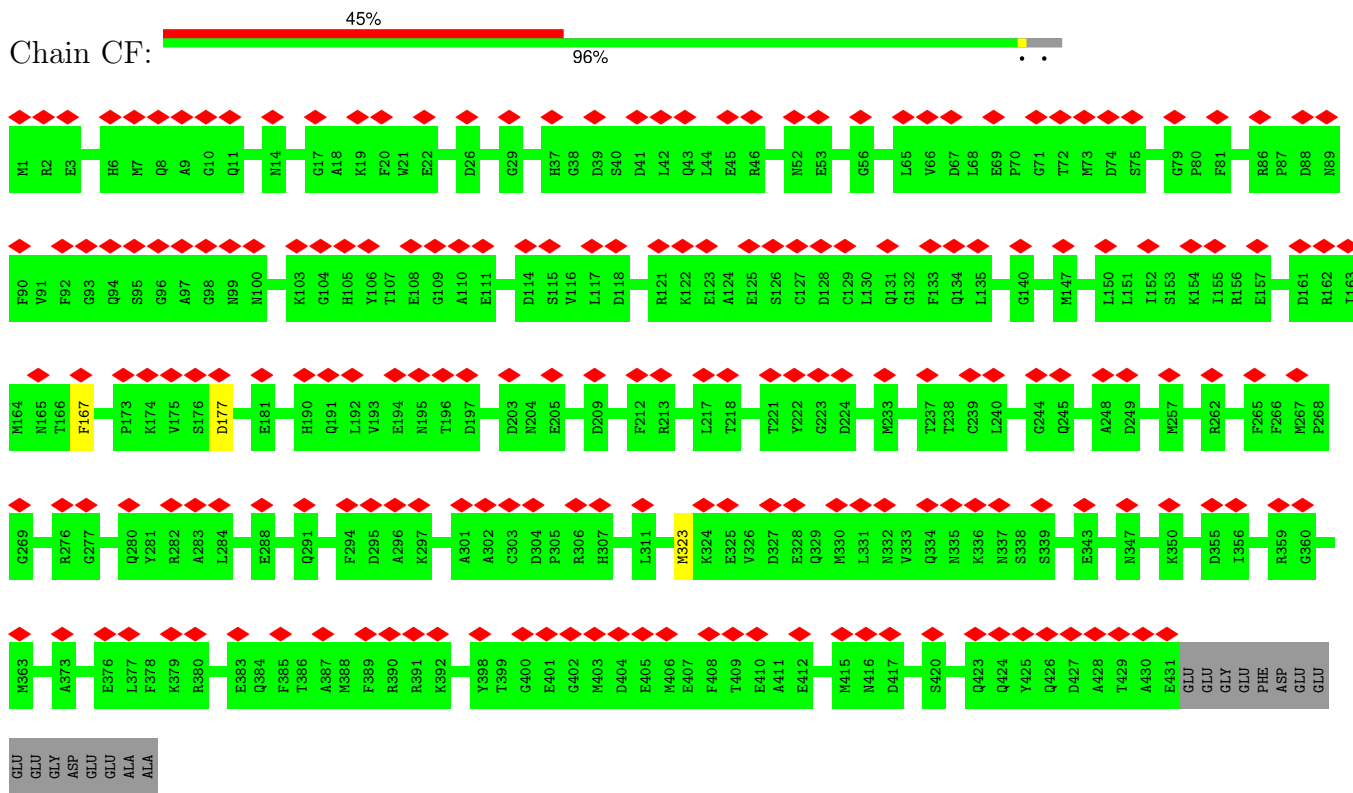
• Molecule 55: Tubulin beta chain



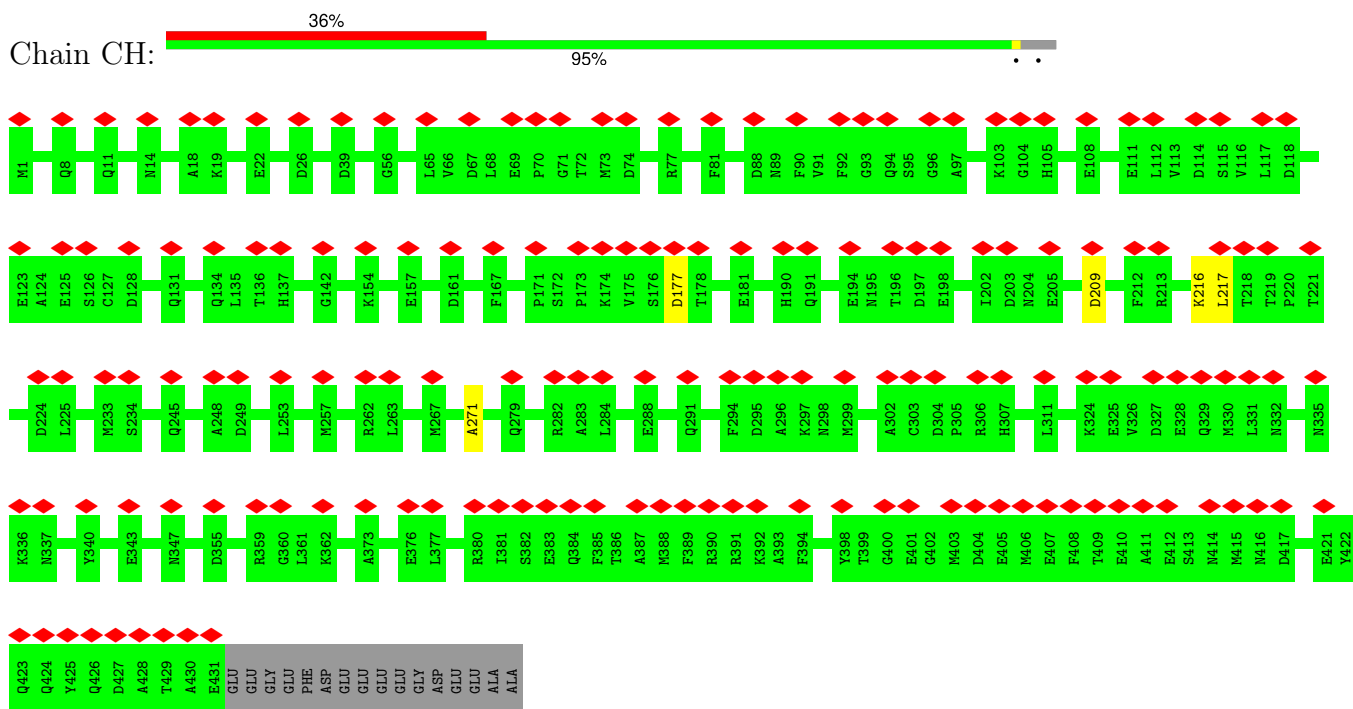
• Molecule 55: Tubulin beta chain



• Molecule 55: Tubulin beta chain



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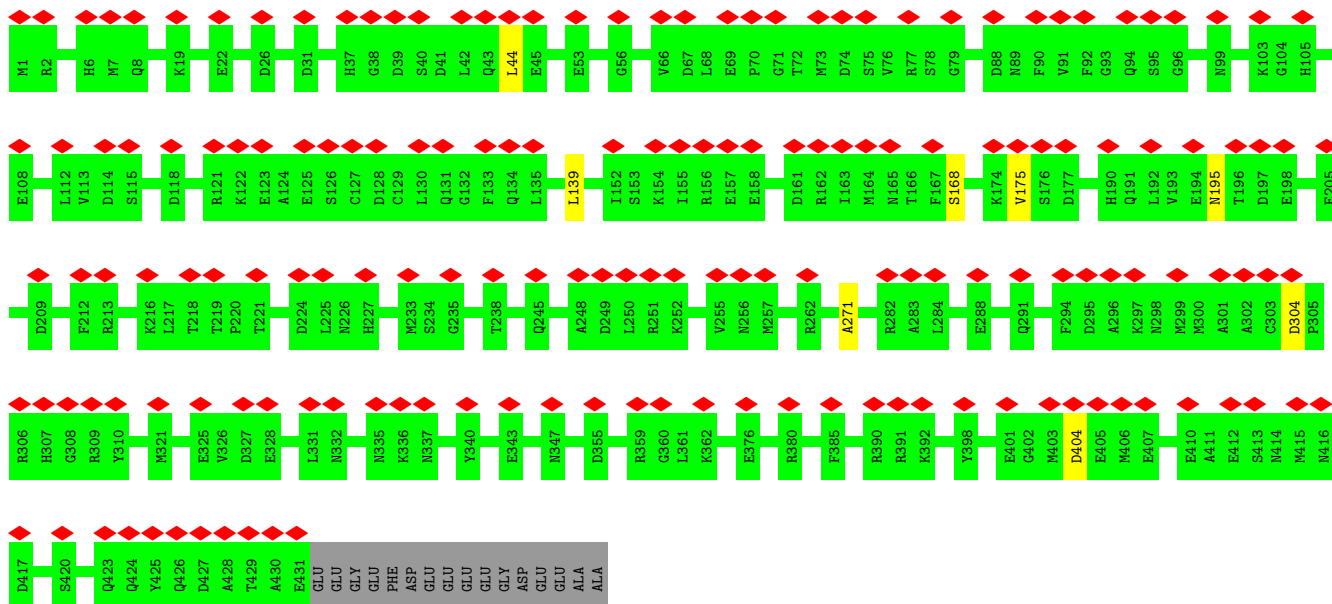


• Molecule 55: Tubulin beta chain

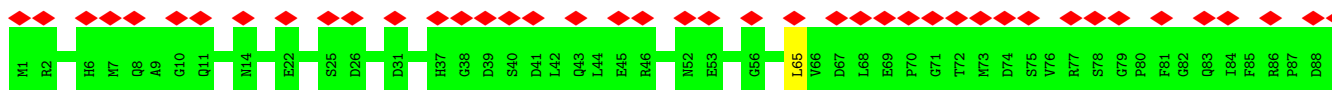


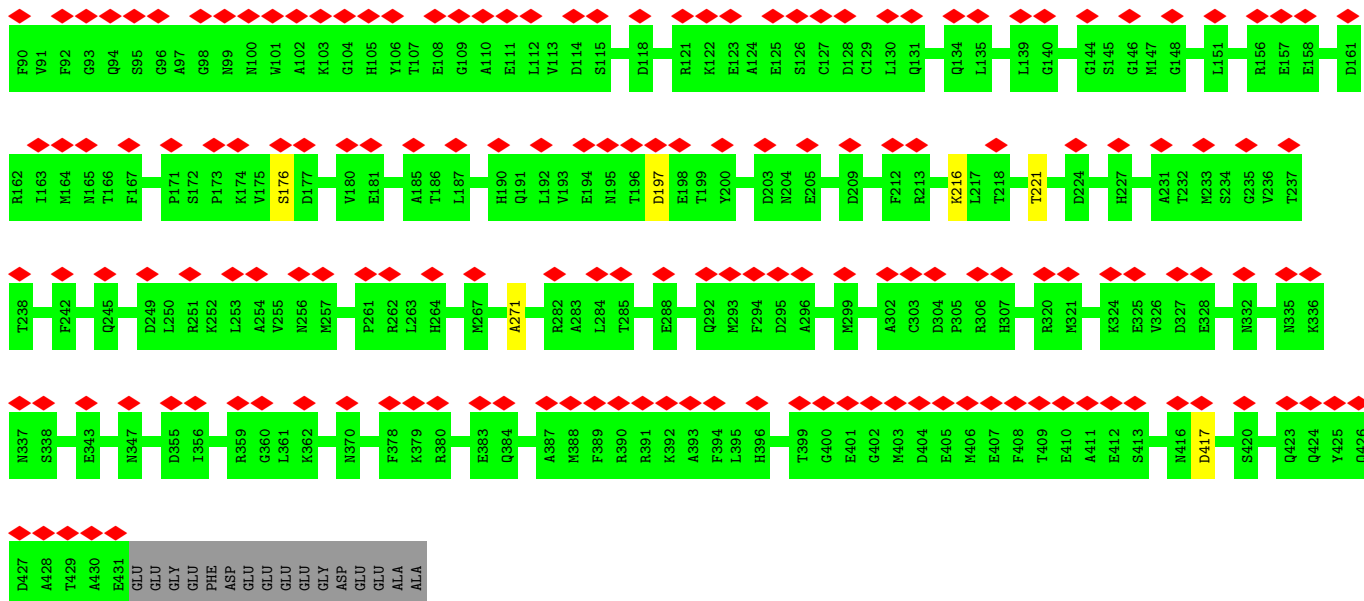


• Molecule 55: Tubulin beta chain

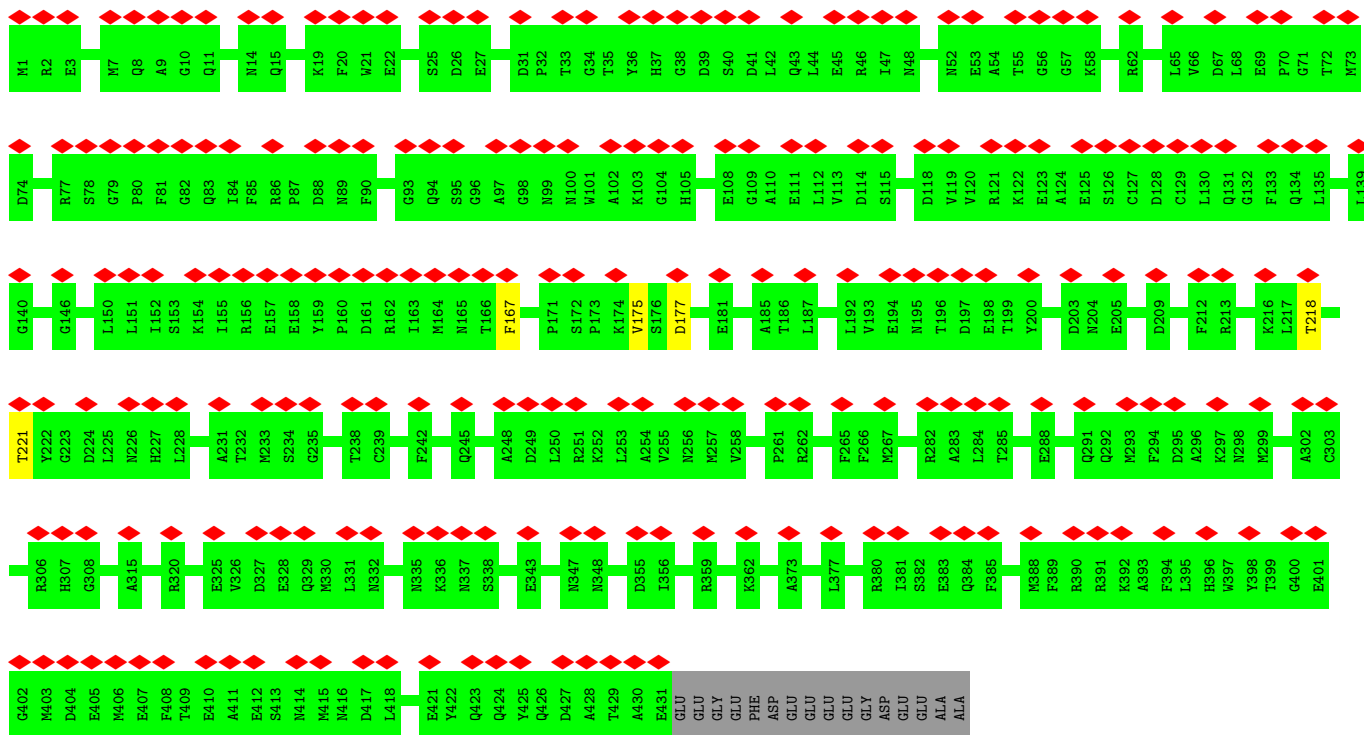


• Molecule 55: Tubulin beta chain

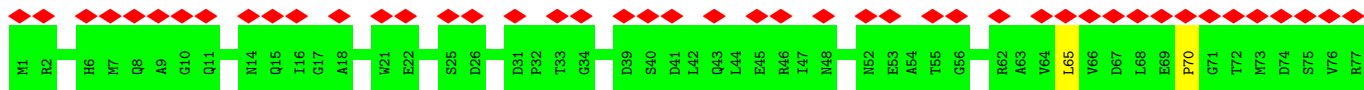


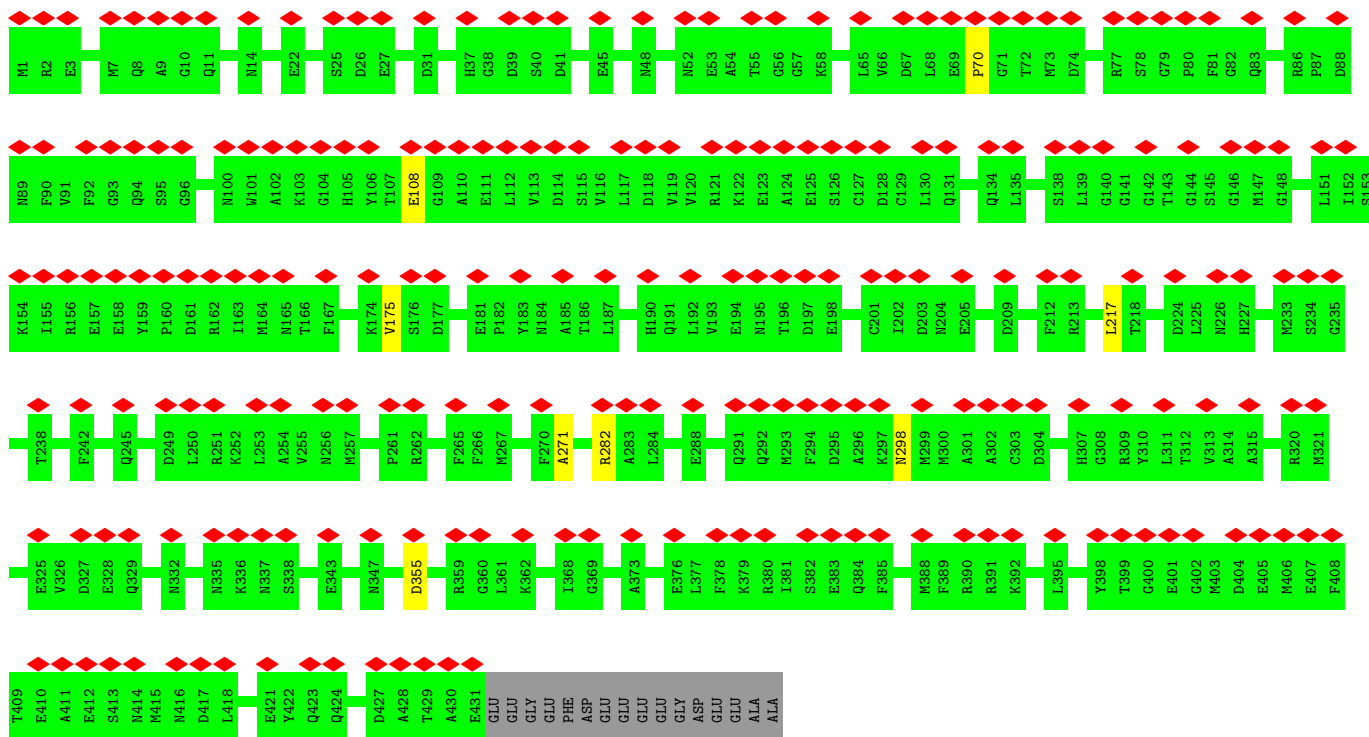


• Molecule 55: Tubulin beta chain

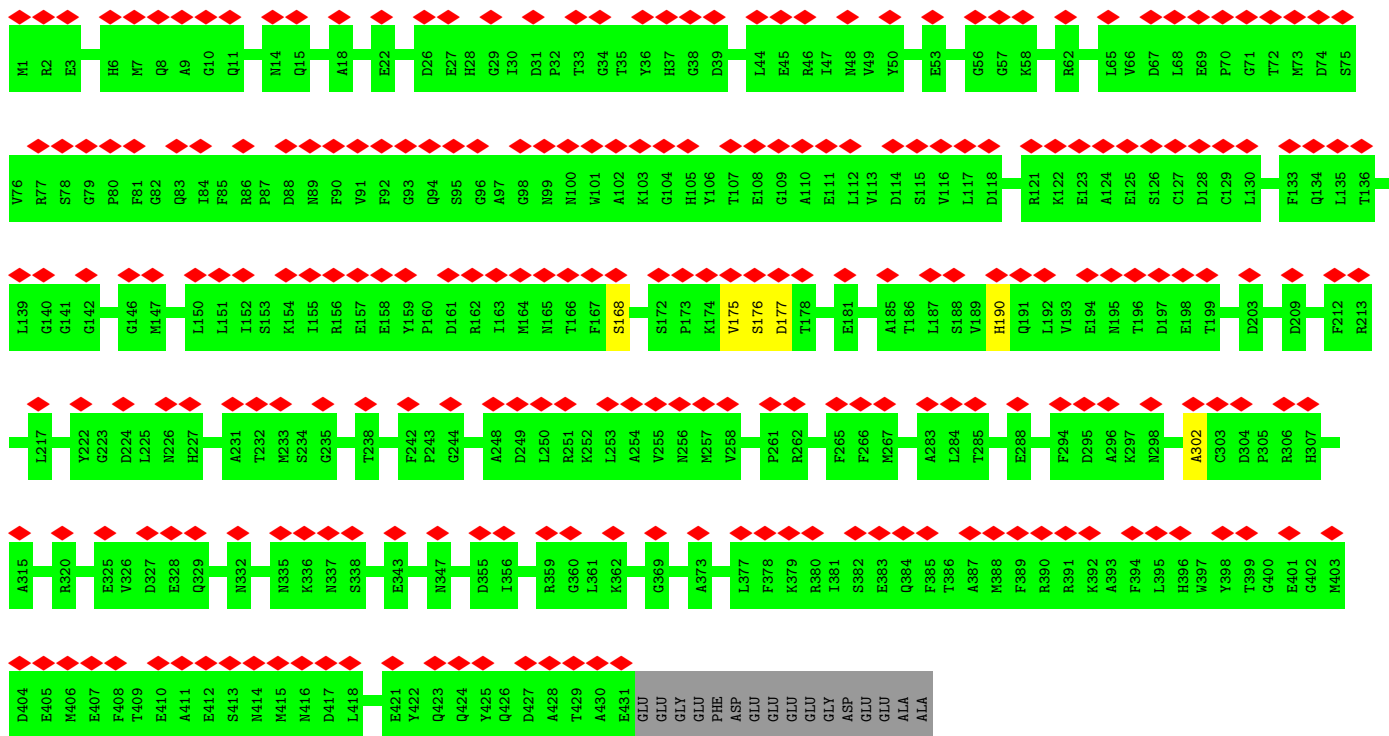


• Molecule 55: Tubulin beta chain





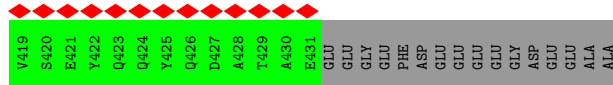
• Molecule 55: Tubulin beta chain



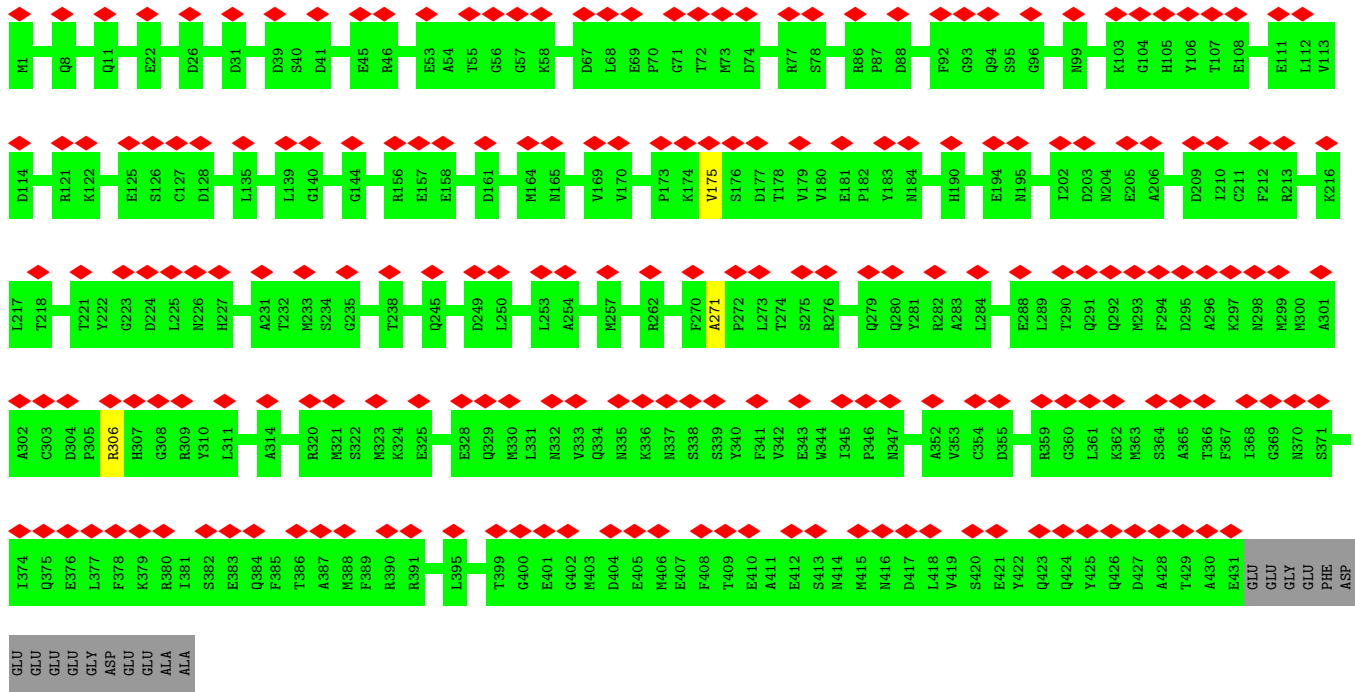
• Molecule 55: Tubulin beta chain



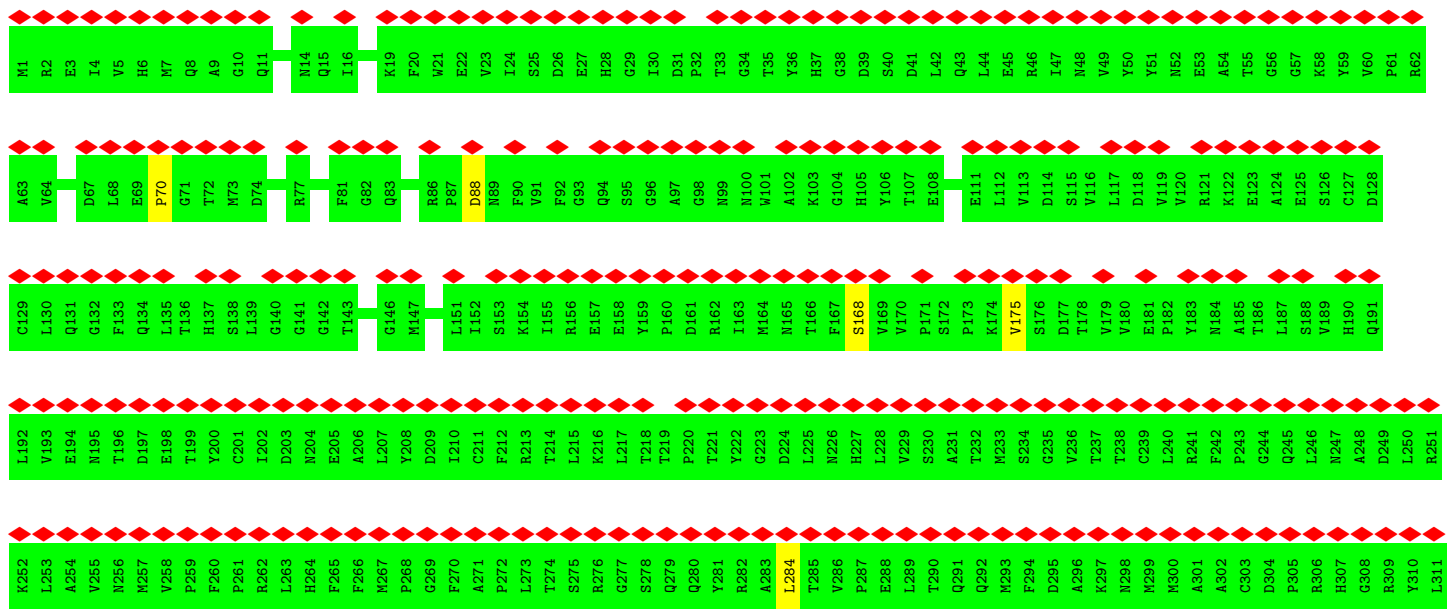
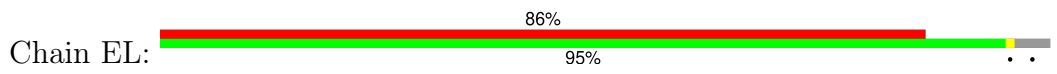


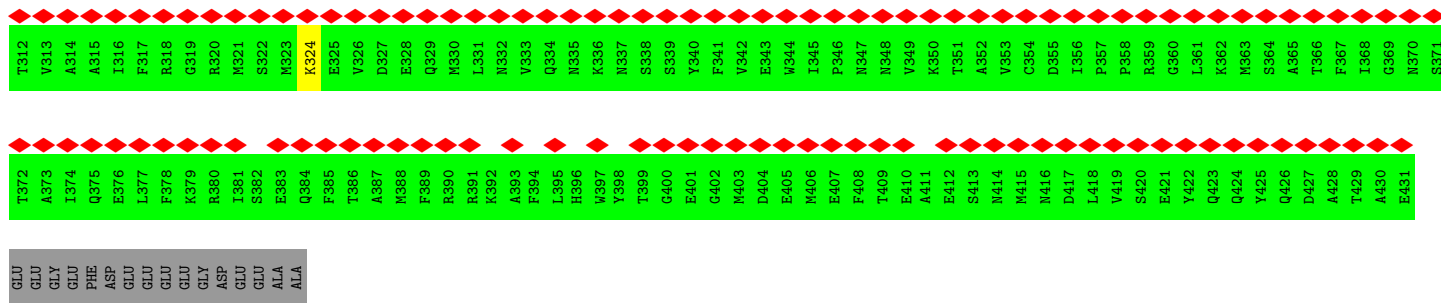


• Molecule 55: Tubulin beta chain

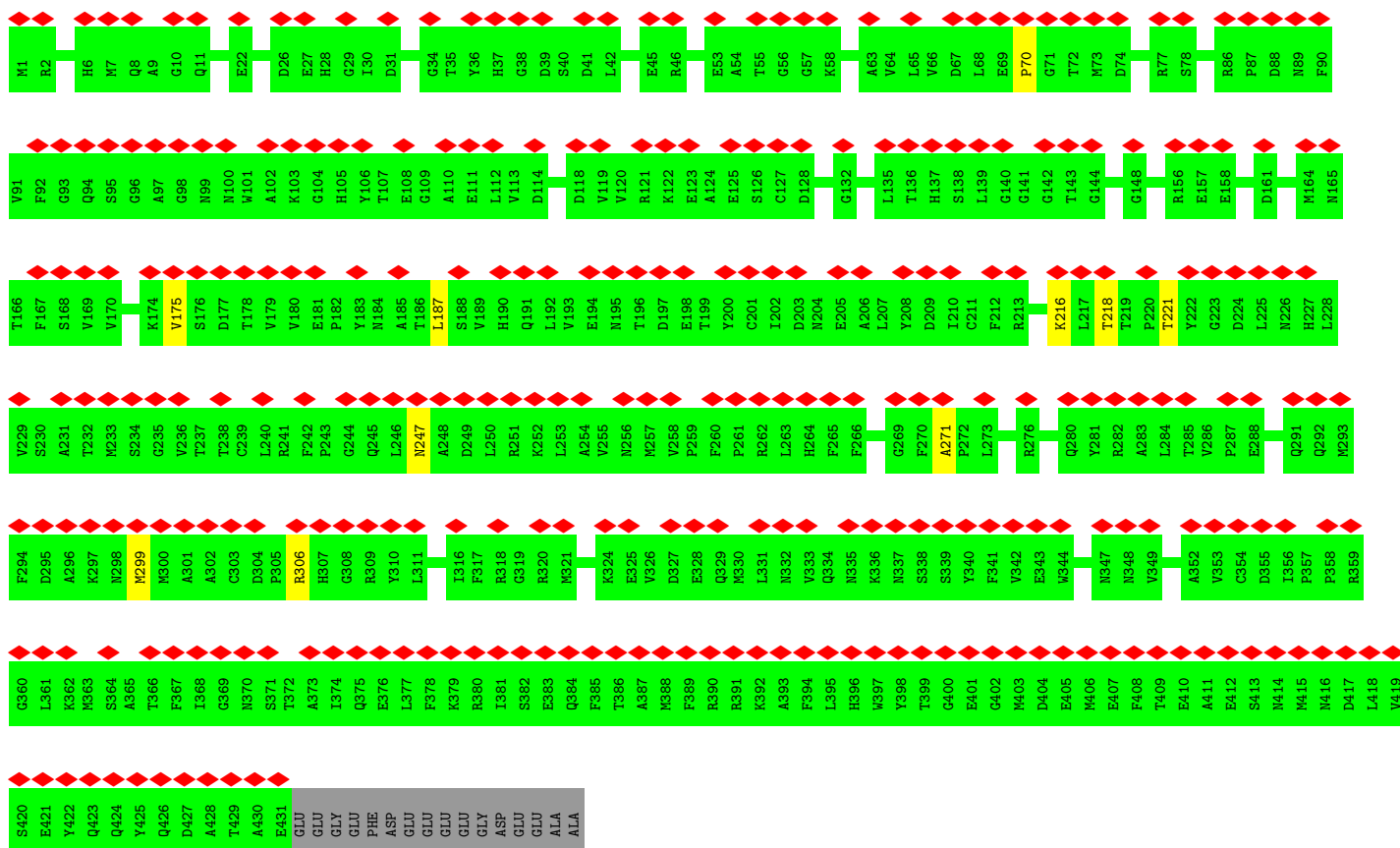


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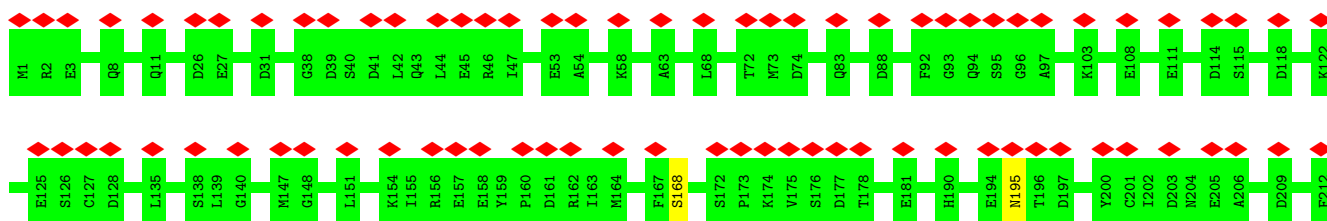


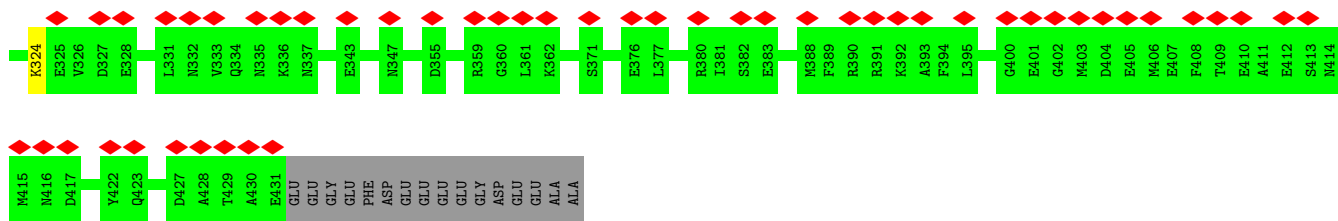


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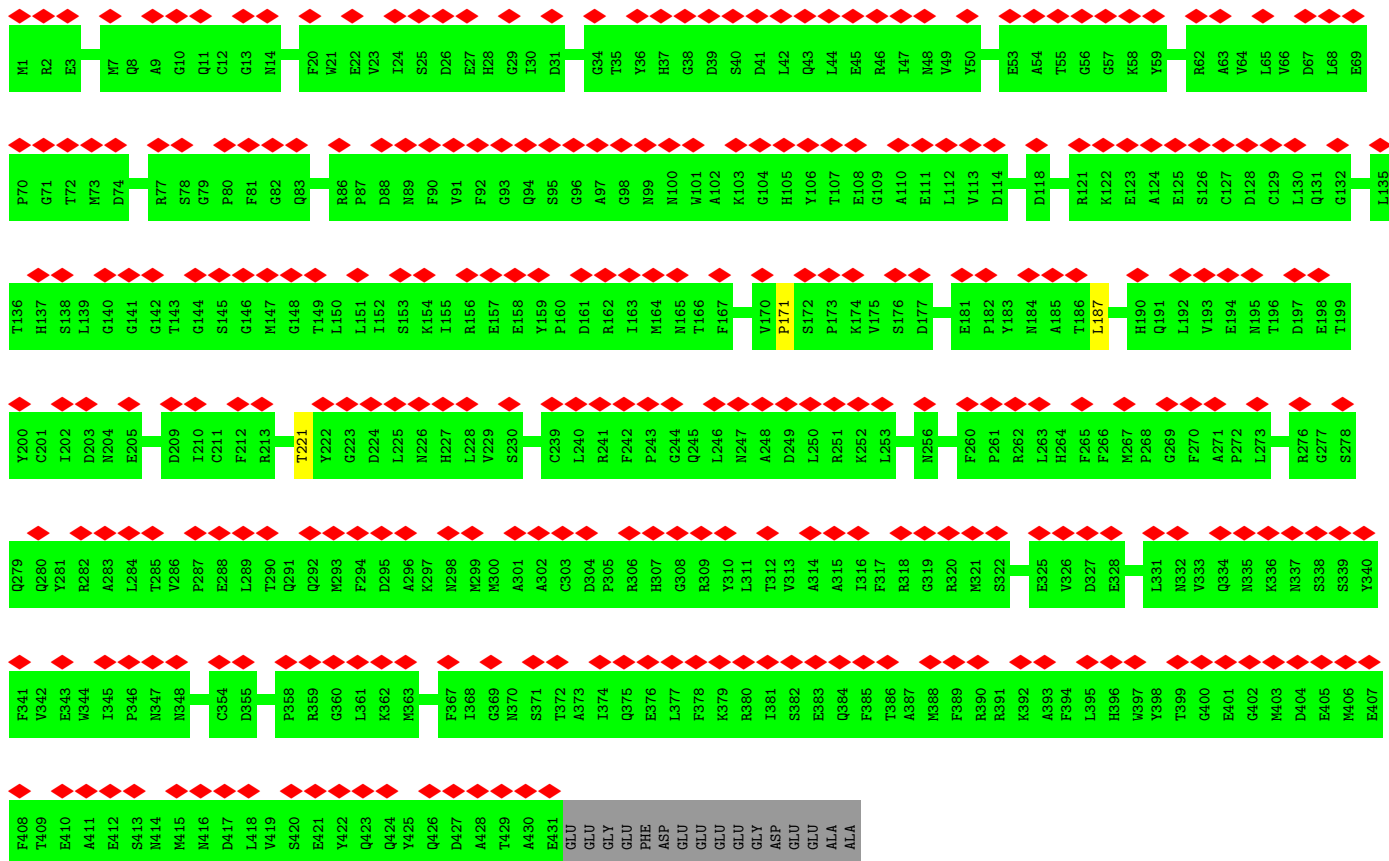
• Molecule 55: Tubulin beta chain





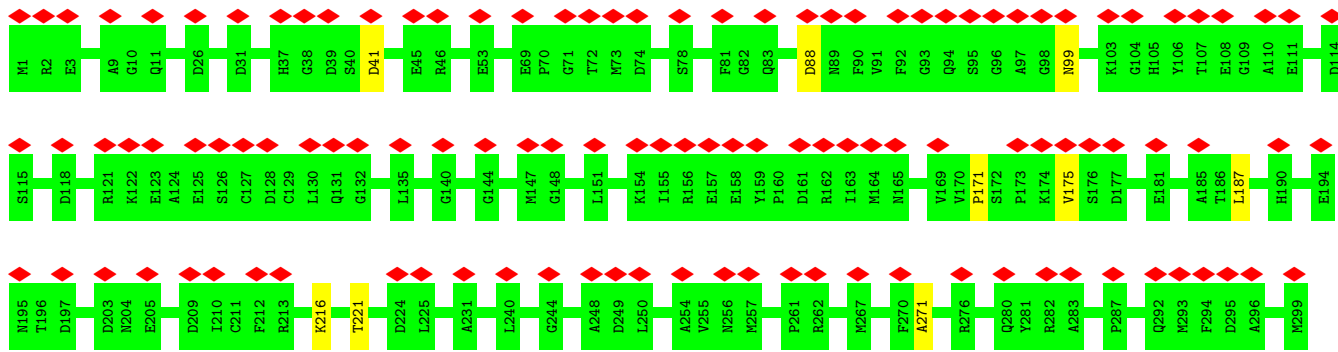
• Molecule 55: Tubulin beta chain

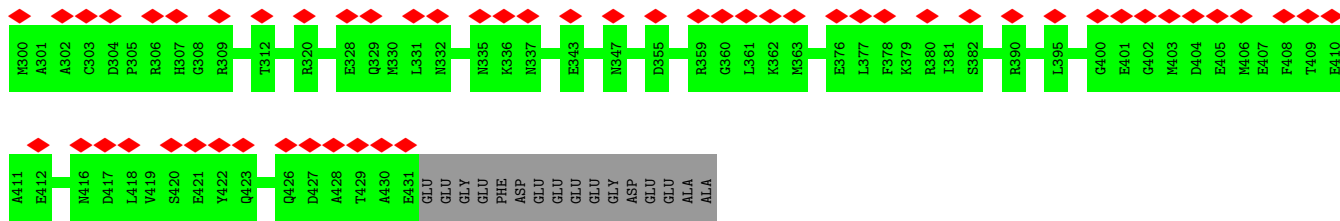
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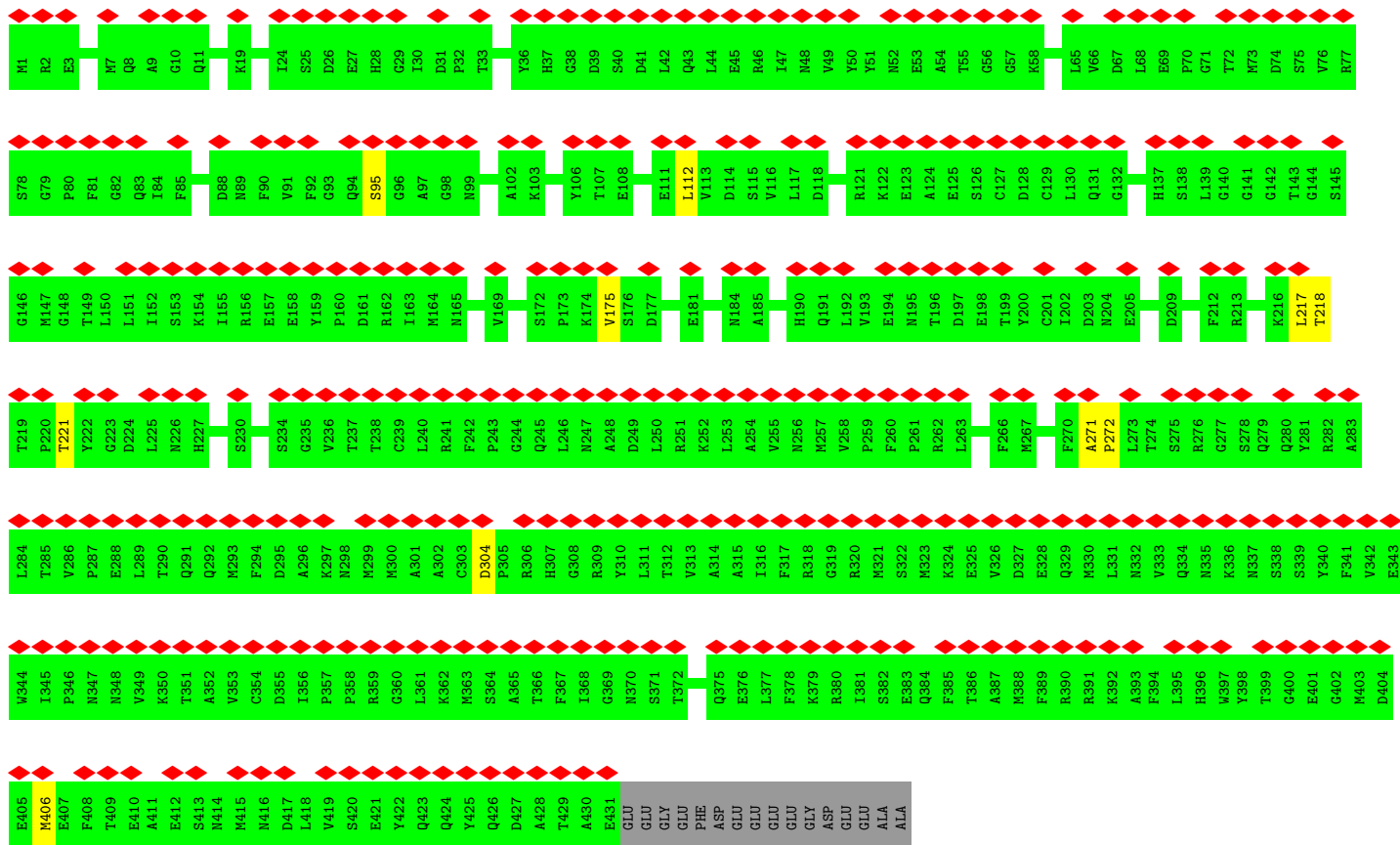
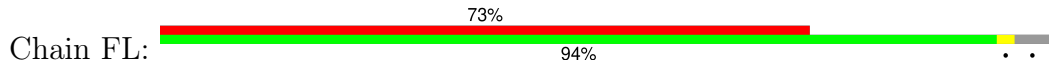
• Molecule 55: Tubulin beta chain

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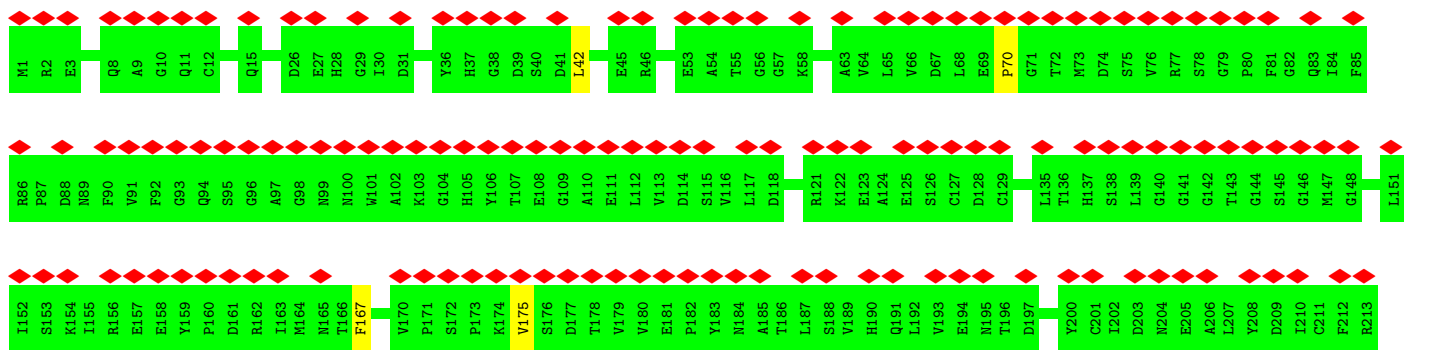


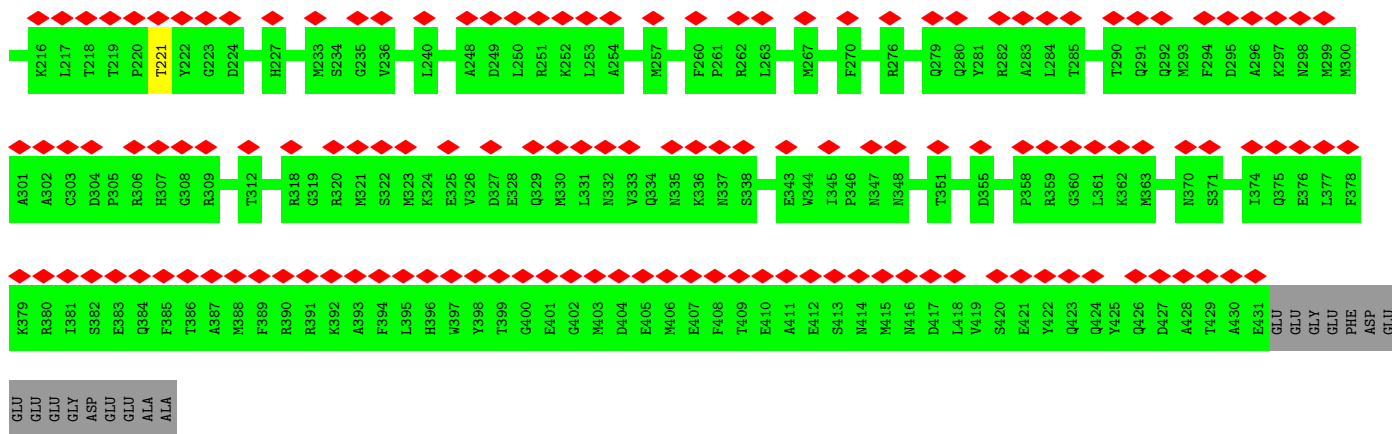


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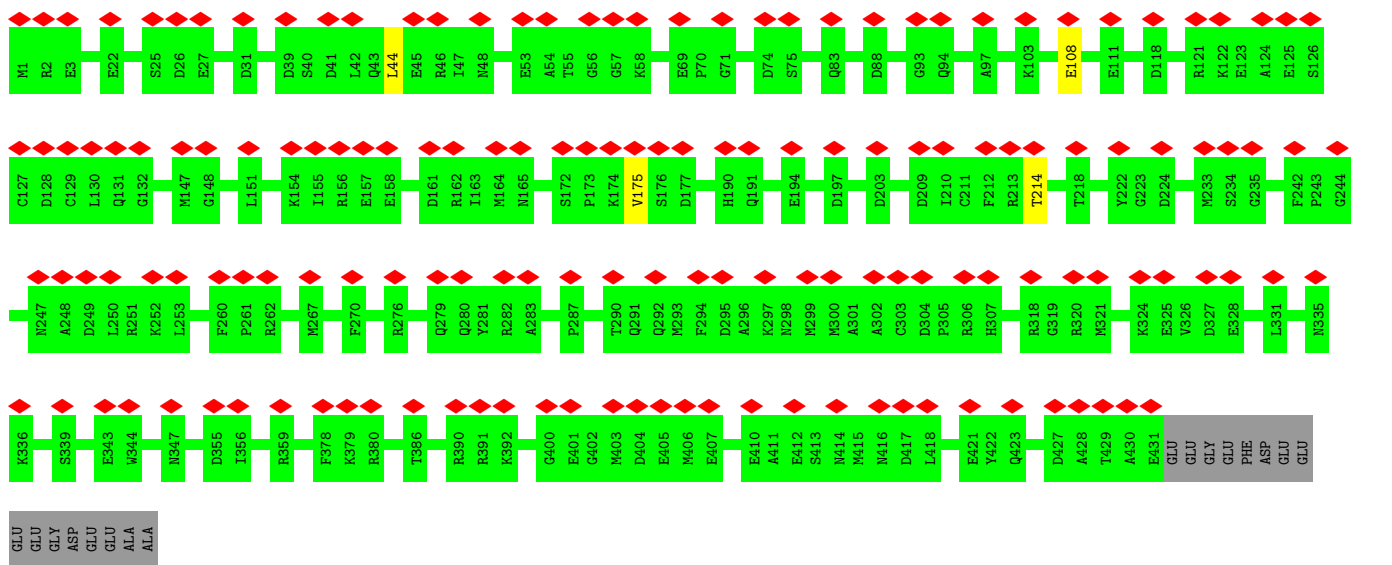


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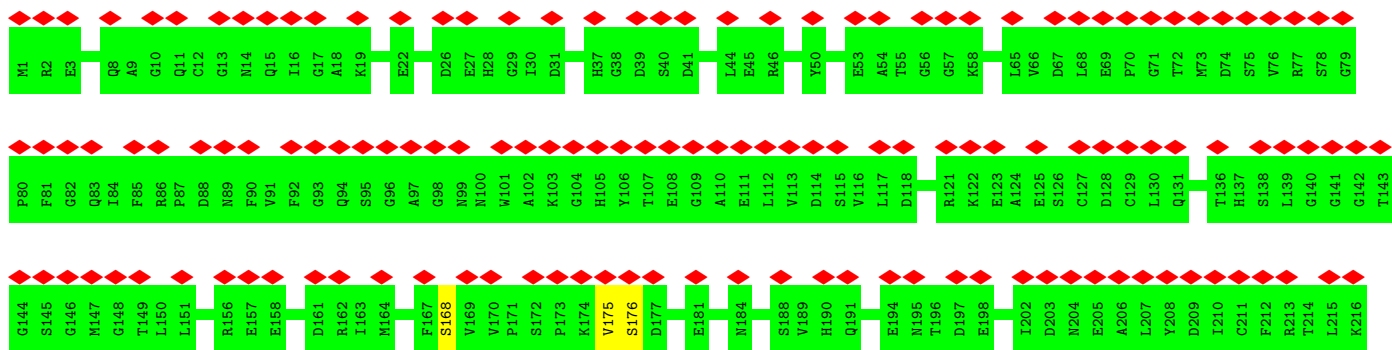


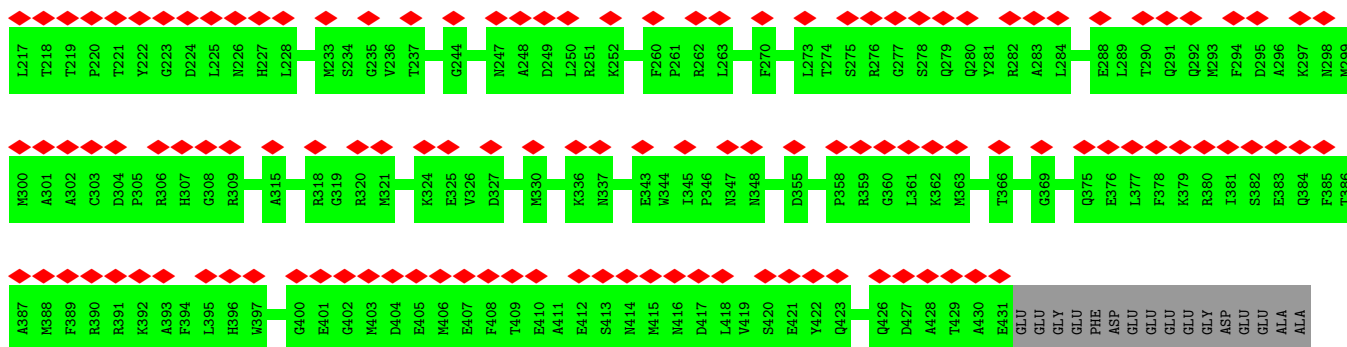


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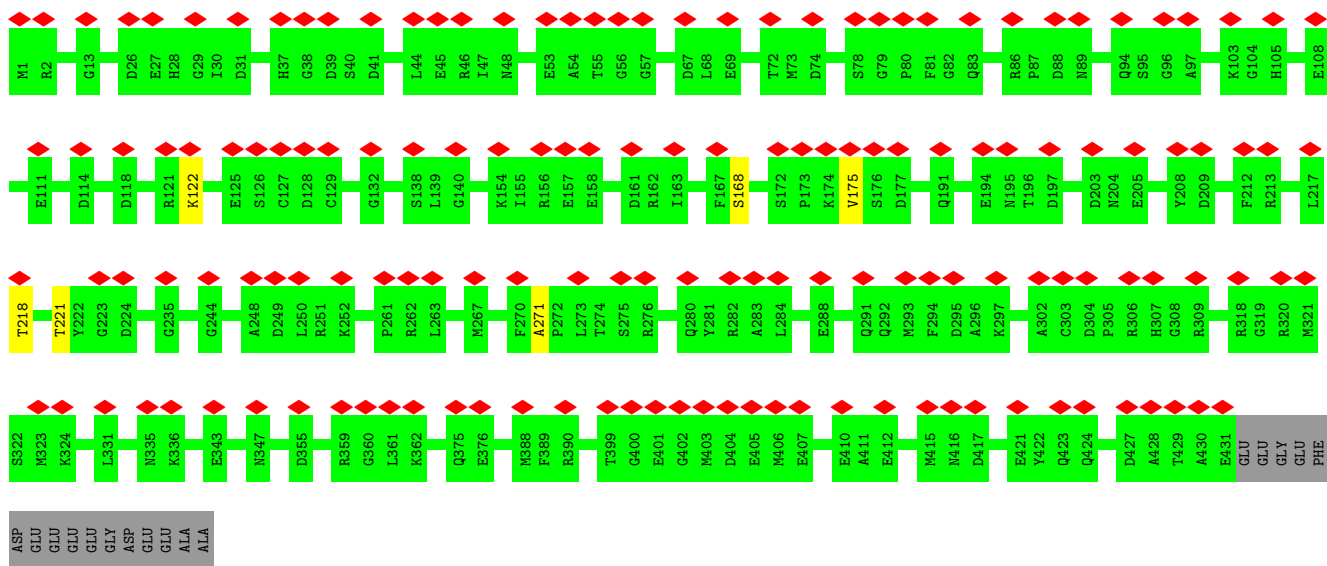


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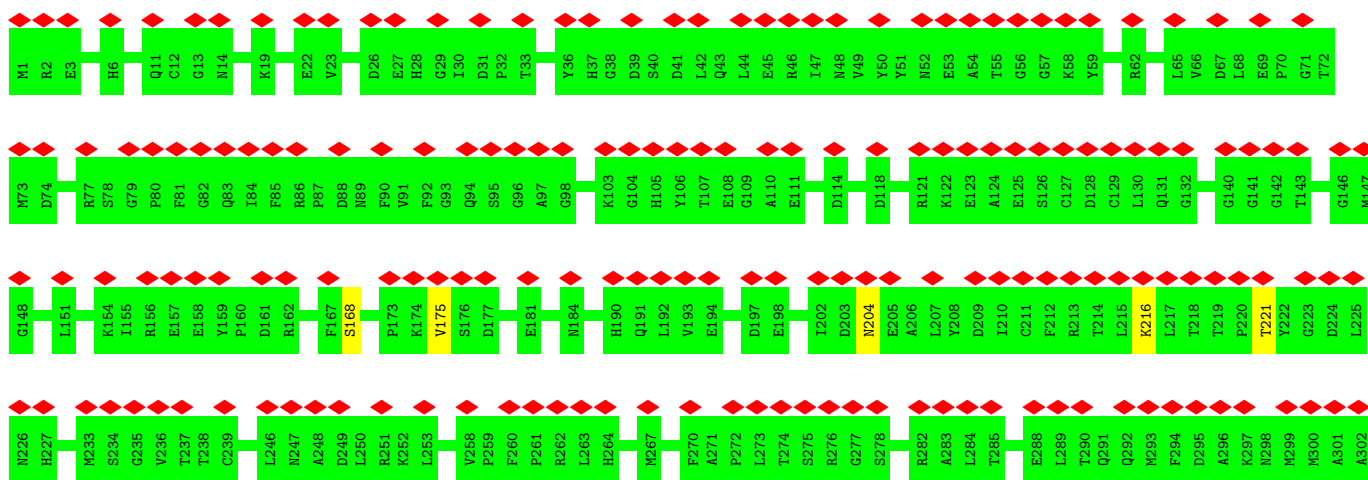




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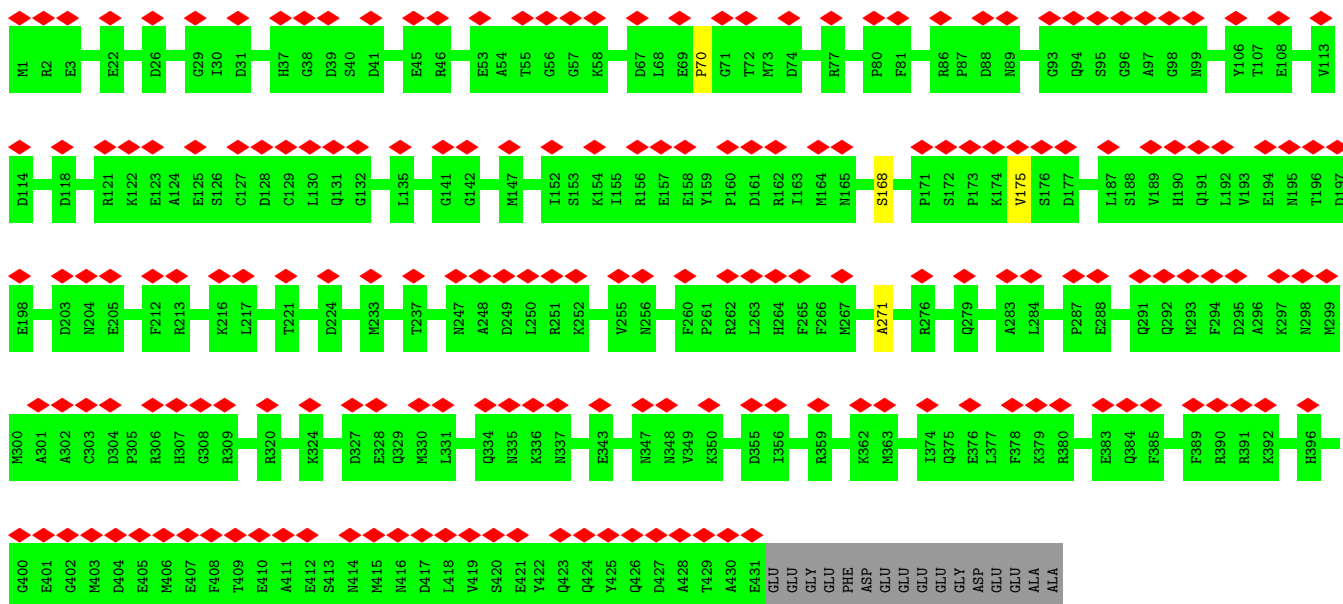
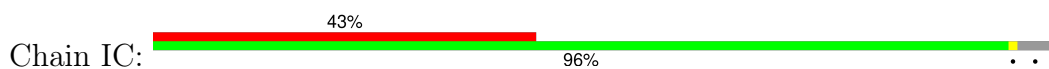


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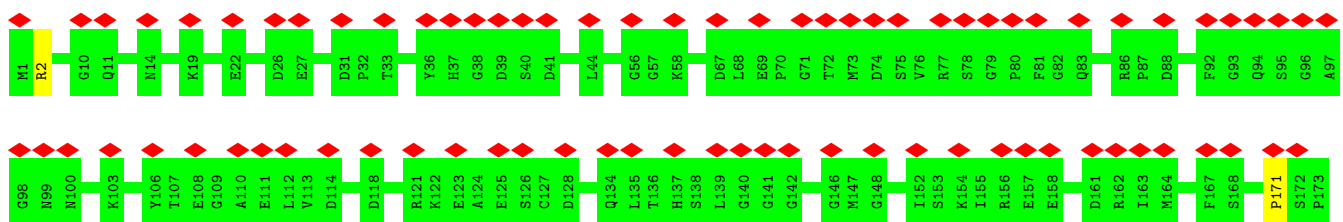


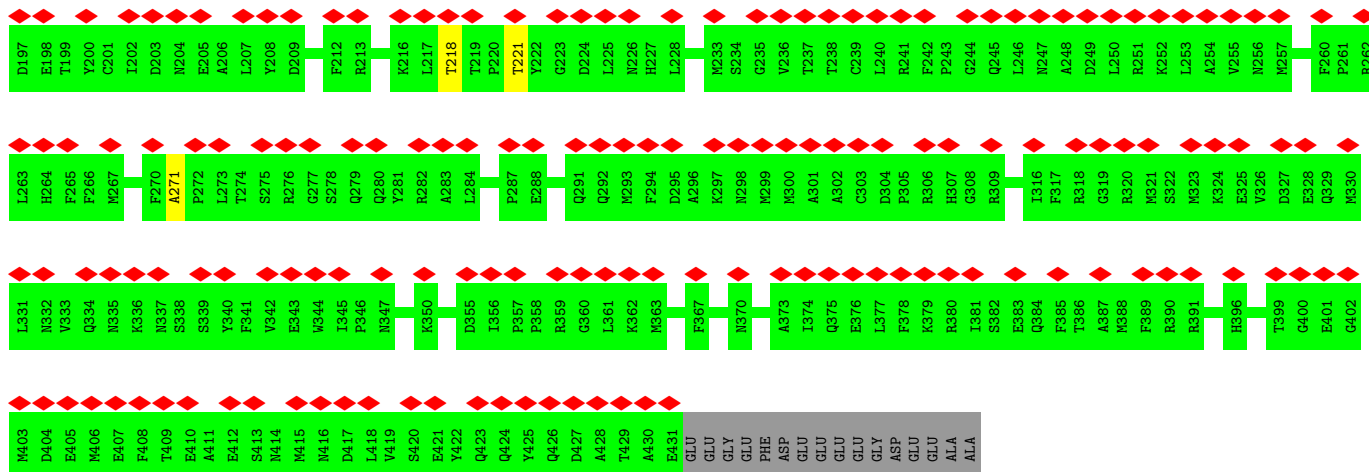


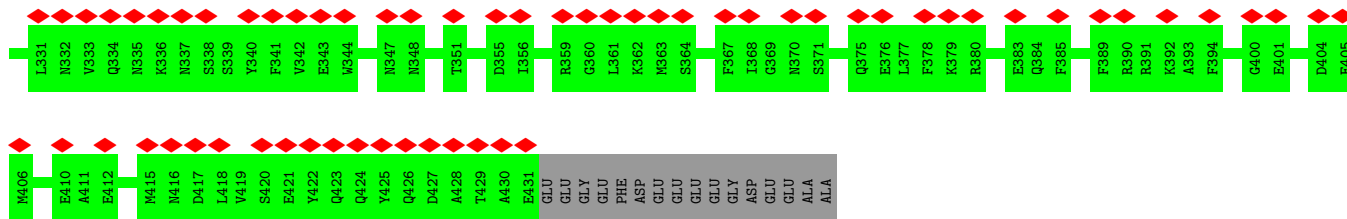
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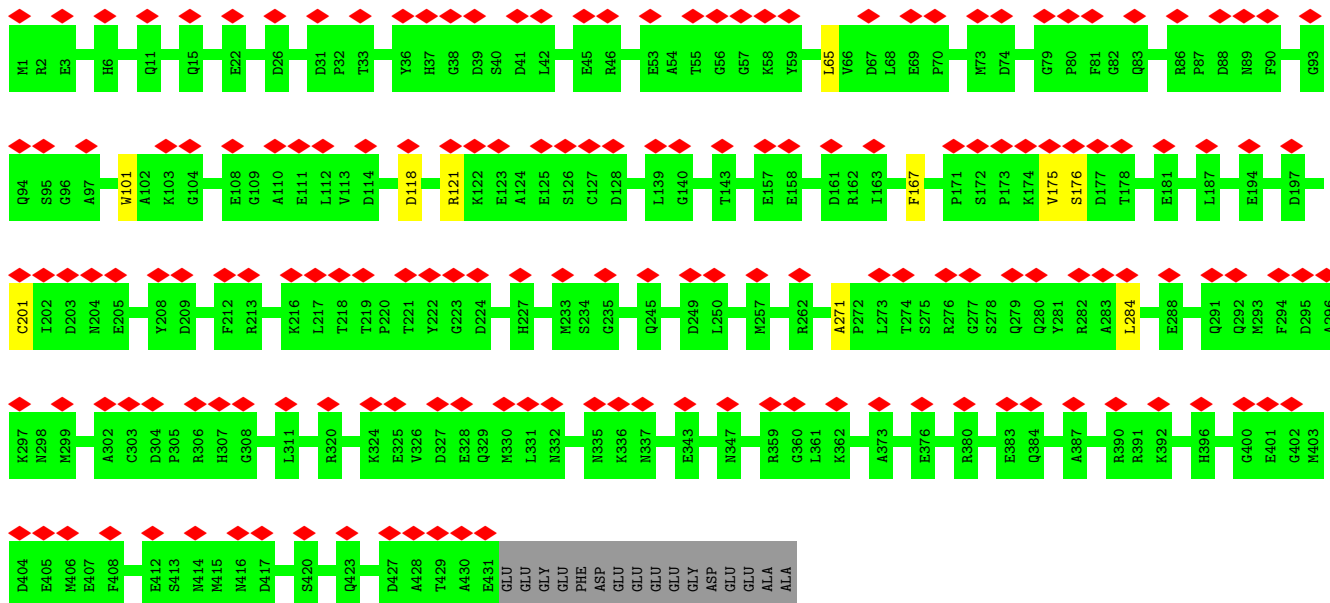
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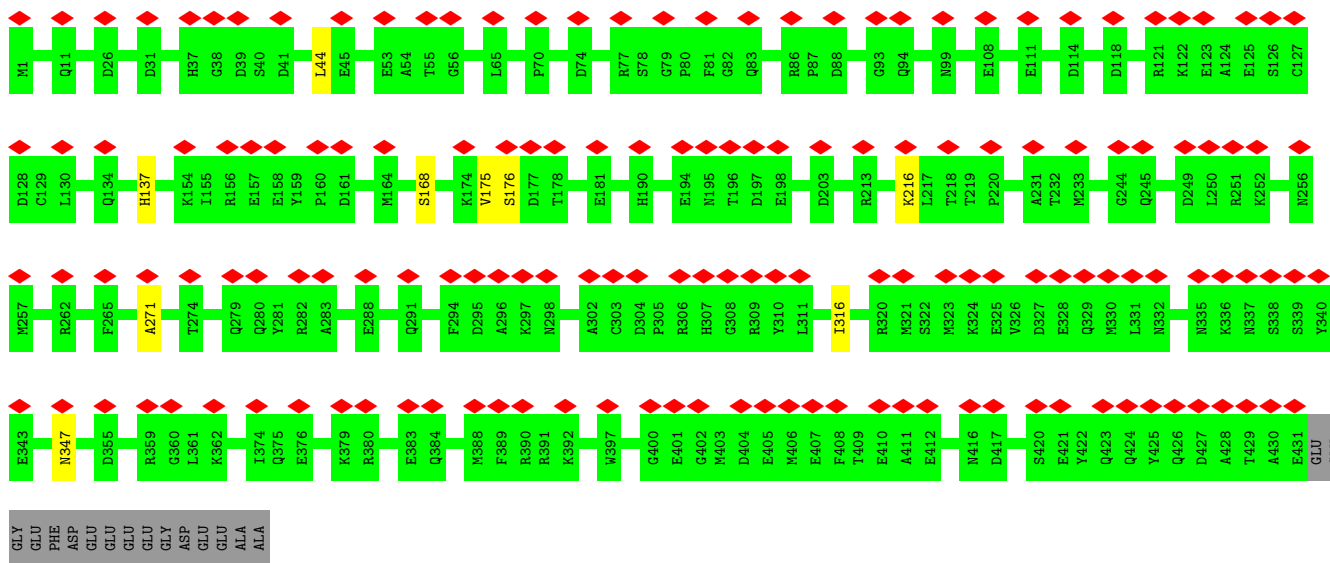




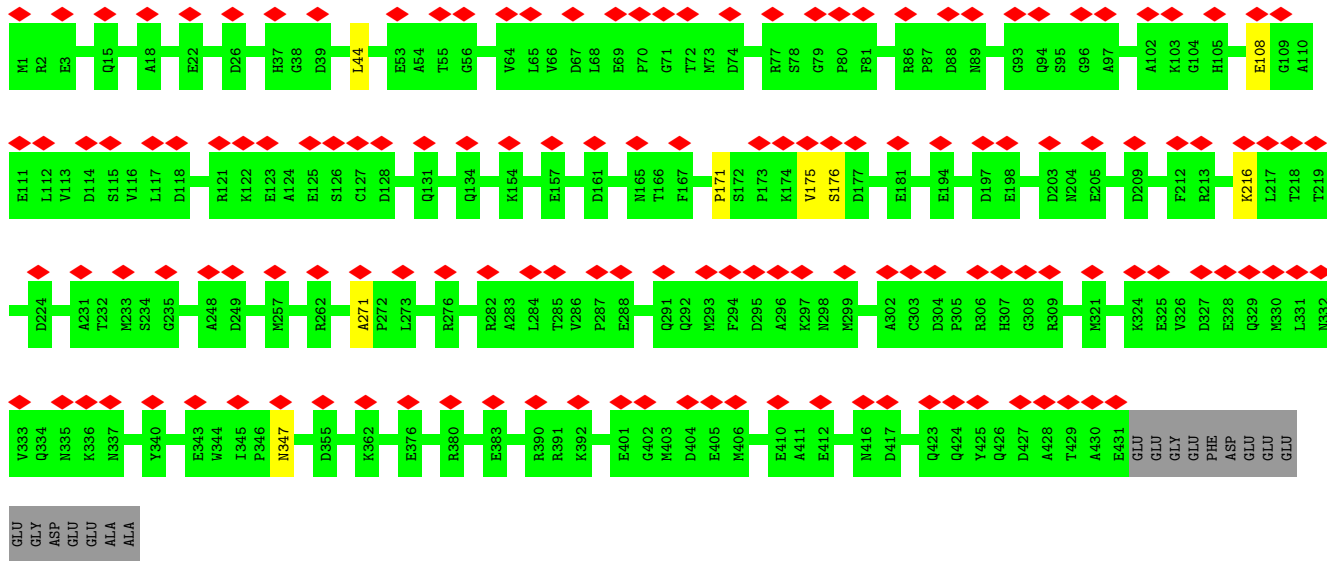
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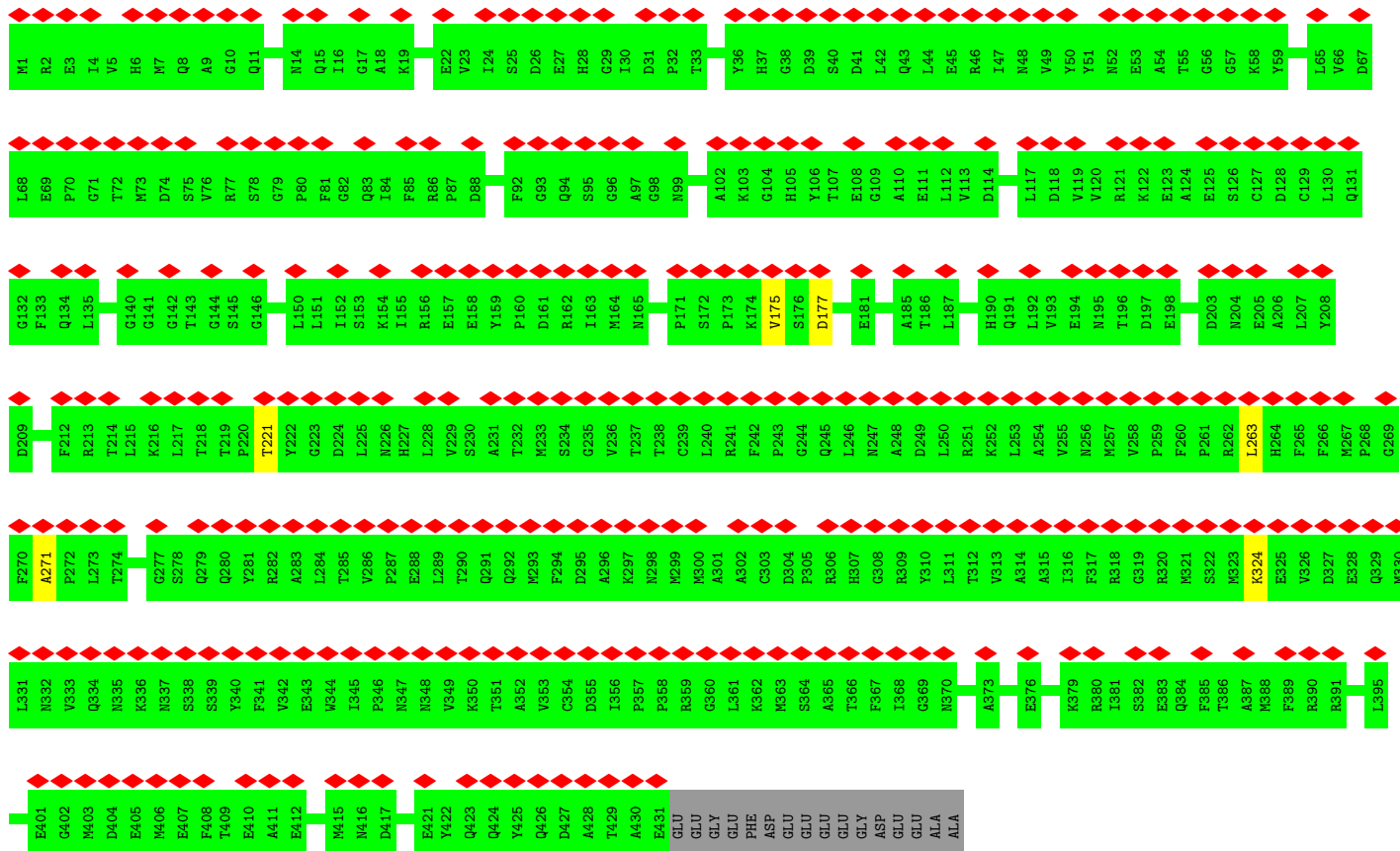
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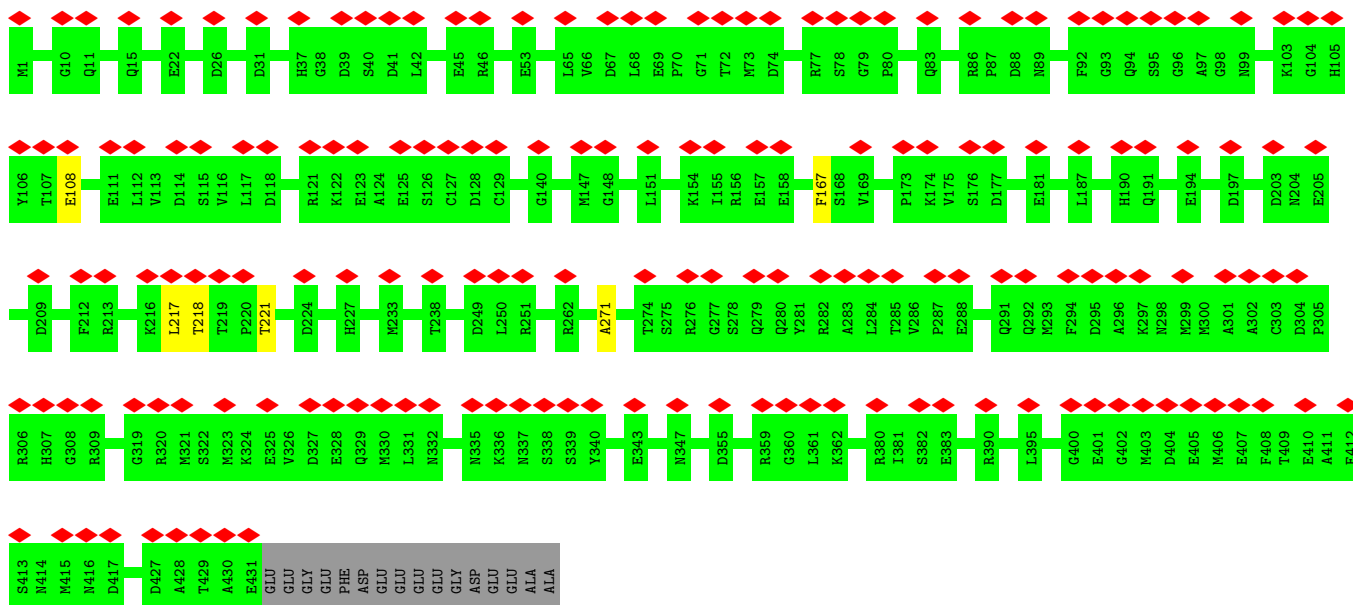


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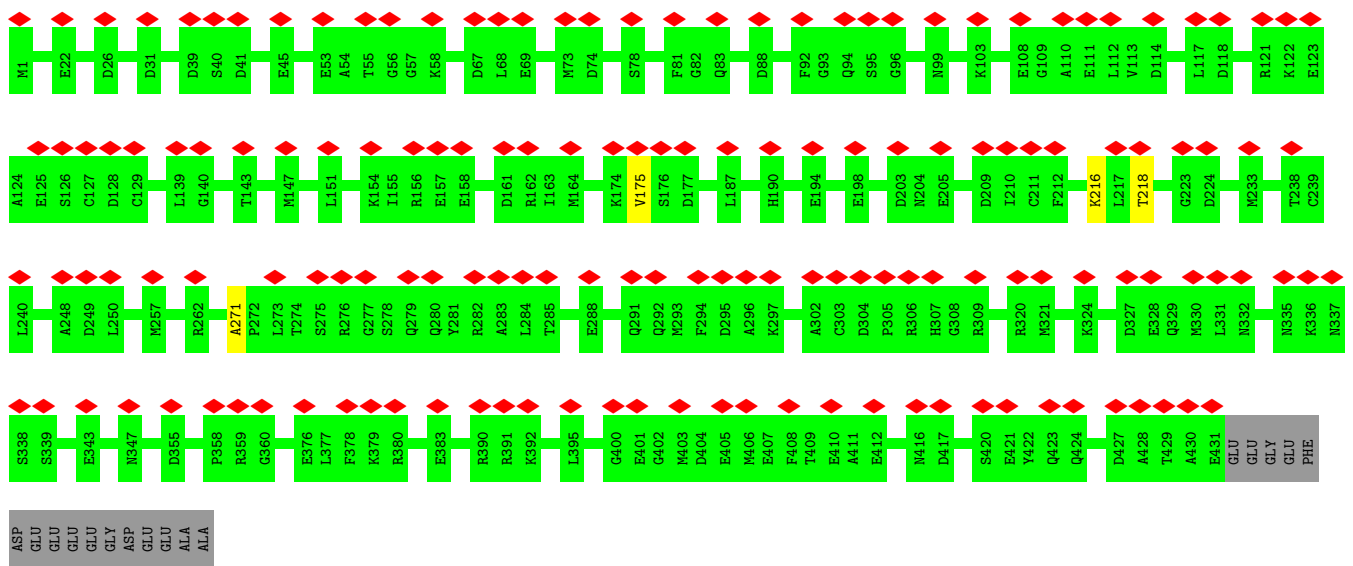


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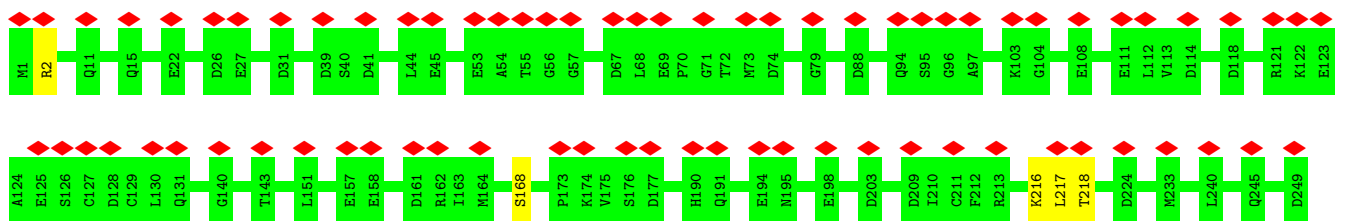


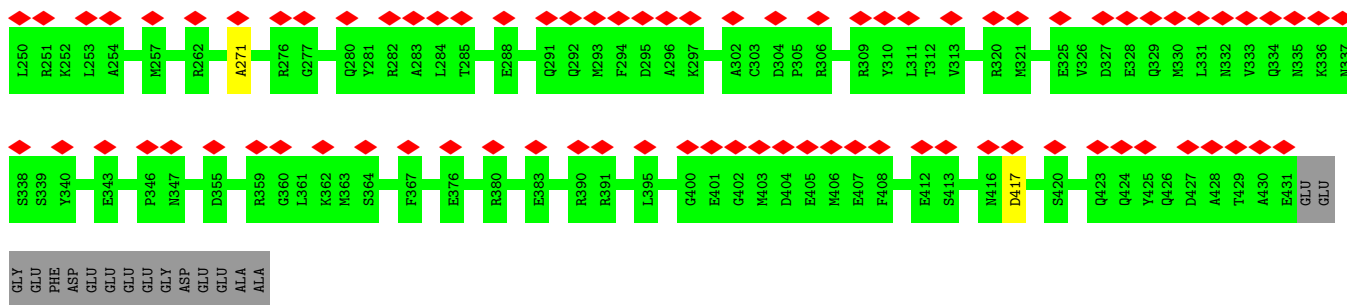


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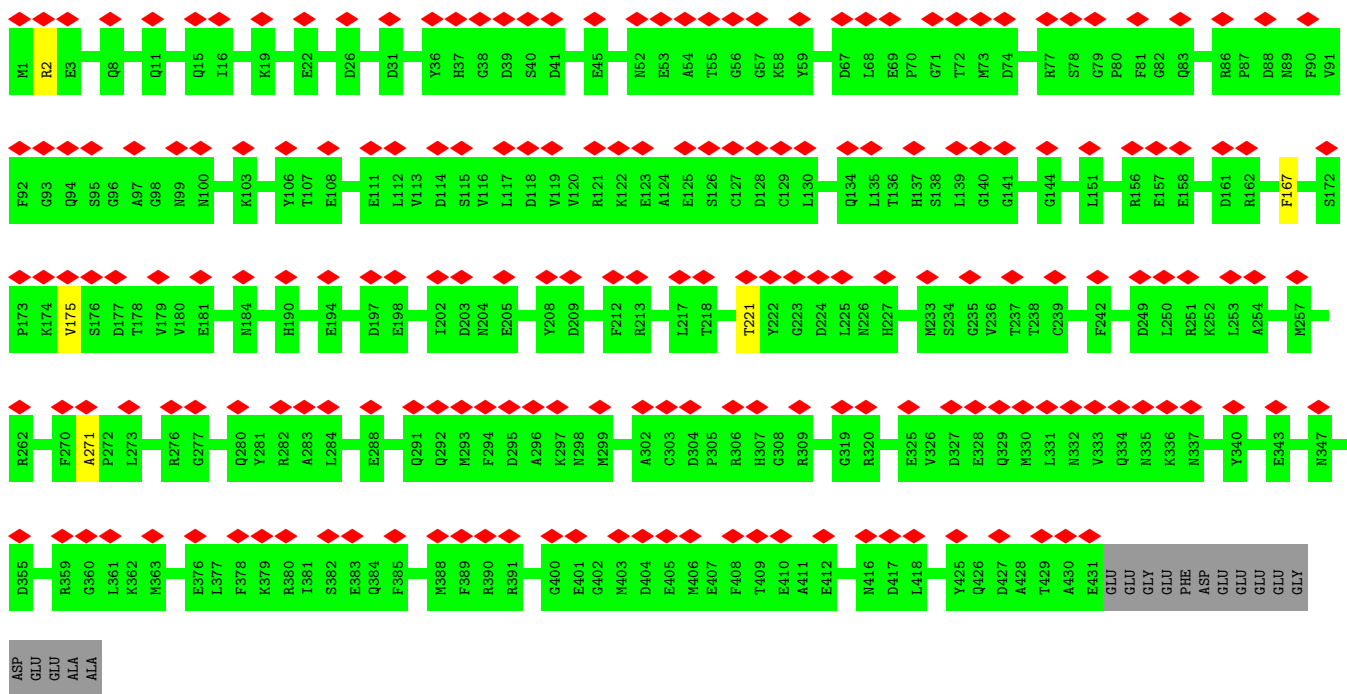
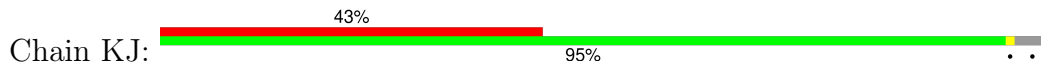


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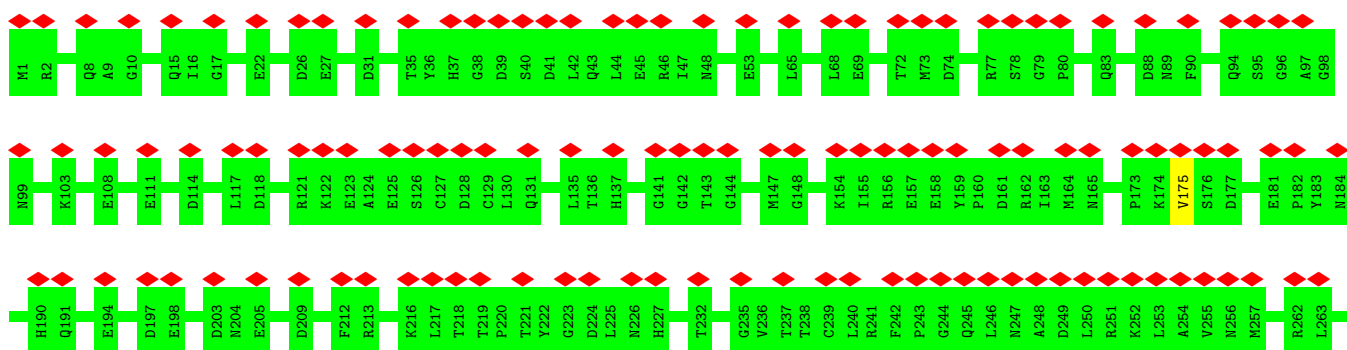


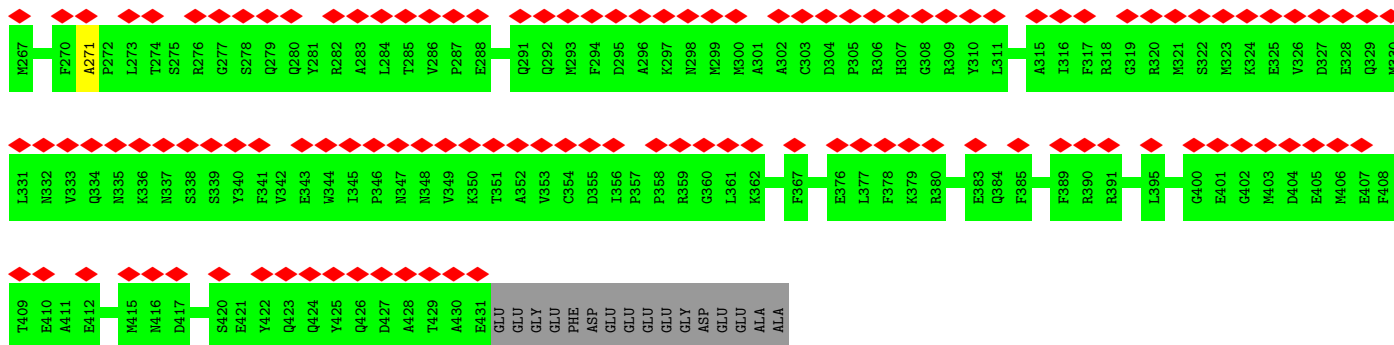


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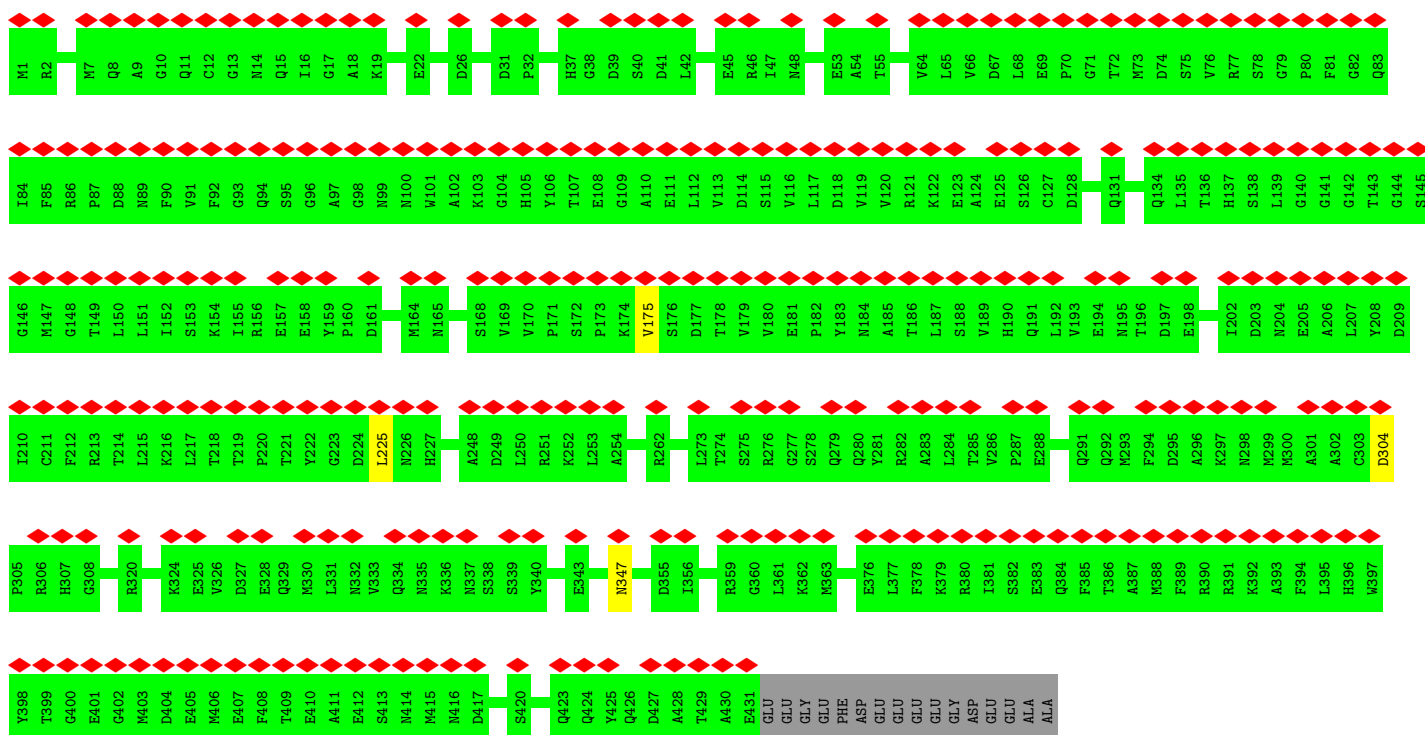


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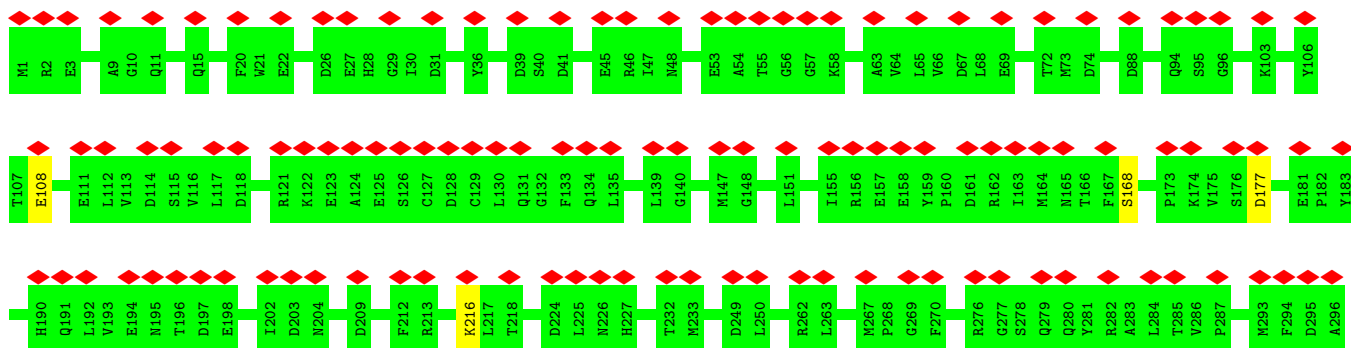
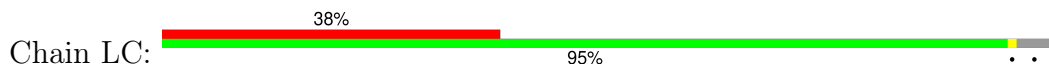


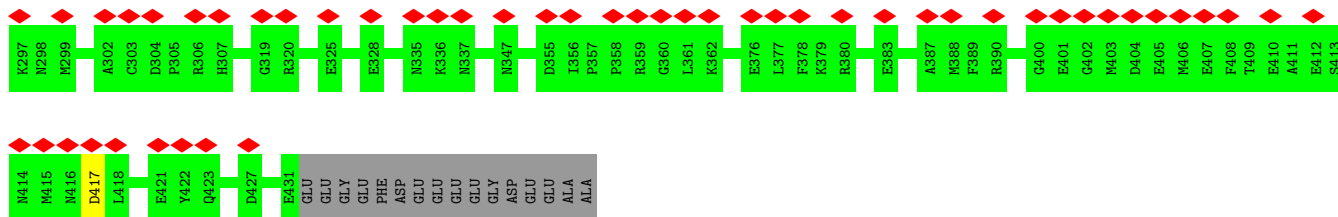


• Molecule 55: Tubulin beta chain



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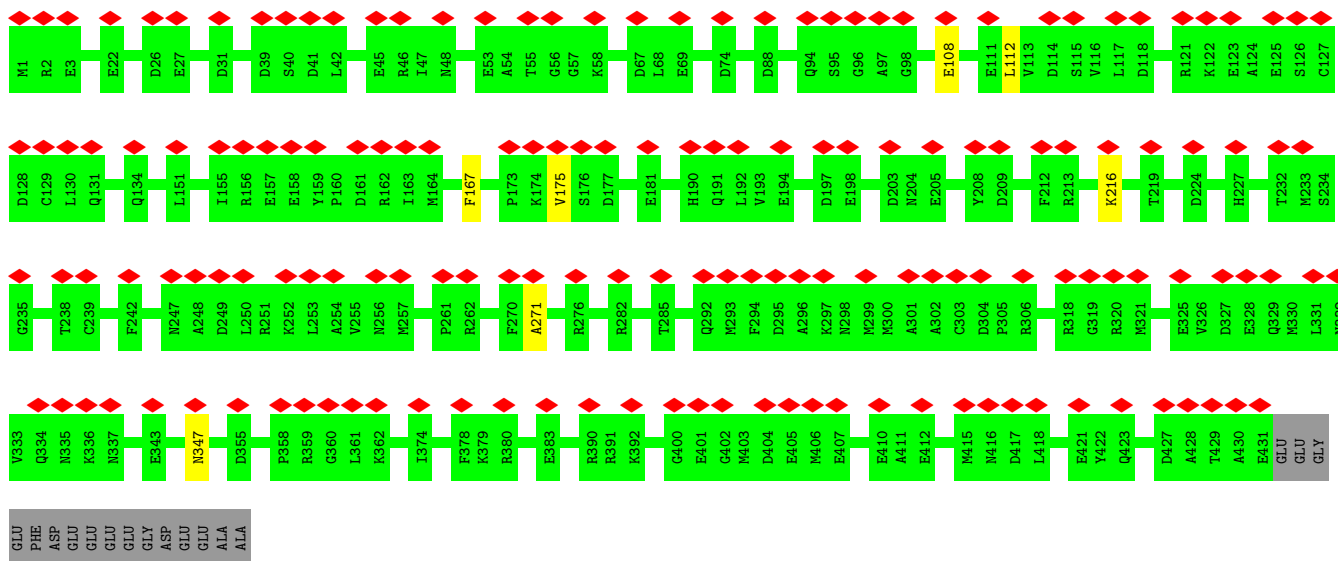




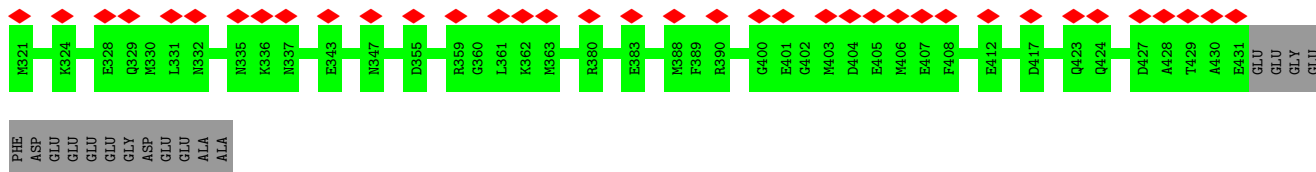
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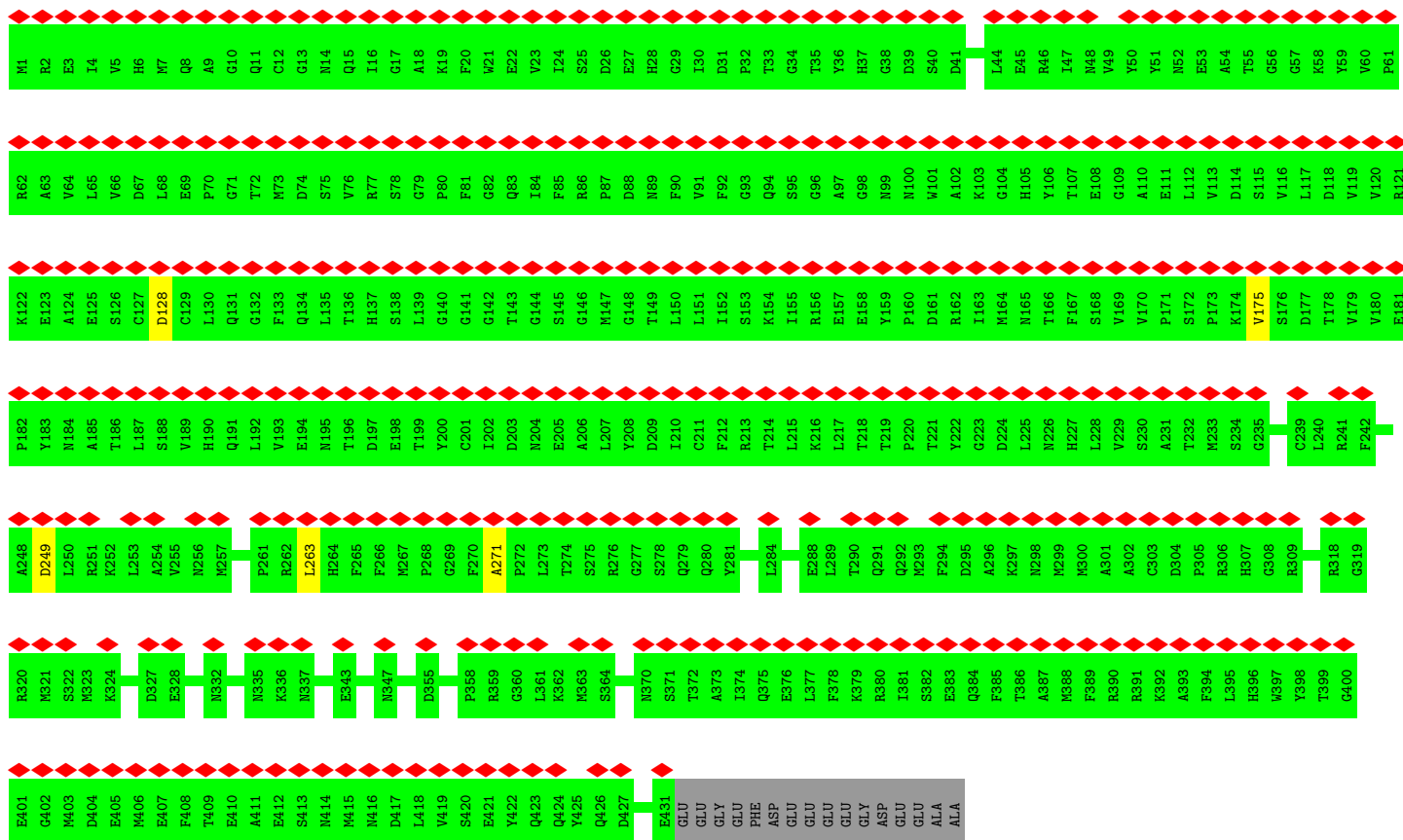
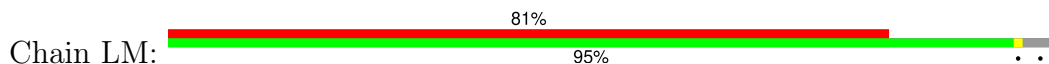
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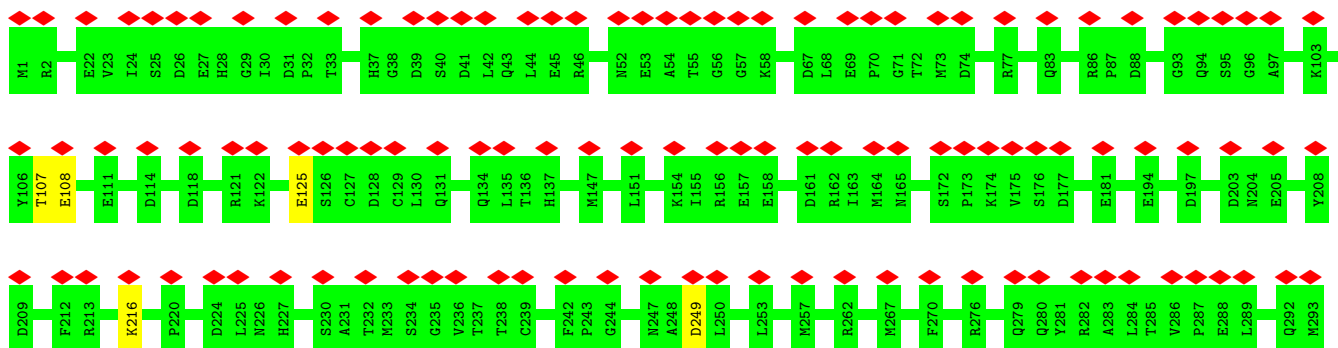
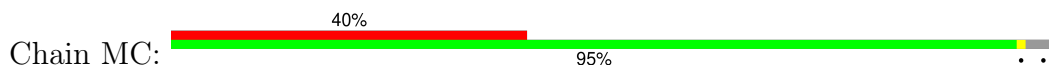
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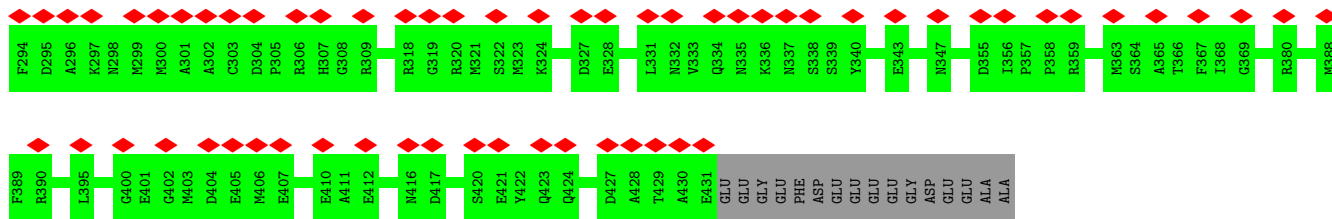


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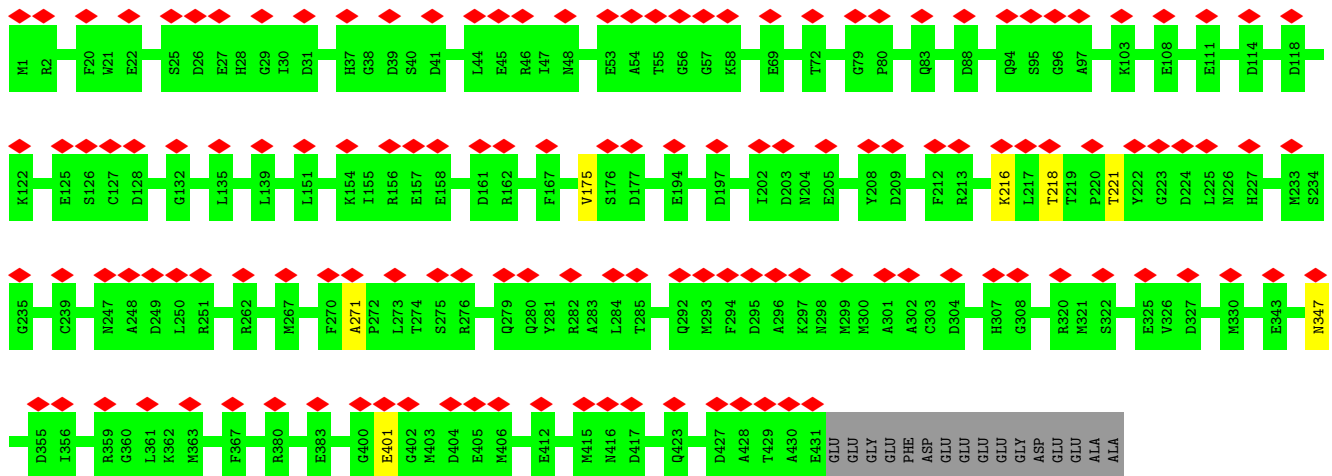


• Molecule 55: Tubulin beta chain

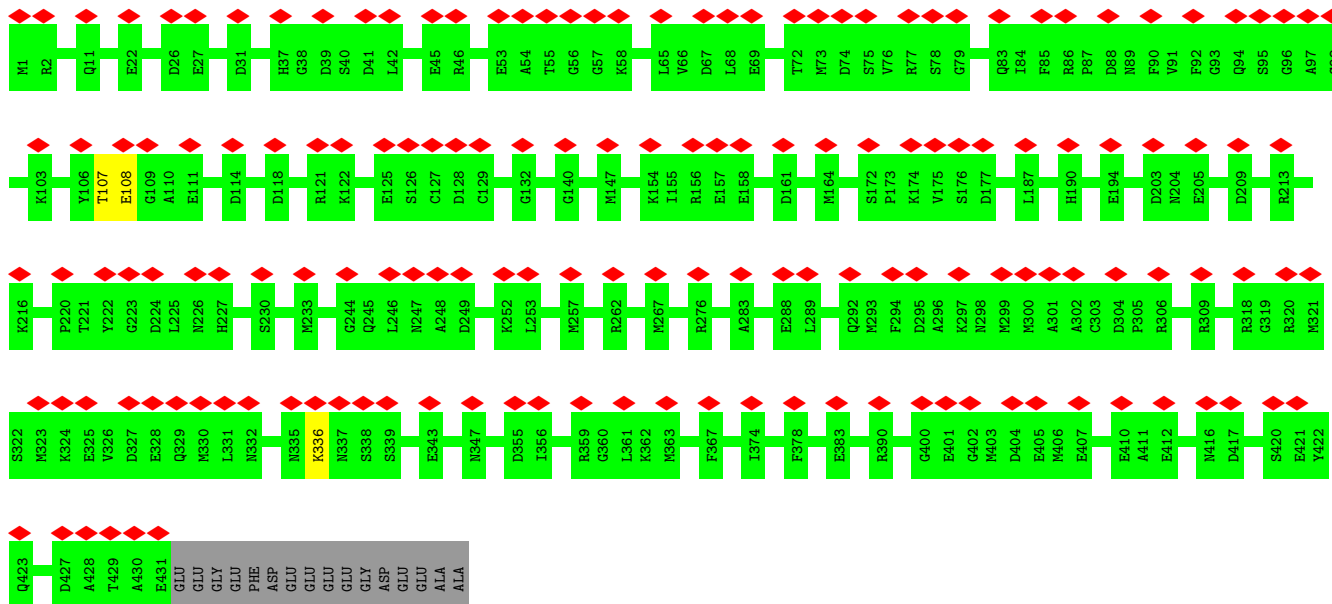




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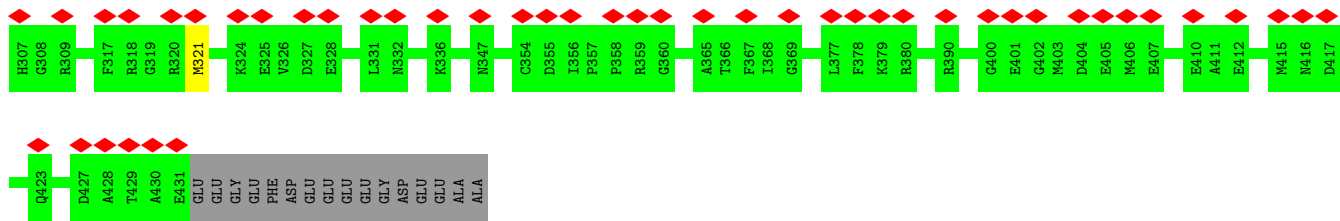


• Molecule 55: Tubulin beta chain



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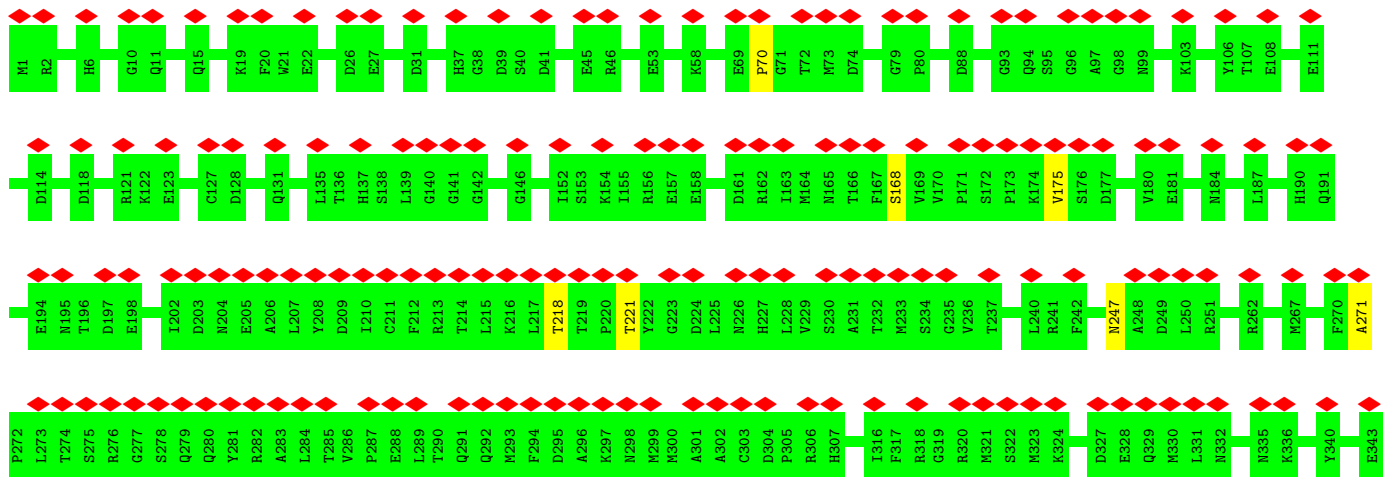


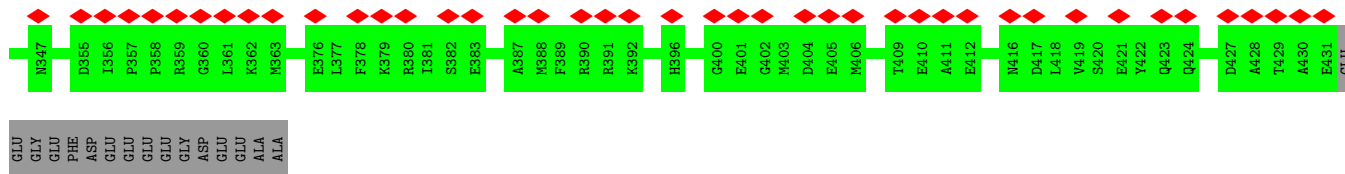


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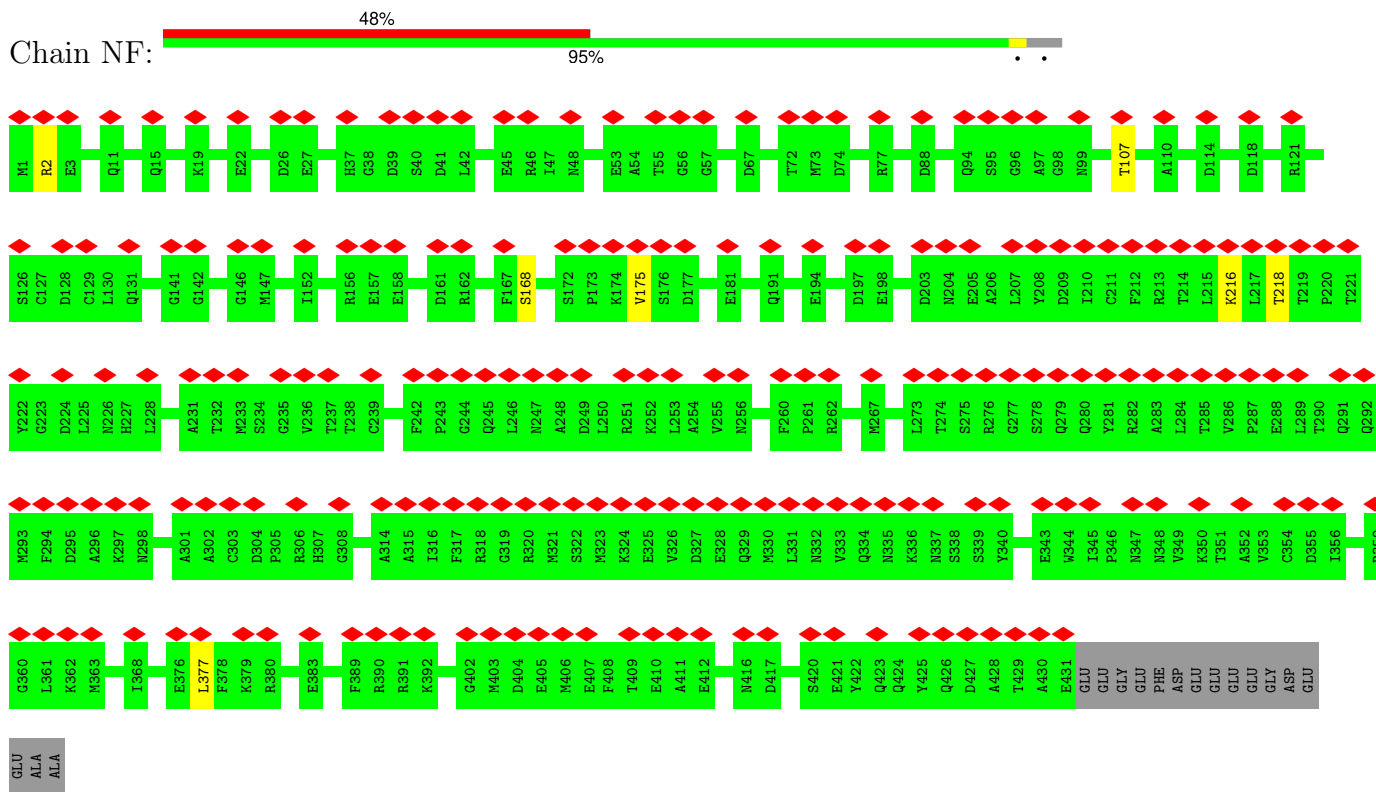


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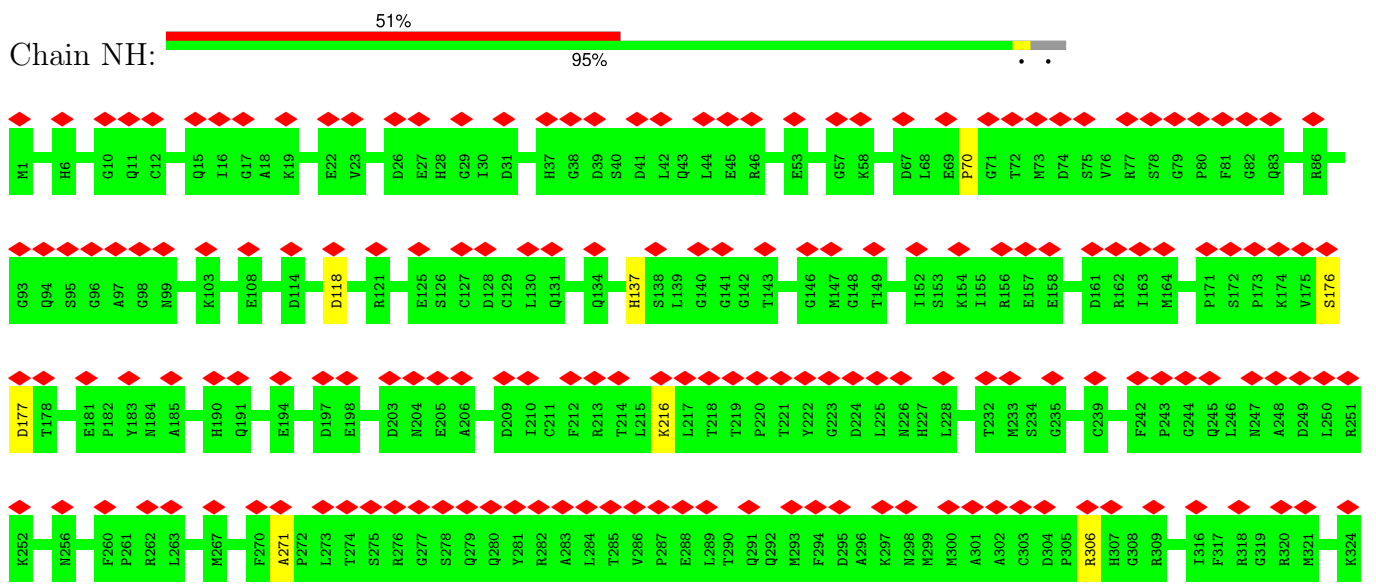


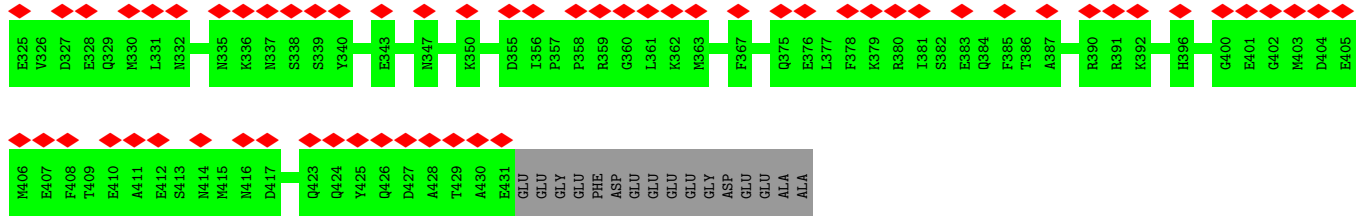


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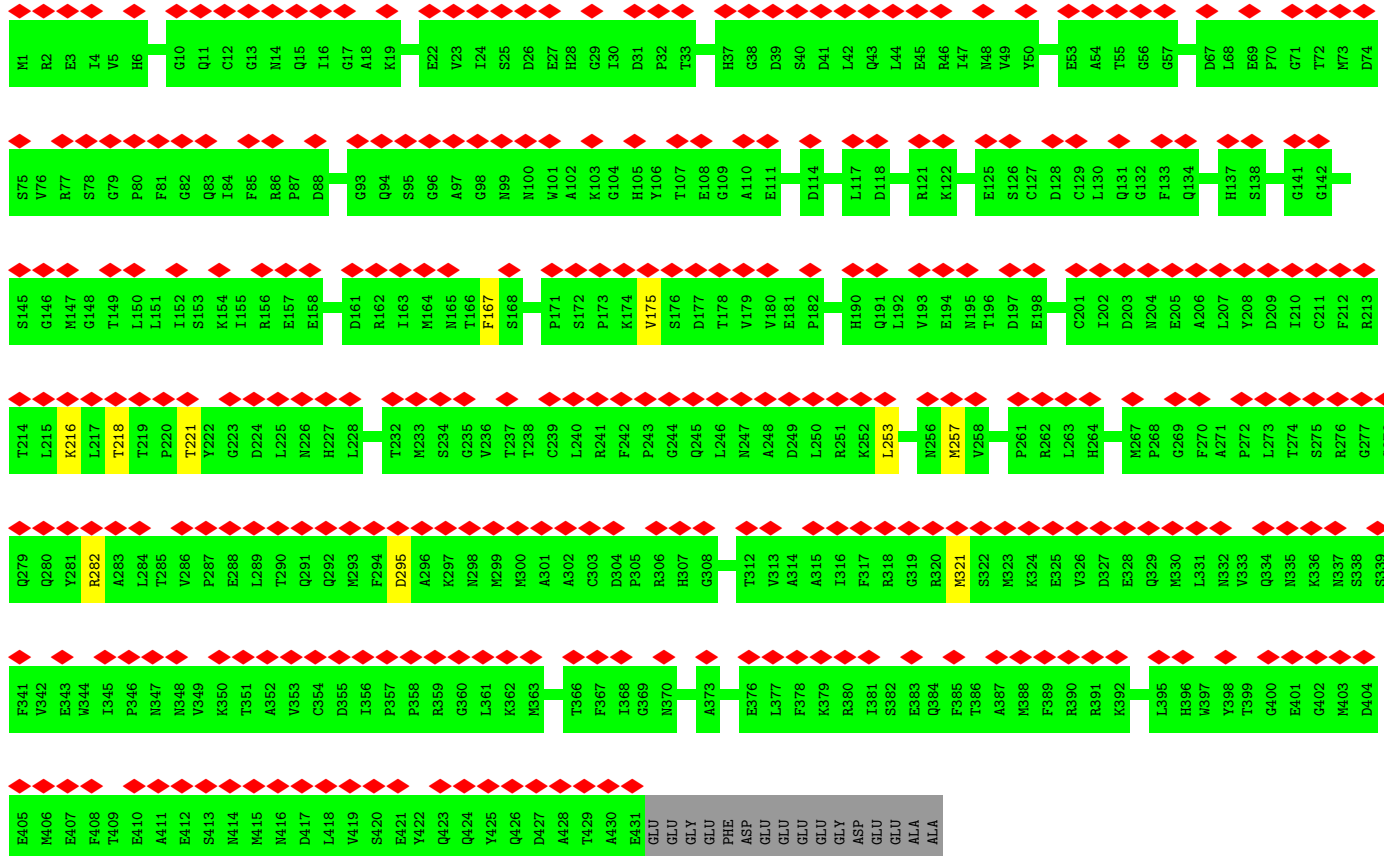


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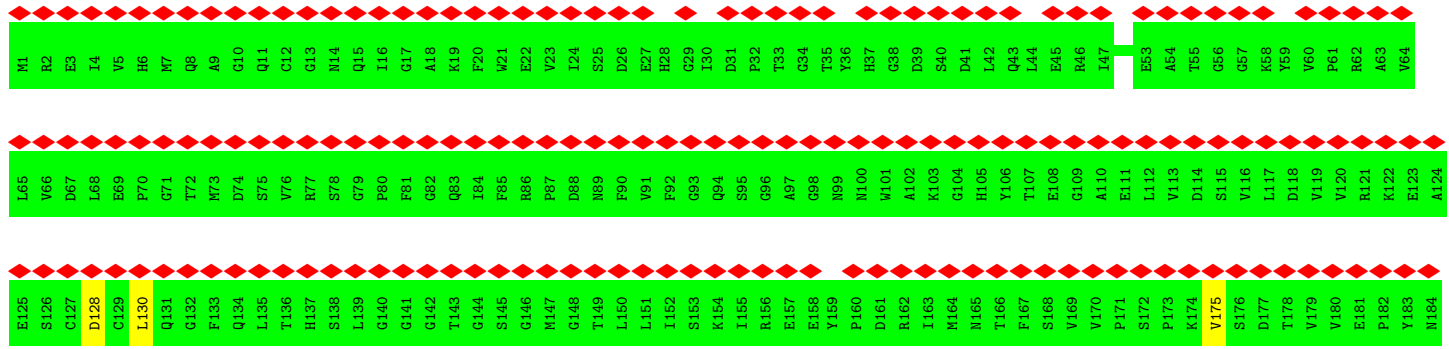
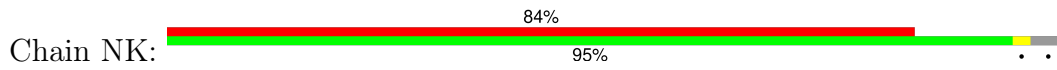


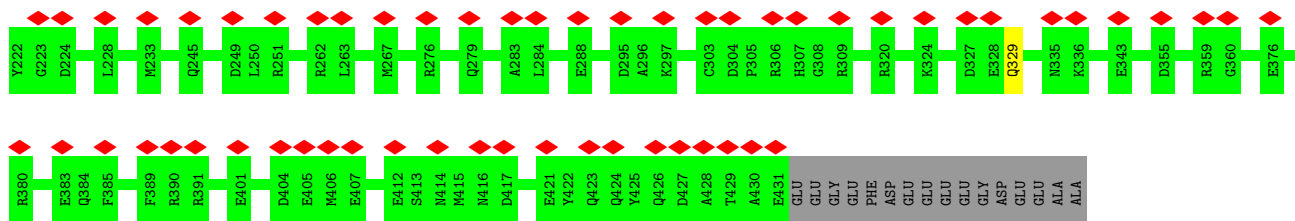


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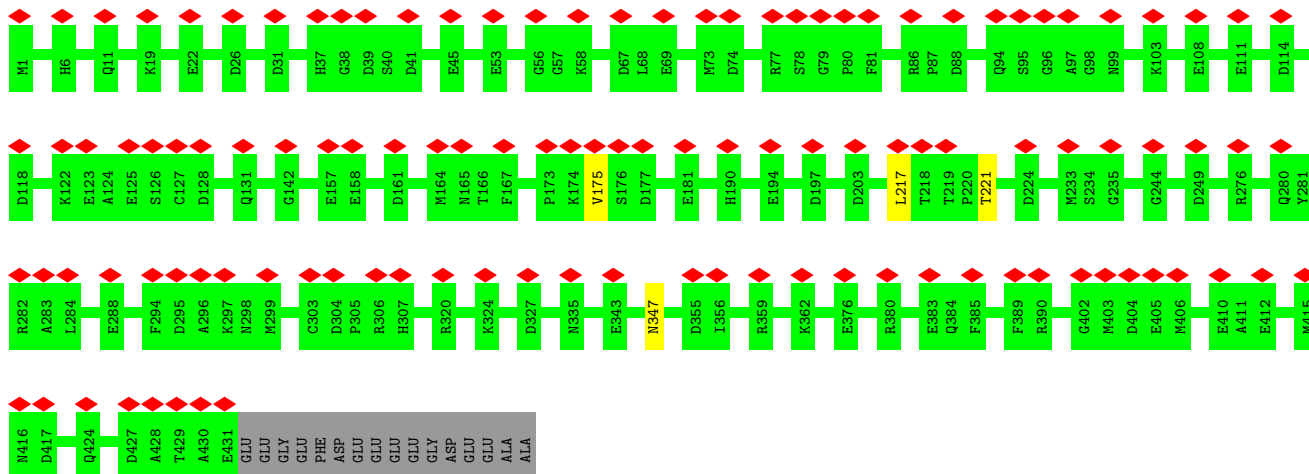


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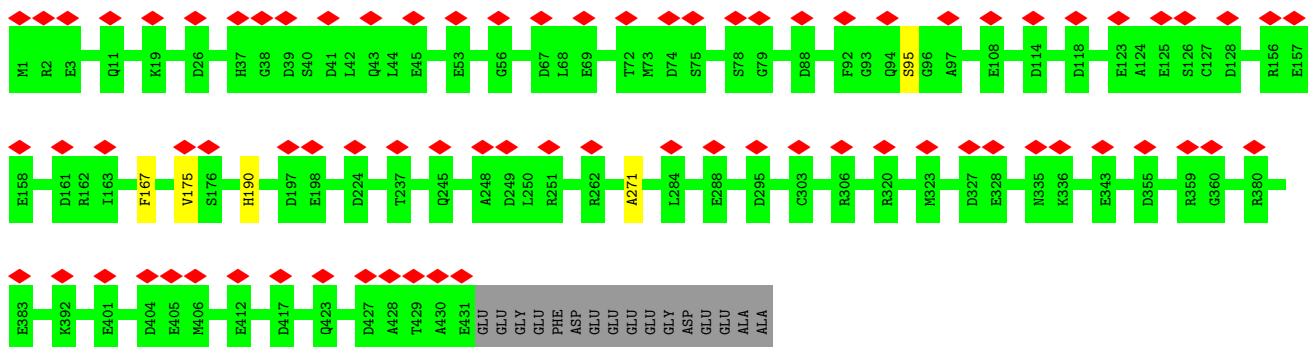




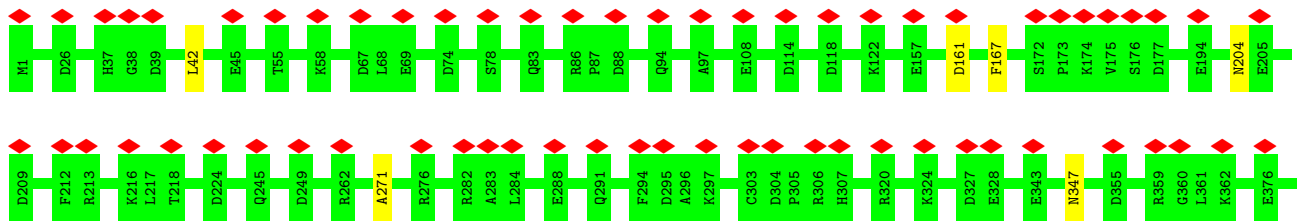
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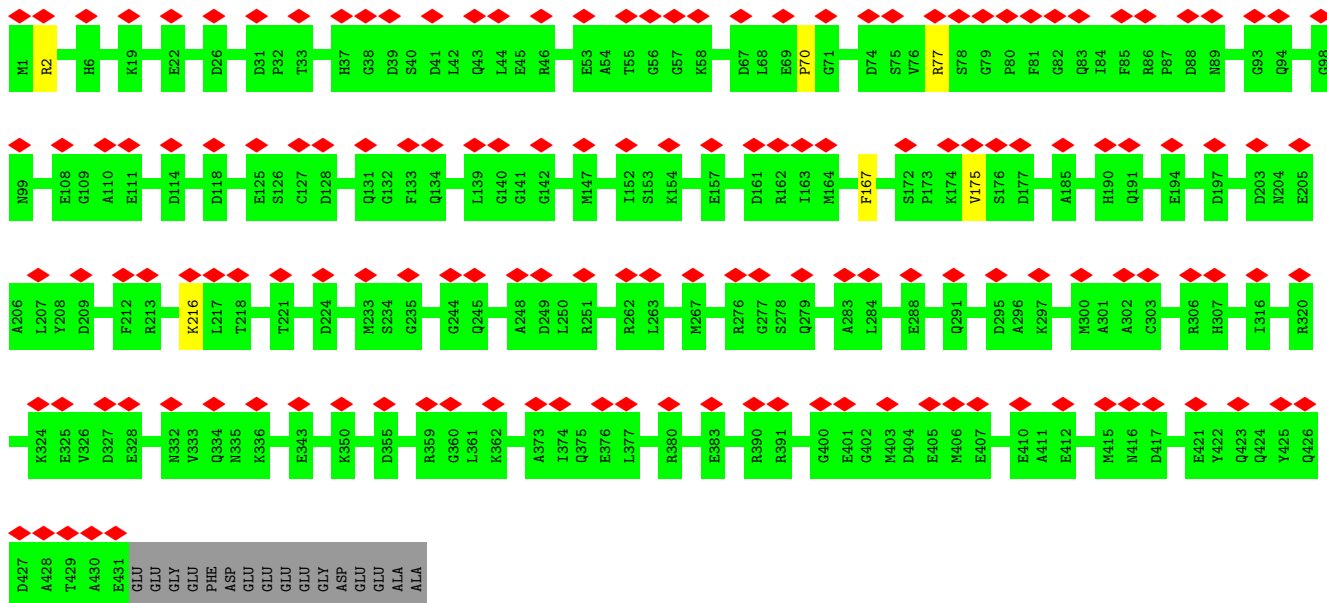


• Molecule 55: Tubulin beta chain

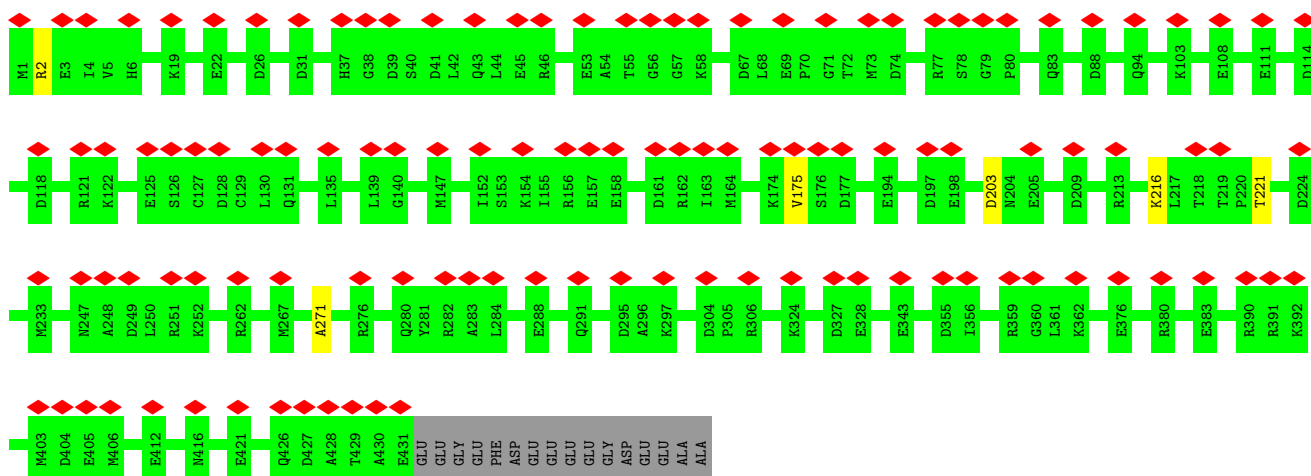




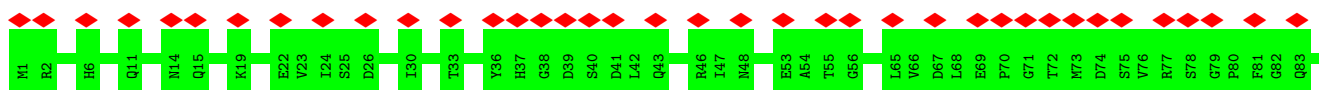
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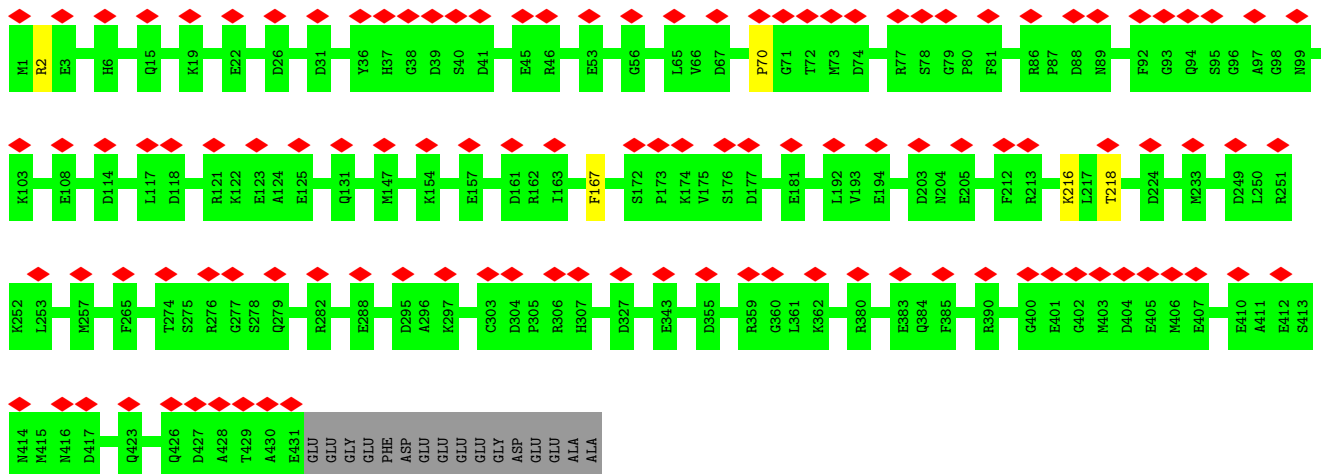
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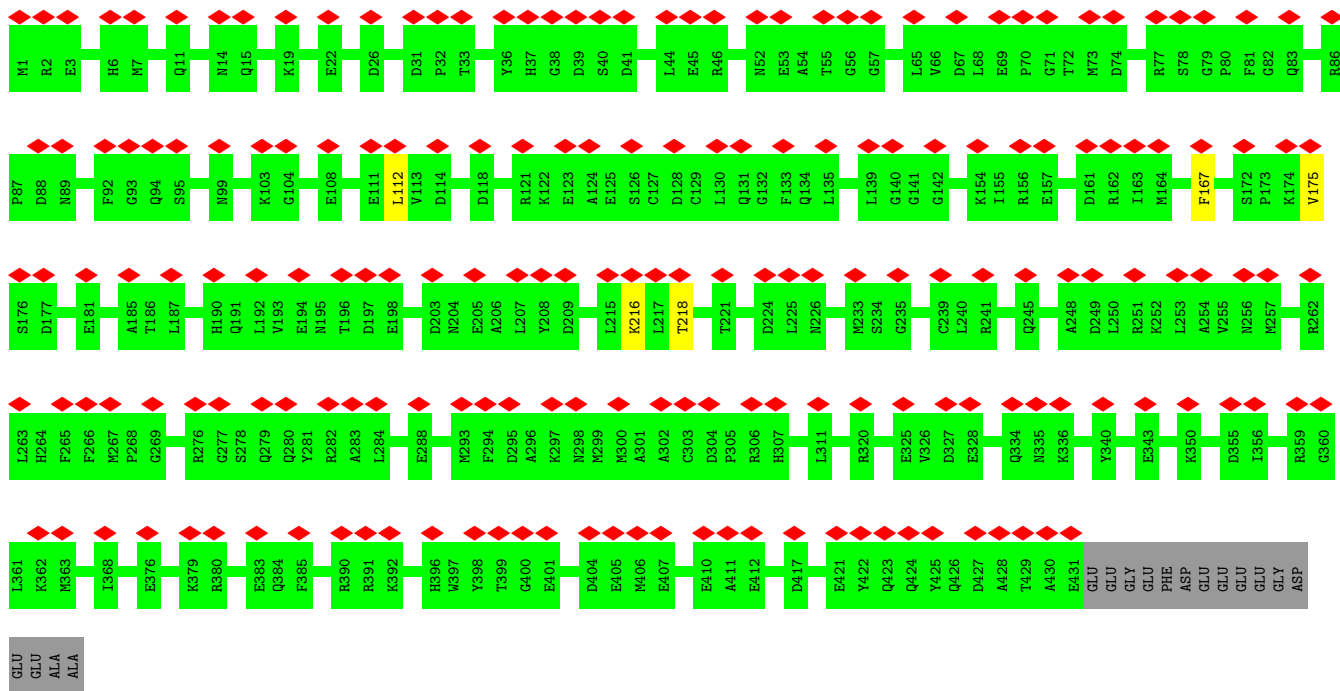
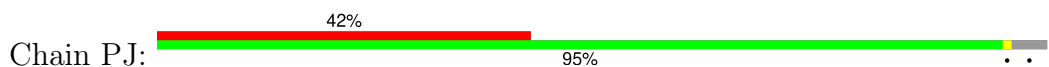
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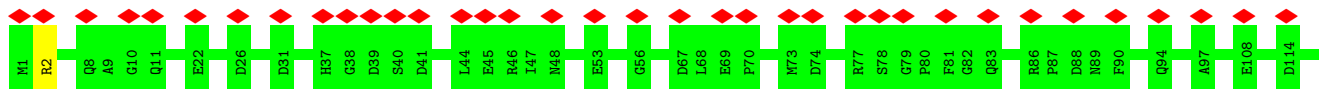
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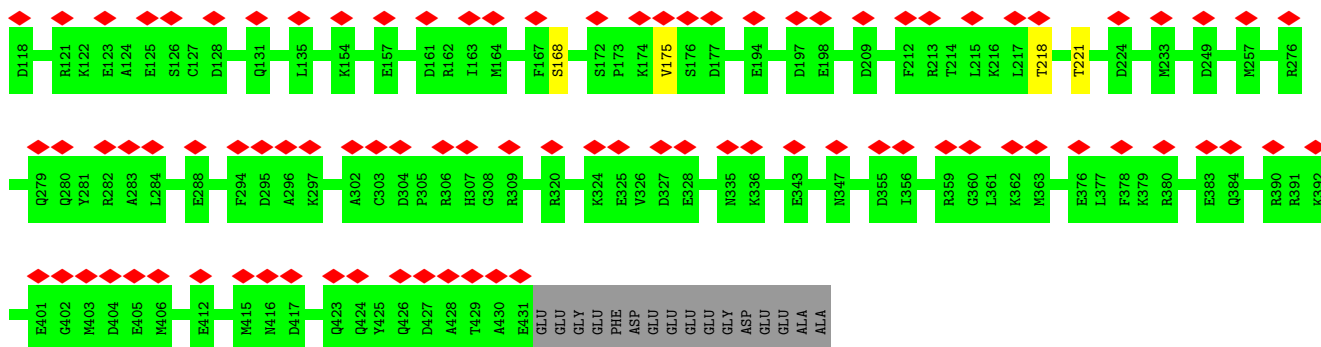


• Molecule 55: Tubulin beta chain

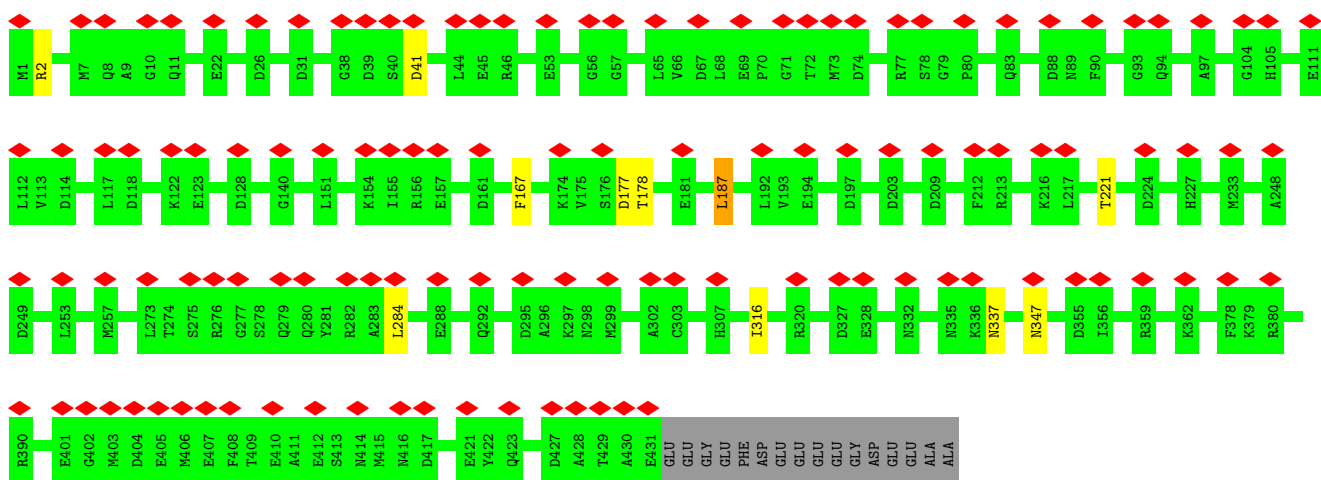


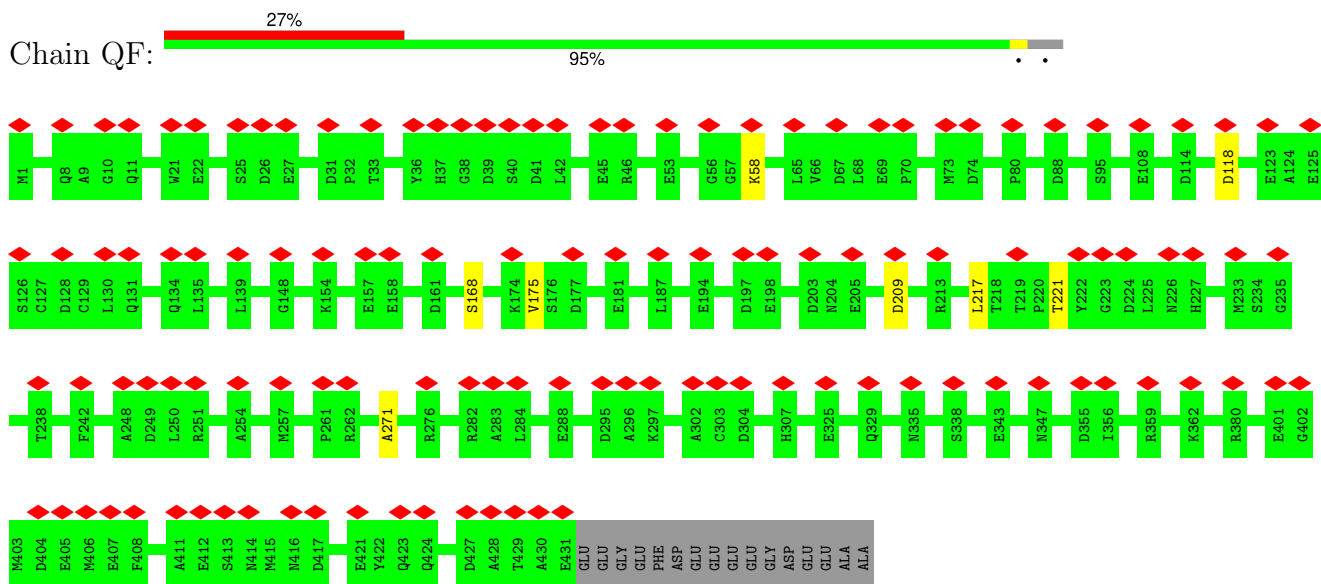
• Molecule 55: Tubulin beta chain



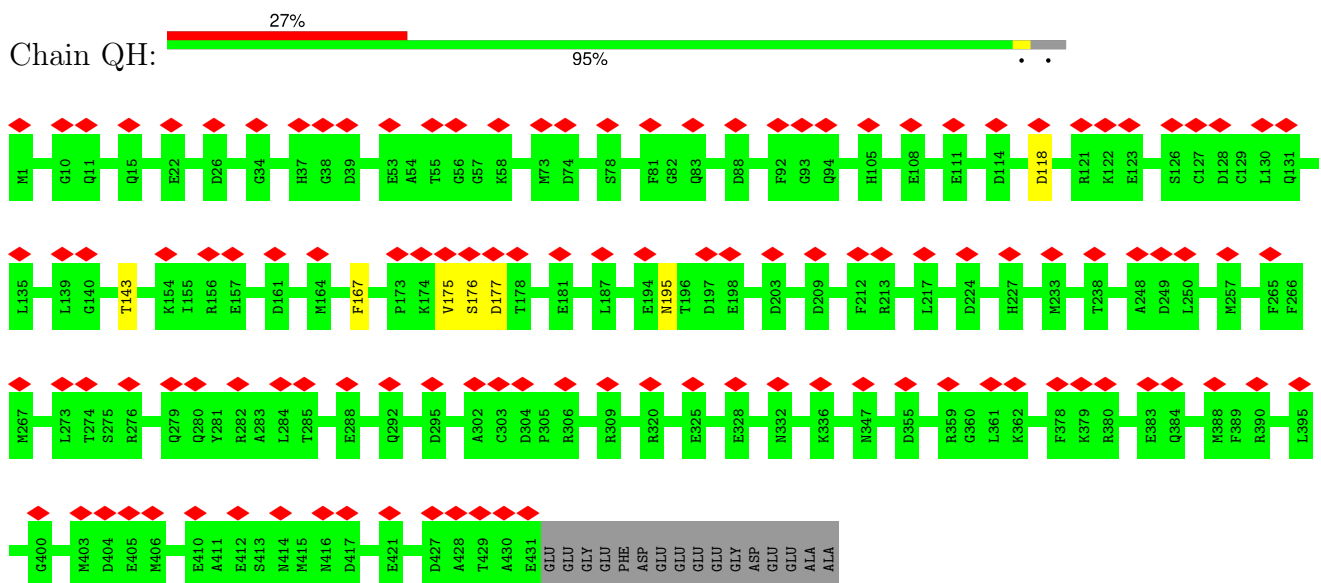


• Molecule 55: Tubulin beta chain

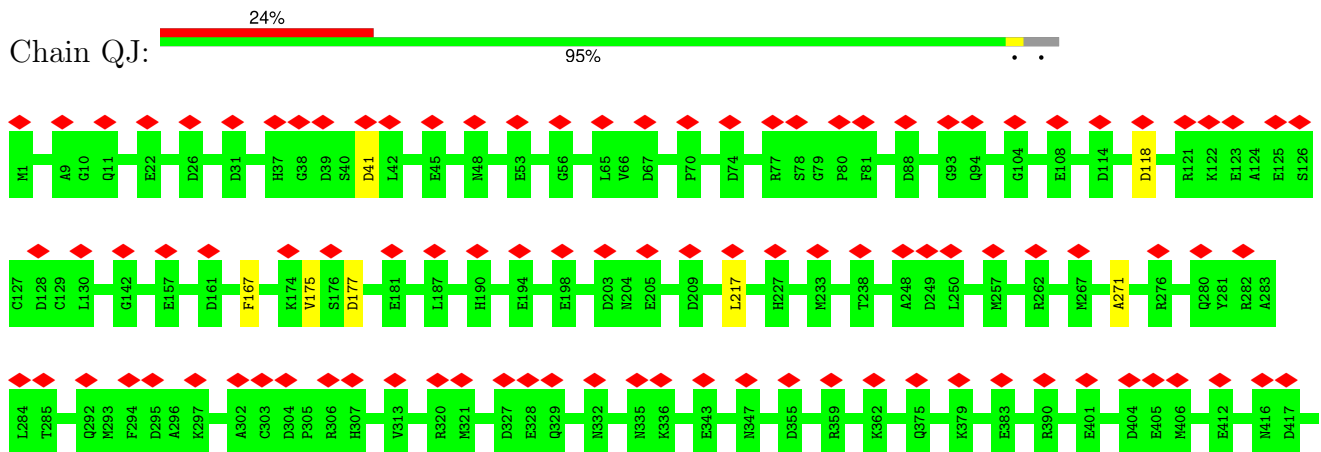


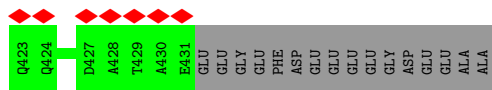


• Molecule 55: Tubulin beta chain

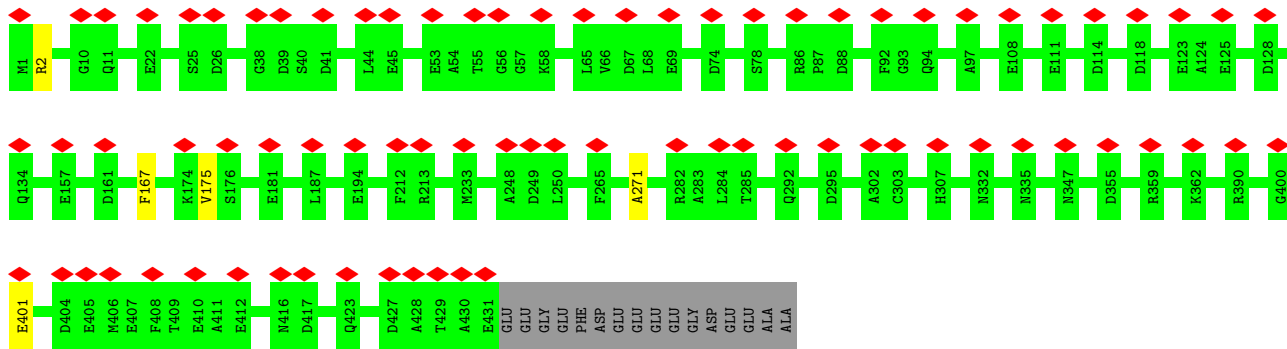


• Molecule 55: Tubulin beta chain

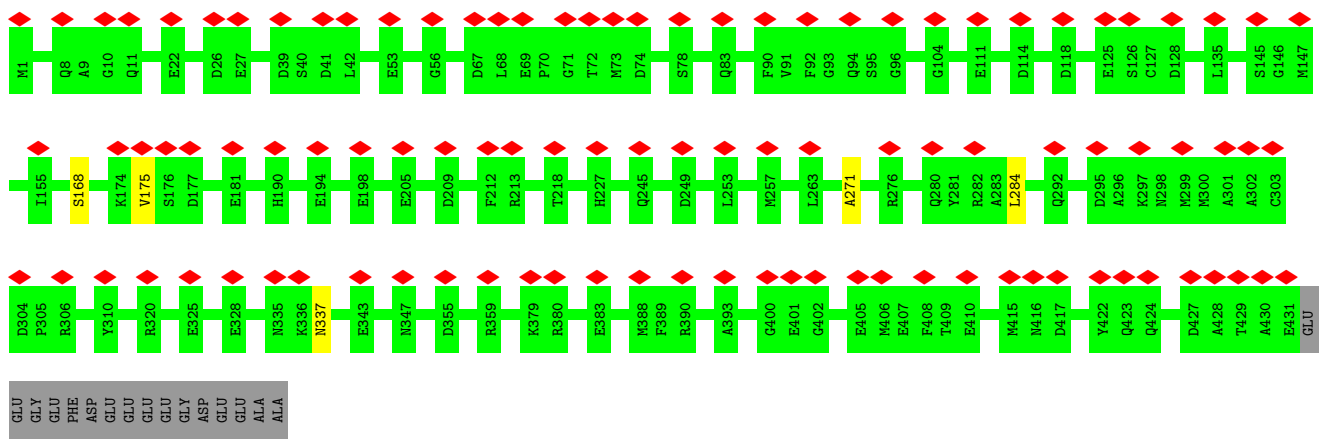




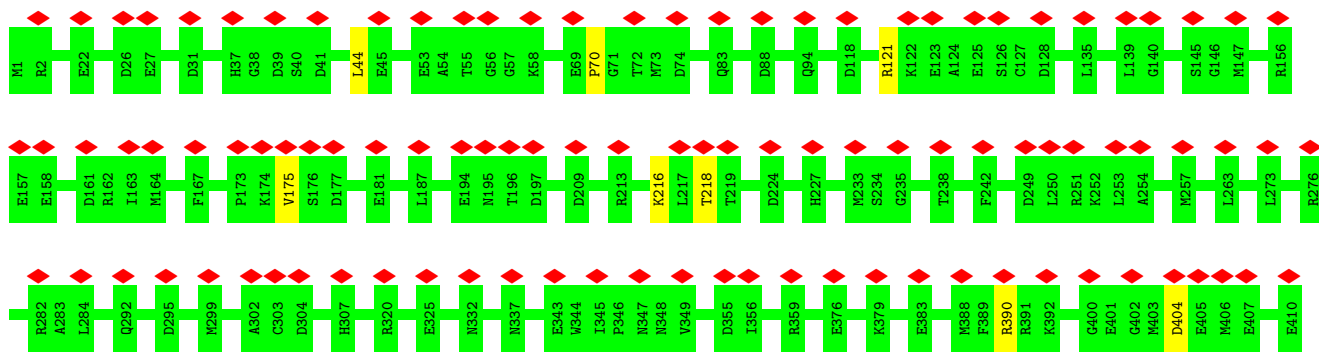
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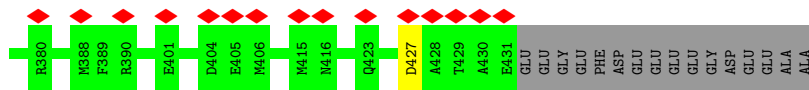


• Molecule 55: Tubulin beta chain

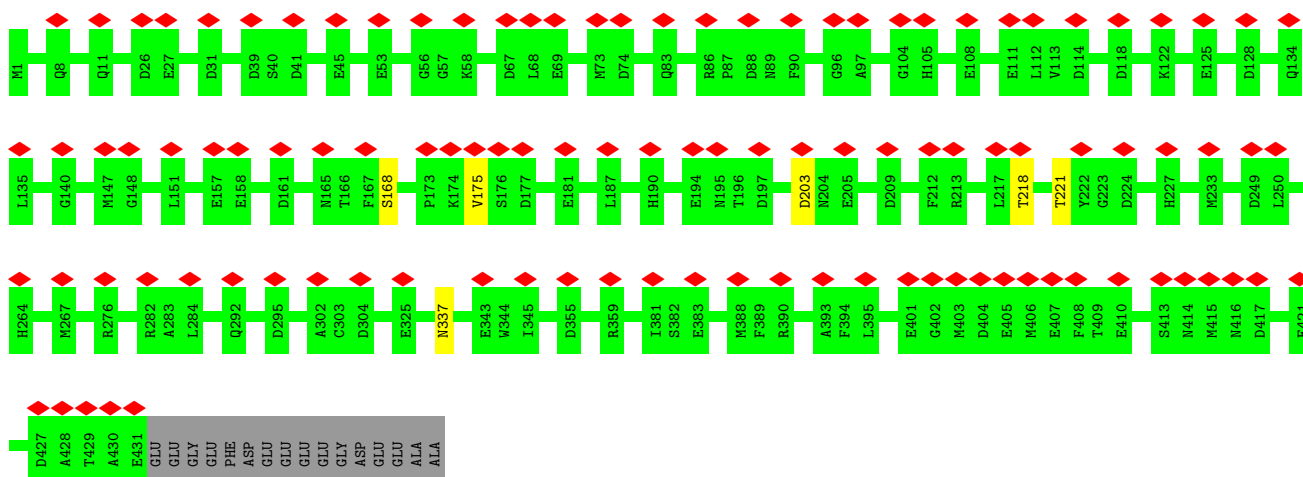


• Molecule 55: Tubulin beta chain

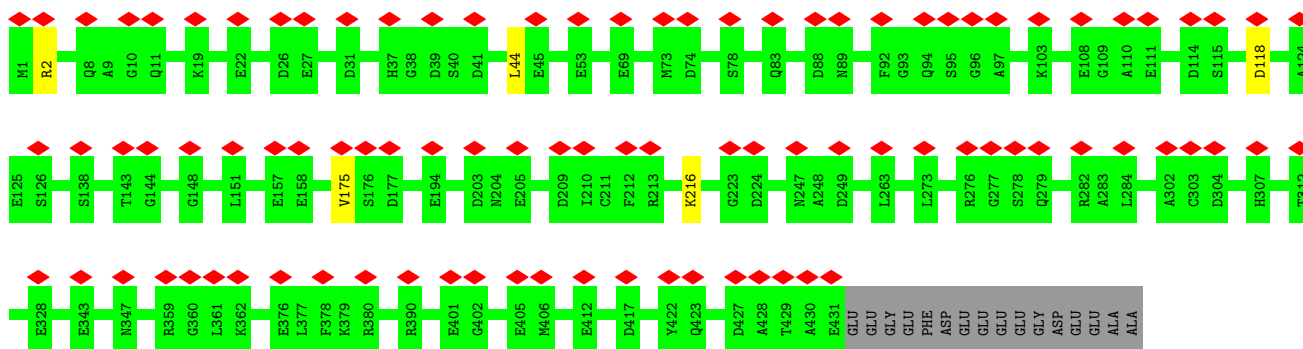




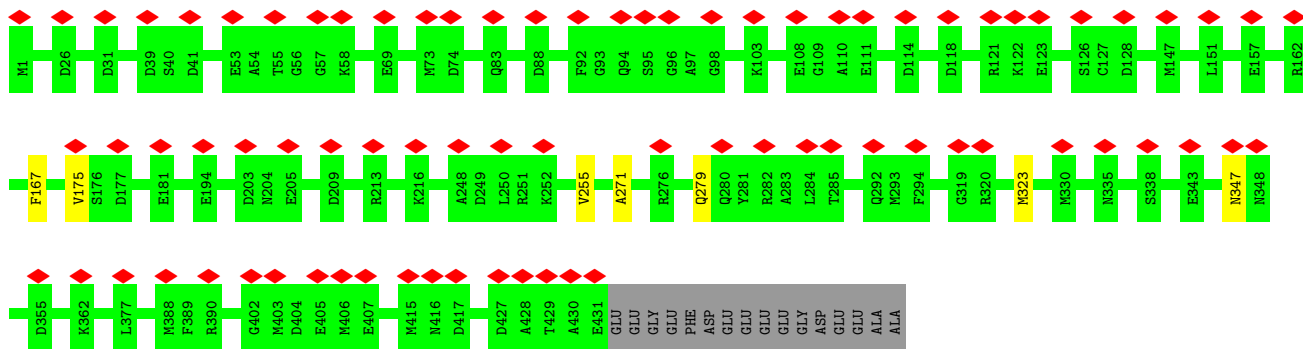
• Molecule 55: Tubulin beta chain



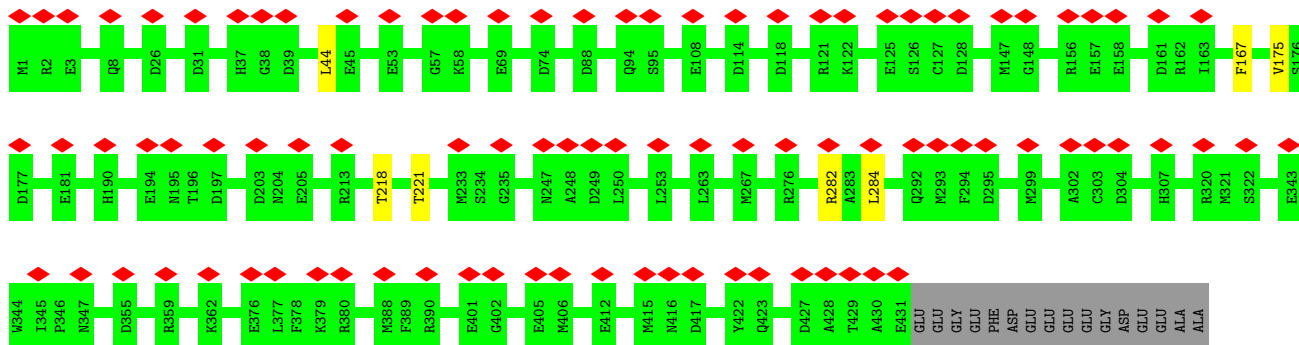
• Molecule 55: Tubulin beta chain



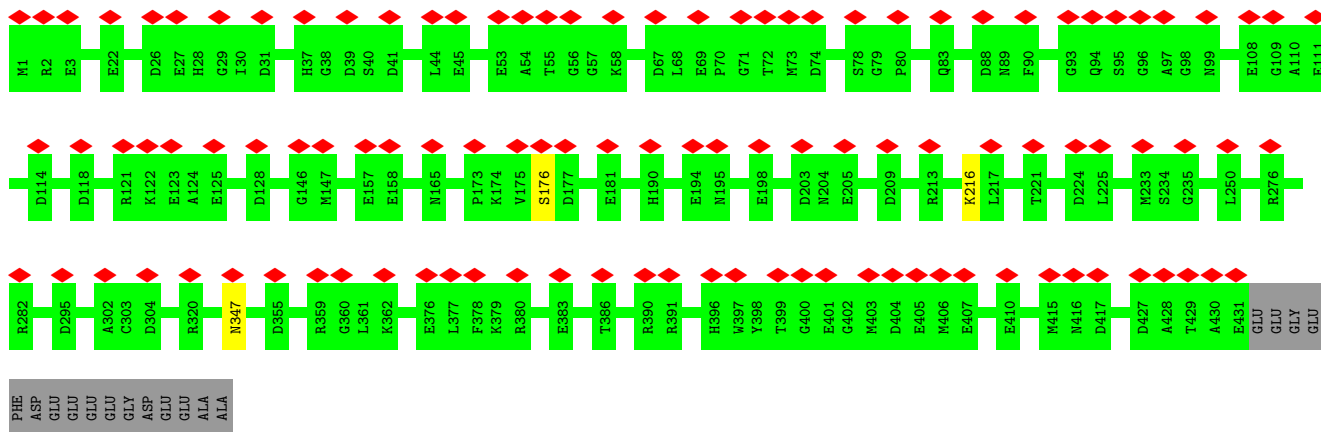
• Molecule 55: Tubulin beta chain



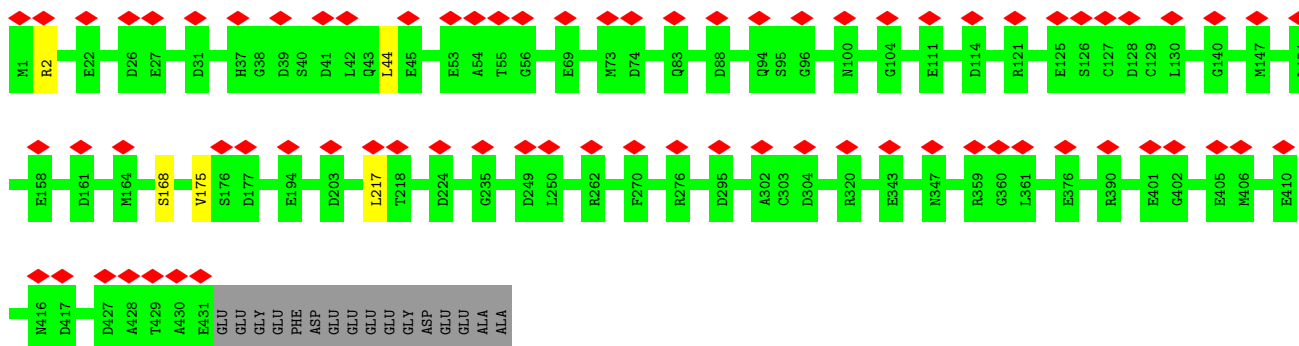
• Molecule 55: Tubulin beta chain



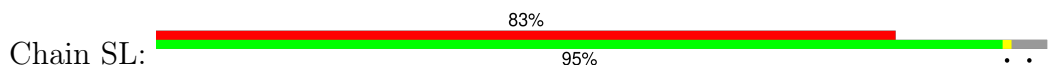
• Molecule 55: Tubulin beta chain

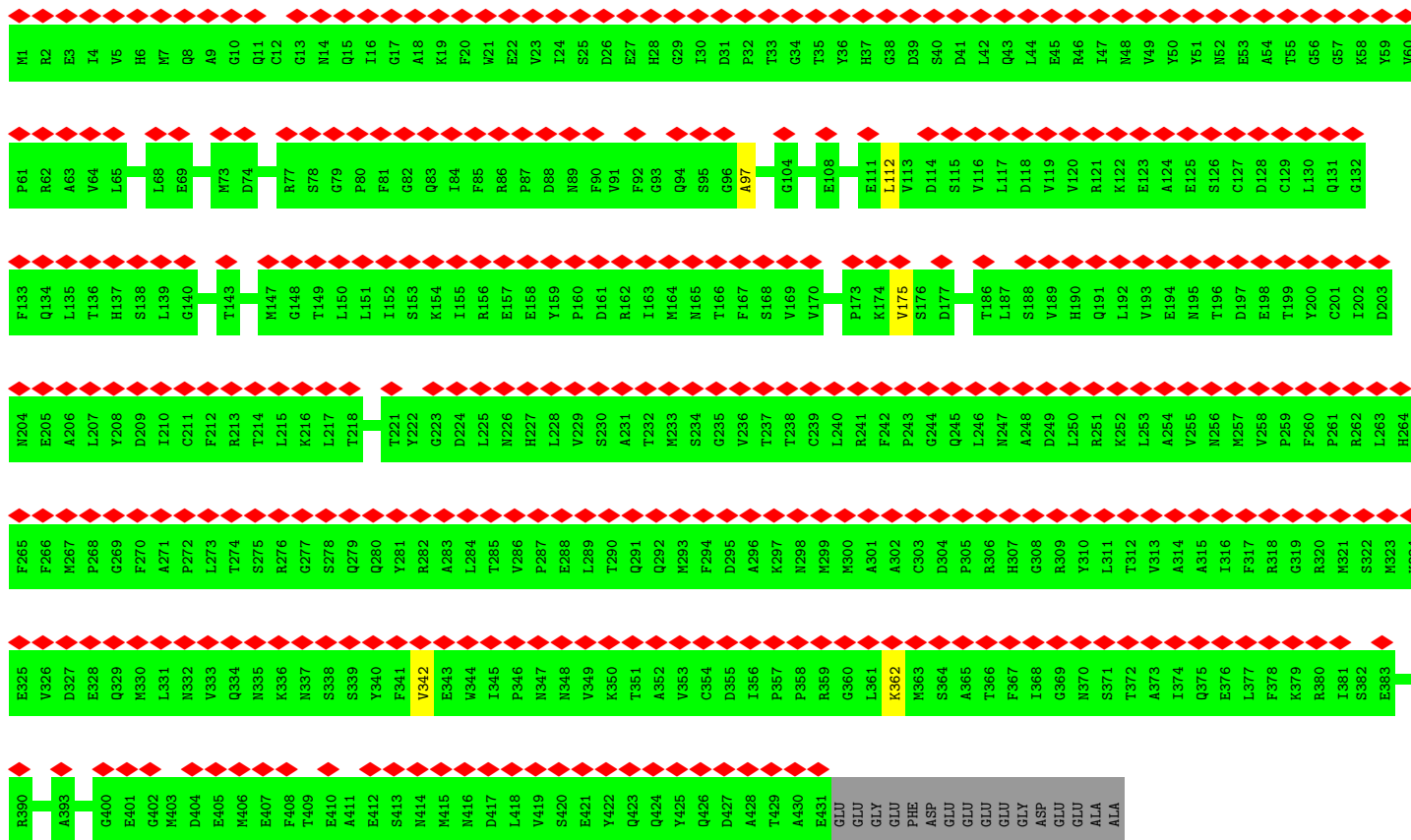


• Molecule 55: Tubulin beta chain

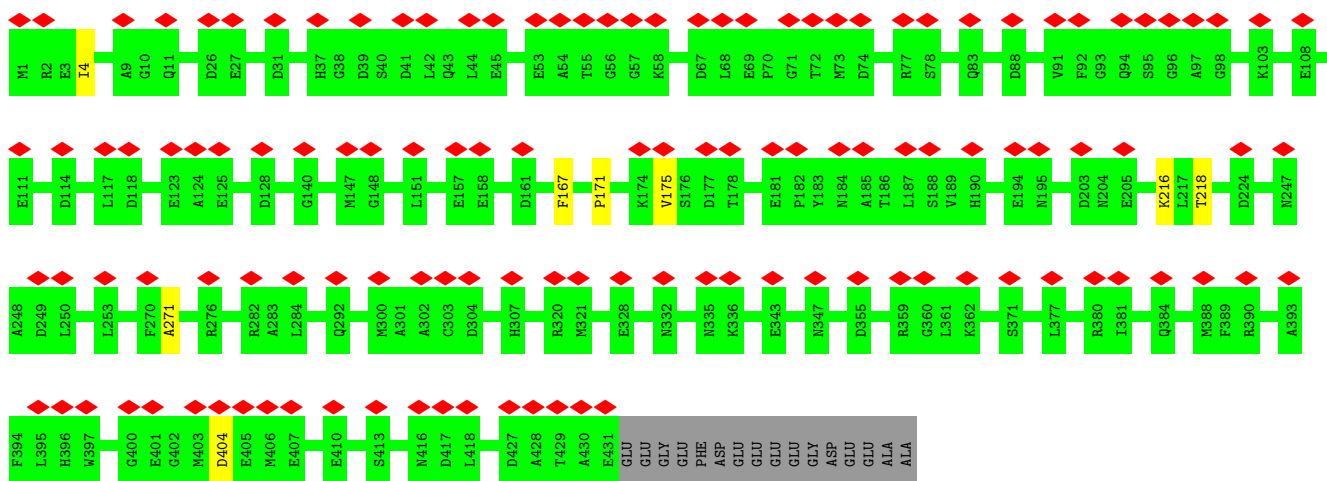


• Molecule 55: Tubulin beta chain

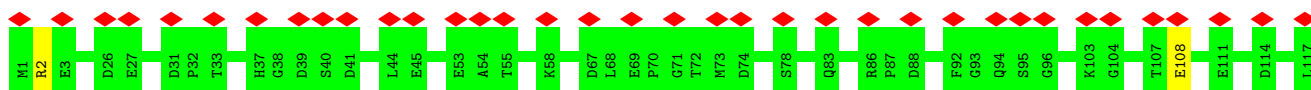


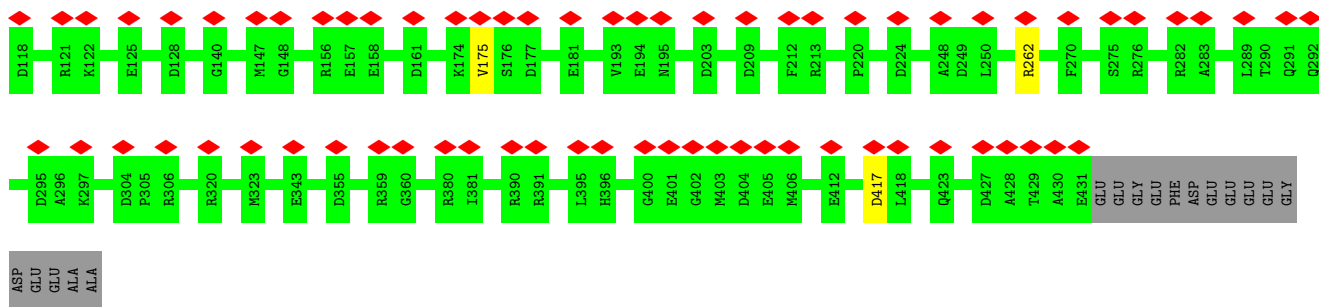


• Molecule 55: Tubulin beta chain

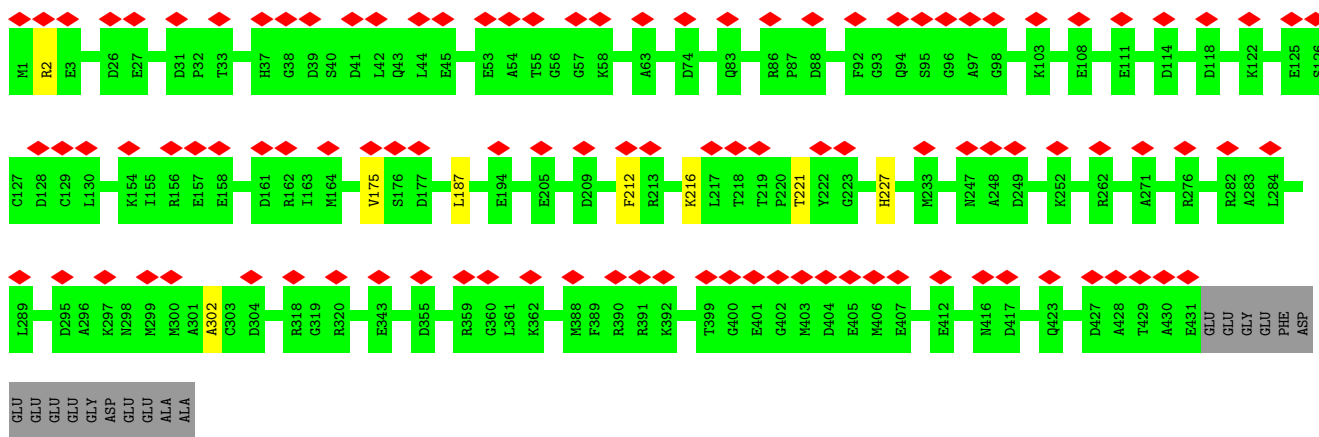


• Molecule 55: Tubulin beta chain

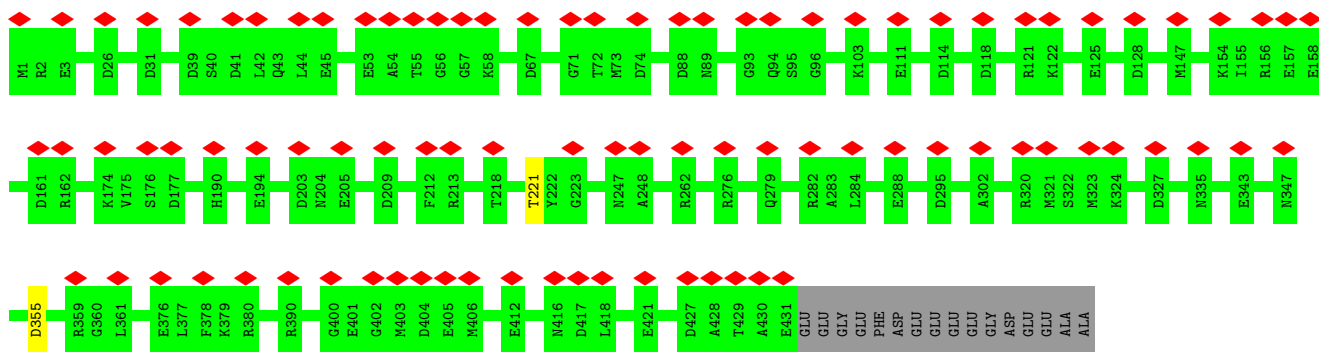




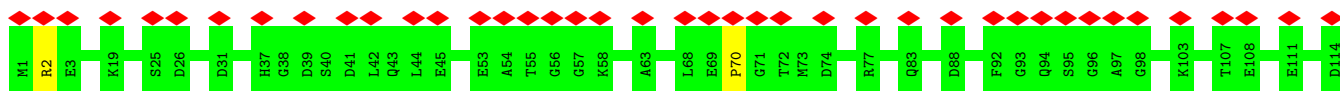
• Molecule 55: Tubulin beta chain

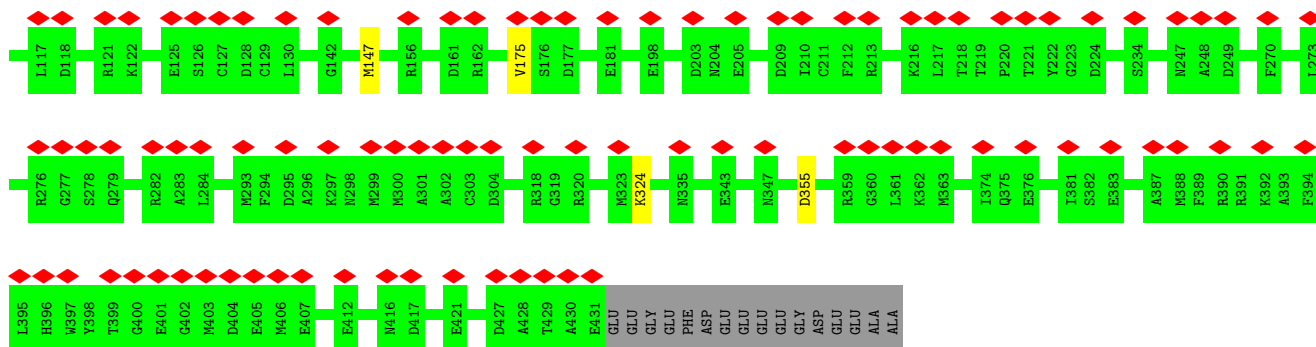


• Molecule 55: Tubulin beta chain

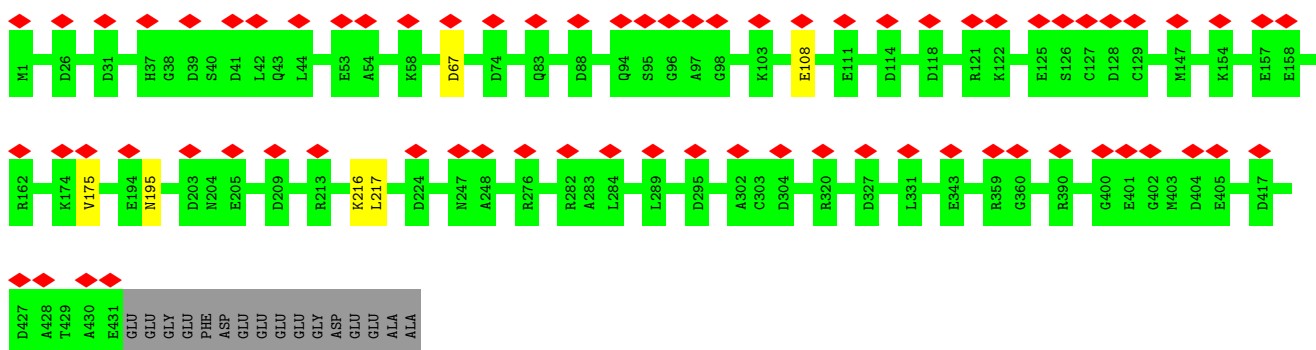


• Molecule 55: Tubulin beta chain

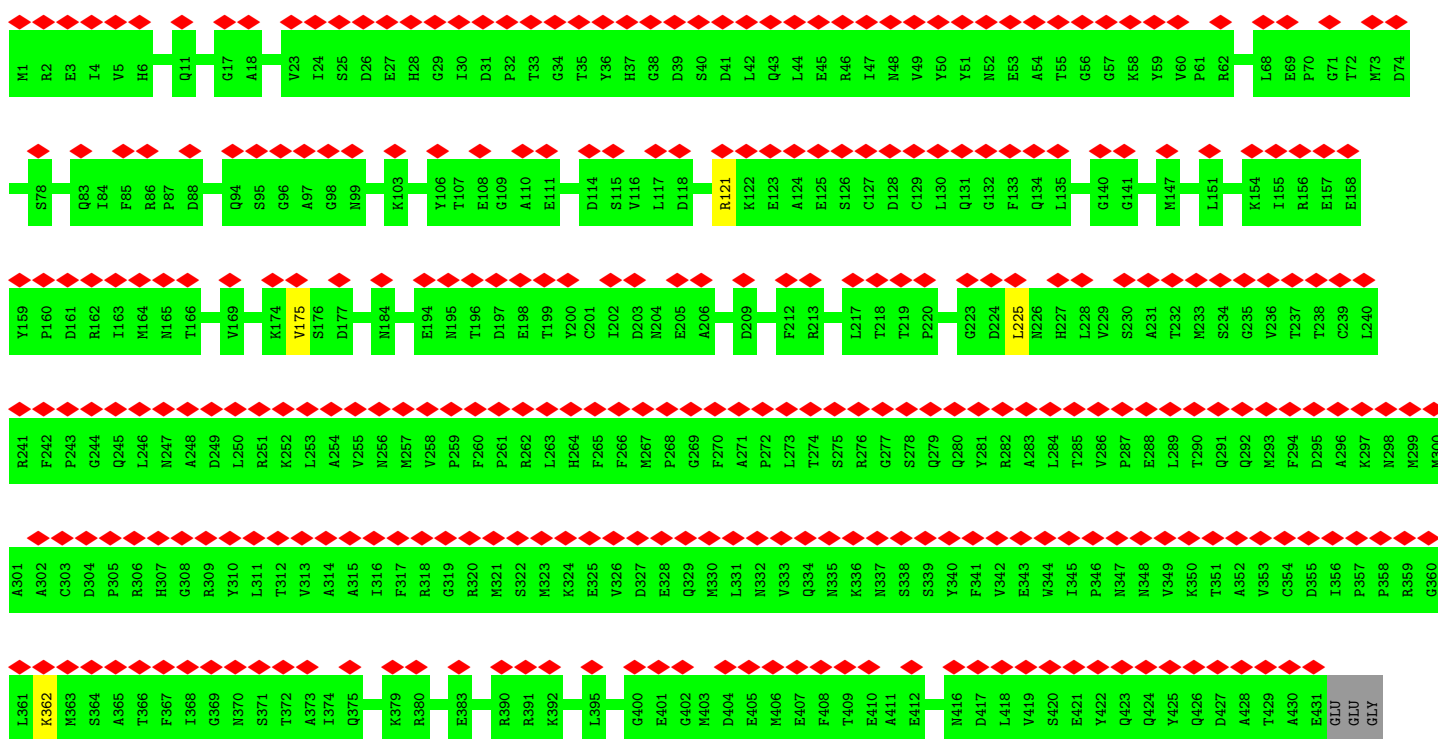




• Molecule 55: Tubulin beta chain

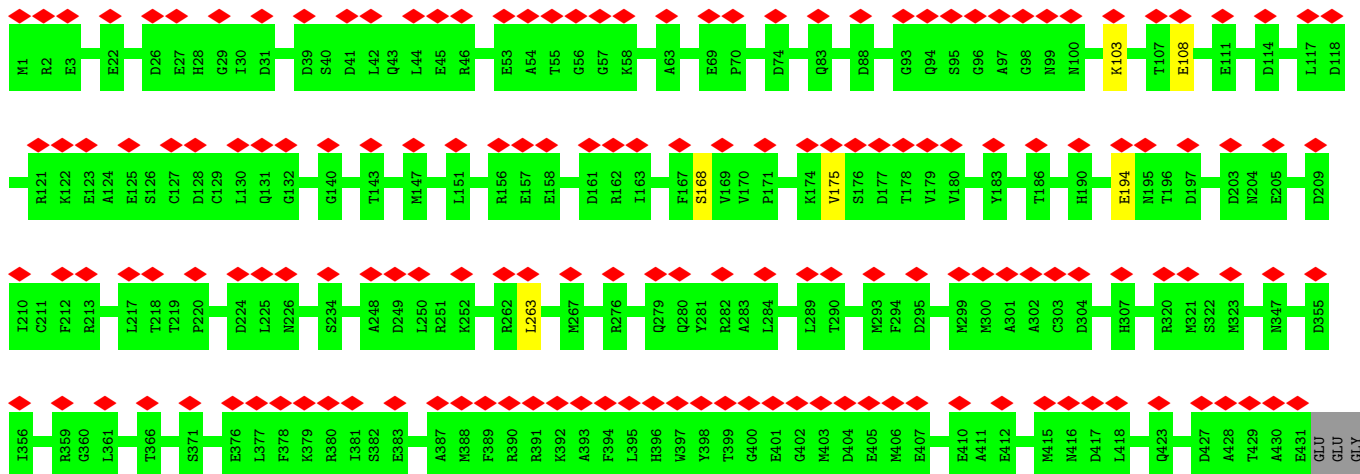


• Molecule 55: Tubulin beta chain



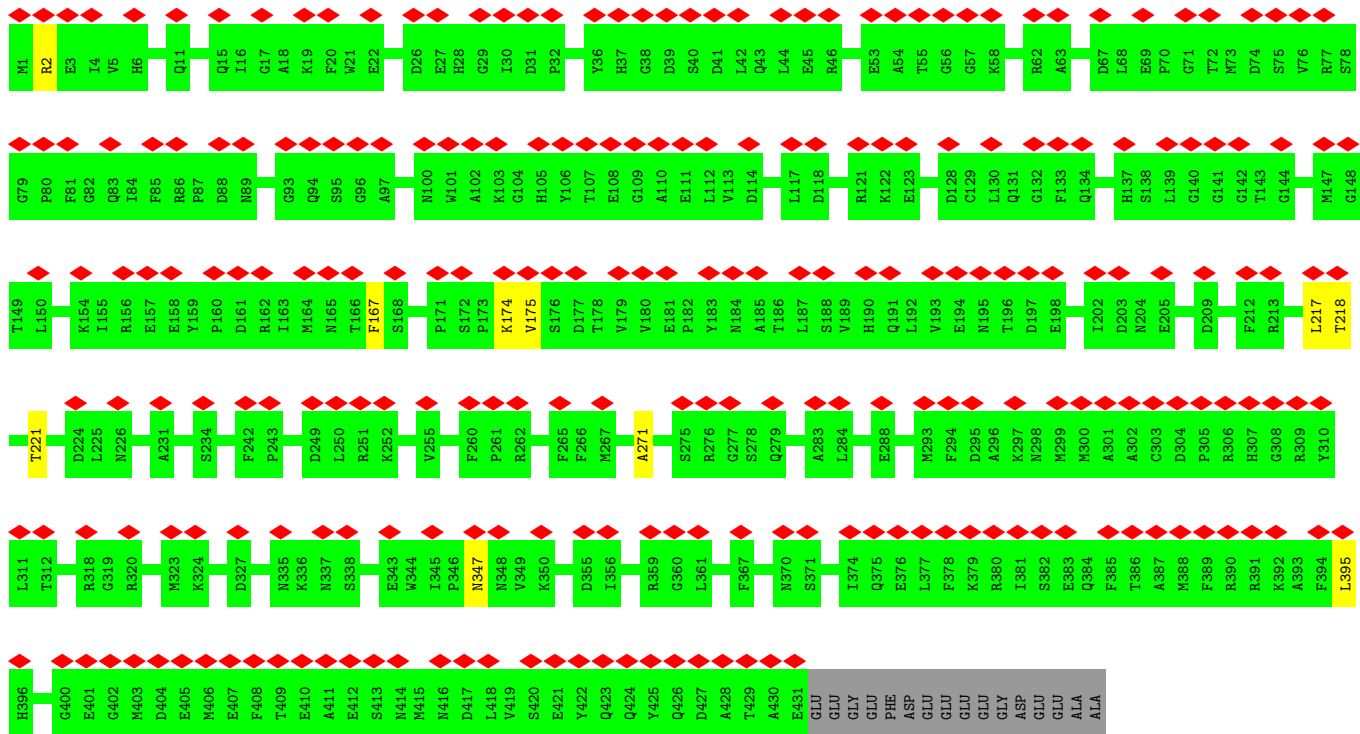
GLU
PHE
ASP
GLU
GLU
GLU
GLY
ASP
GLU
GLU
ALA
ALA

• Molecule 55: Tubulin beta chain

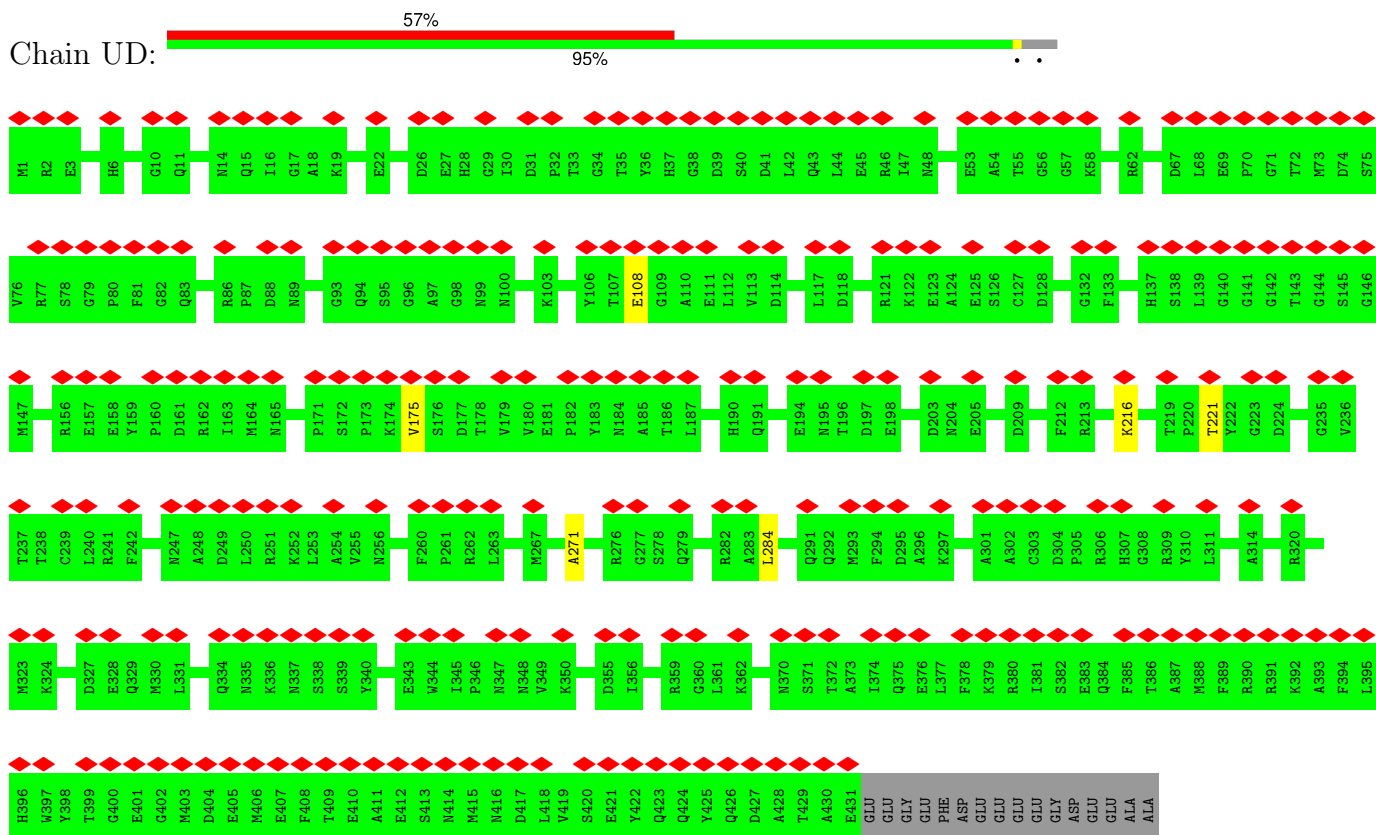


GLU
PHE
ASP
GLU
GLU
GLU
GLY
ASP
GLU
GLU
ALA
ALA

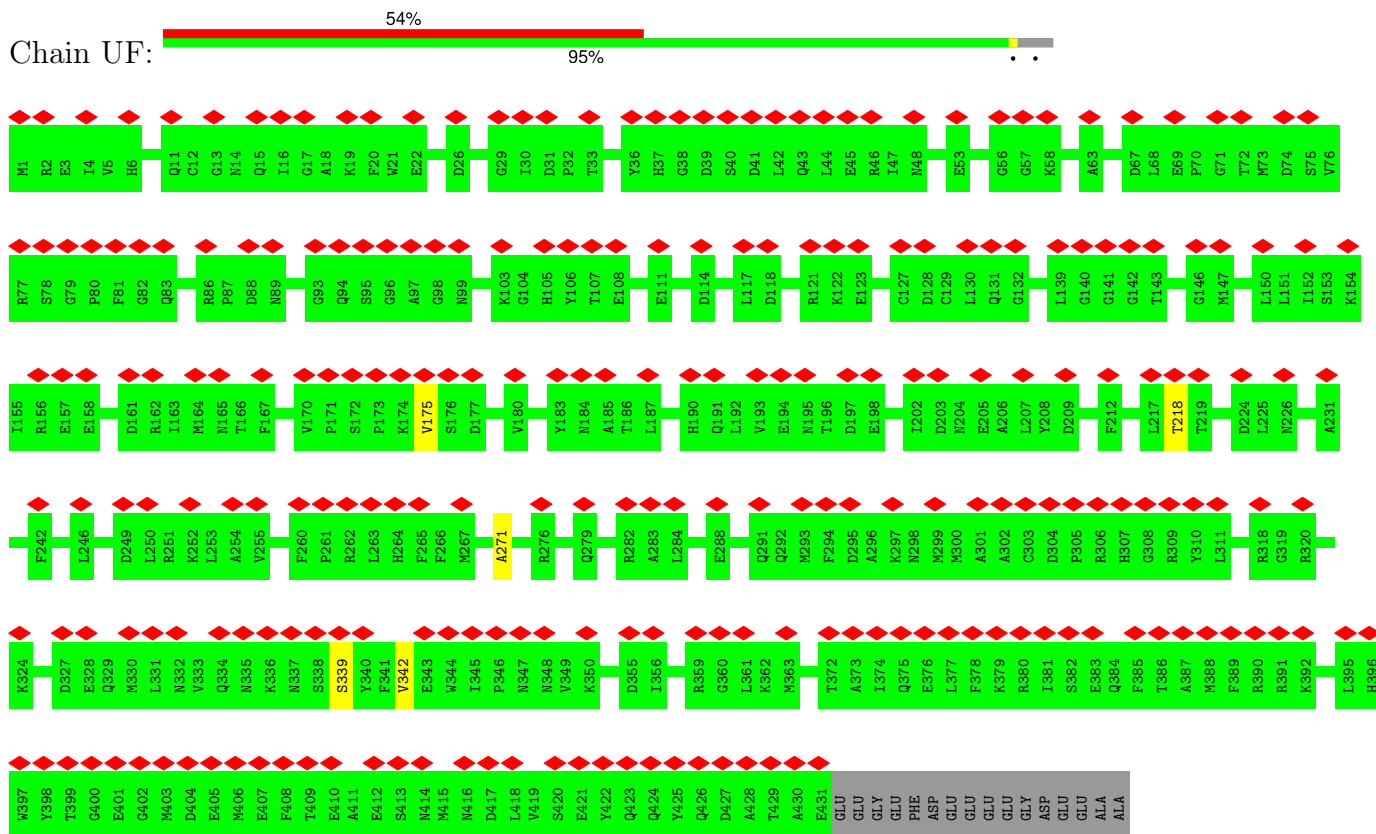
• Molecule 55: Tubulin beta chain



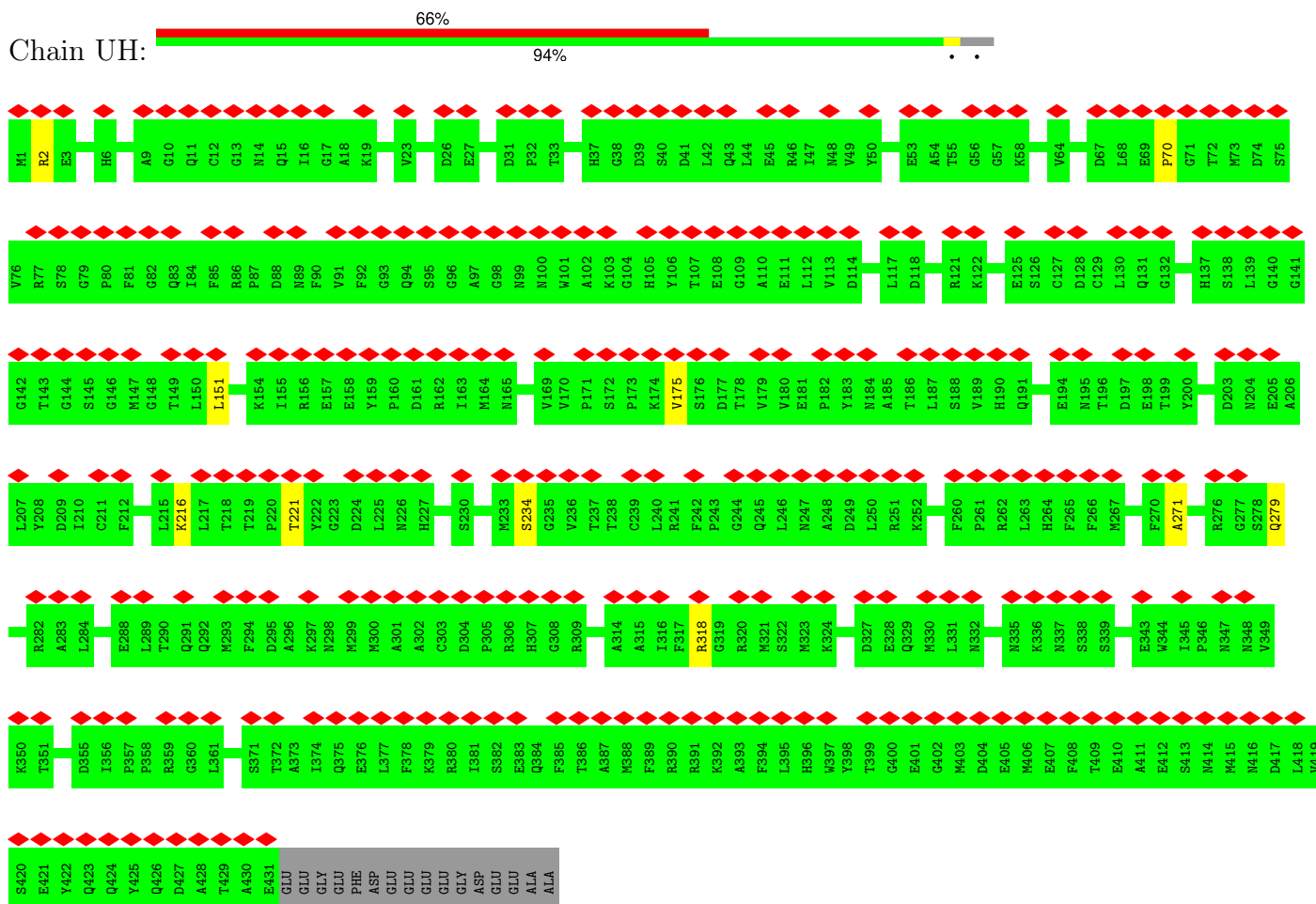
• Molecule 55: Tubulin beta chain



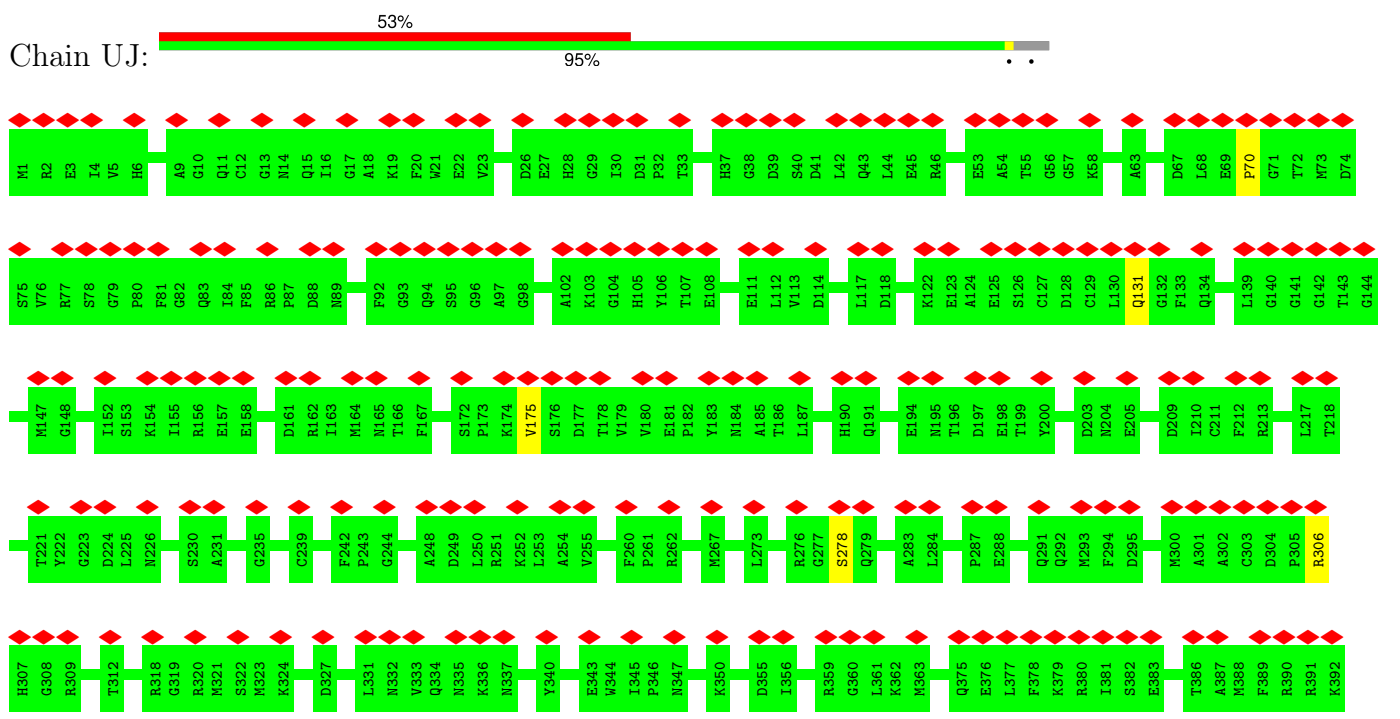
• Molecule 55: Tubulin beta chain

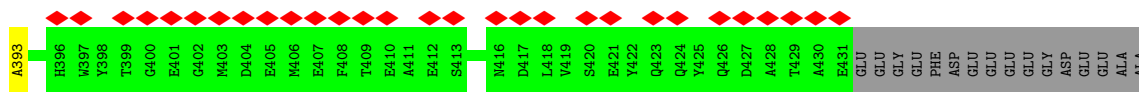


• Molecule 55: Tubulin beta chain

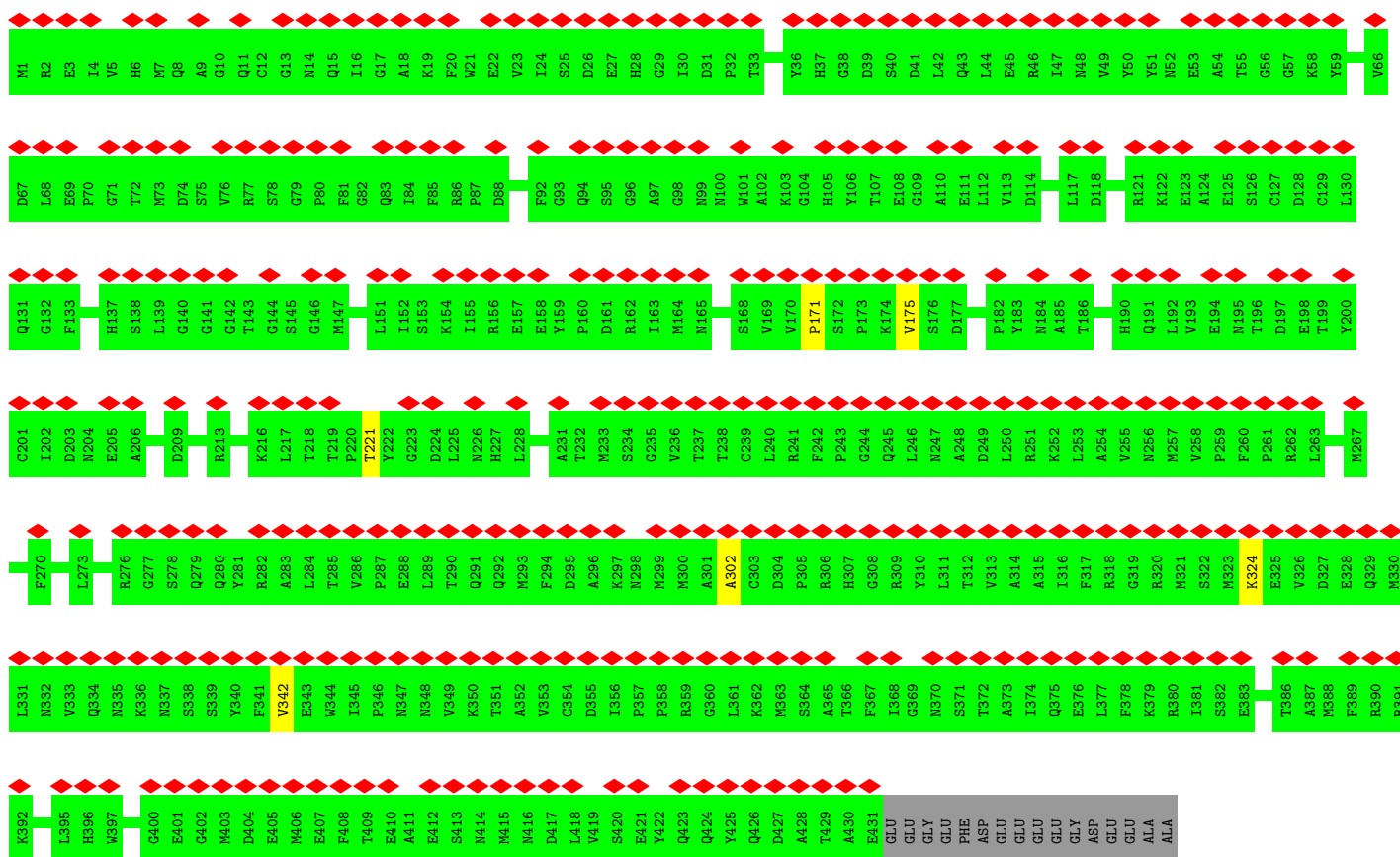
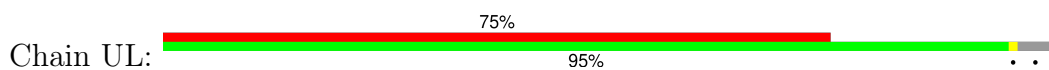


• Molecule 55: Tubulin beta chain

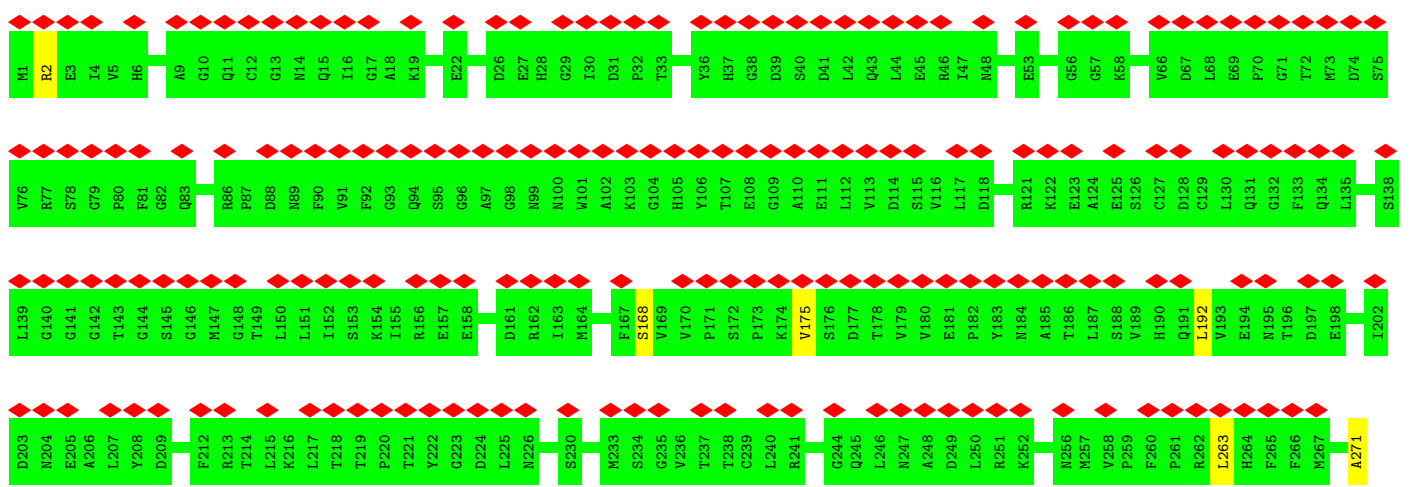
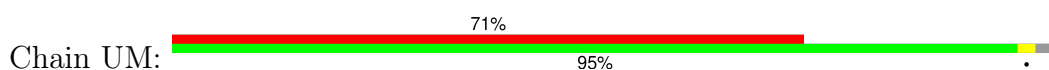


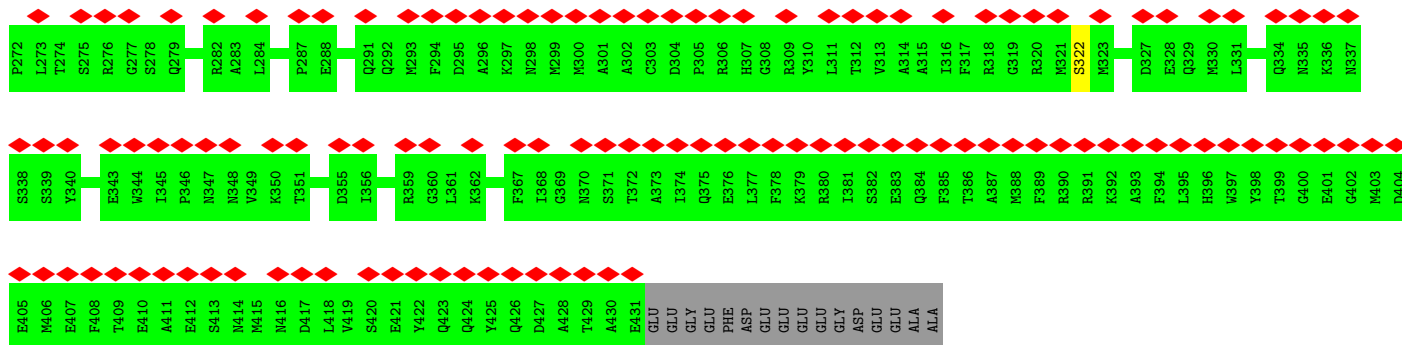


• Molecule 55: Tubulin beta chain

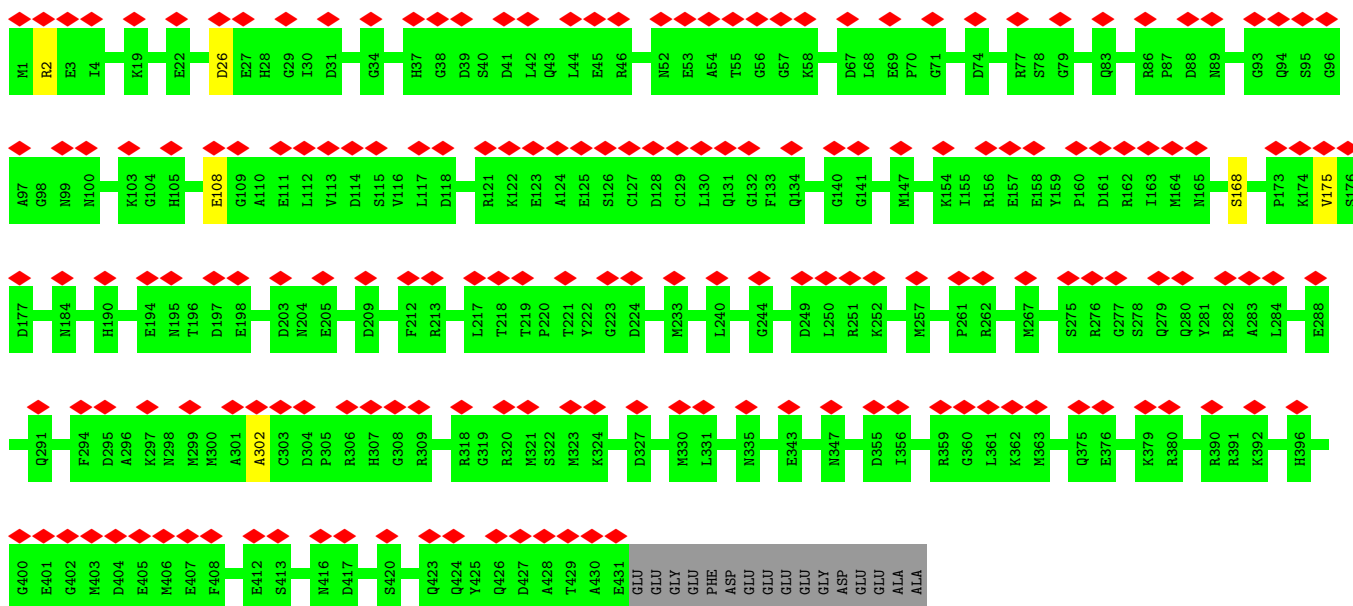
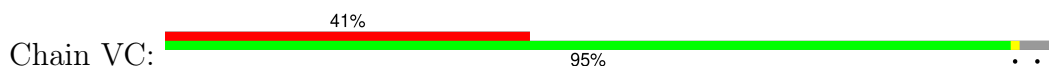


• Molecule 55: Tubulin beta chain

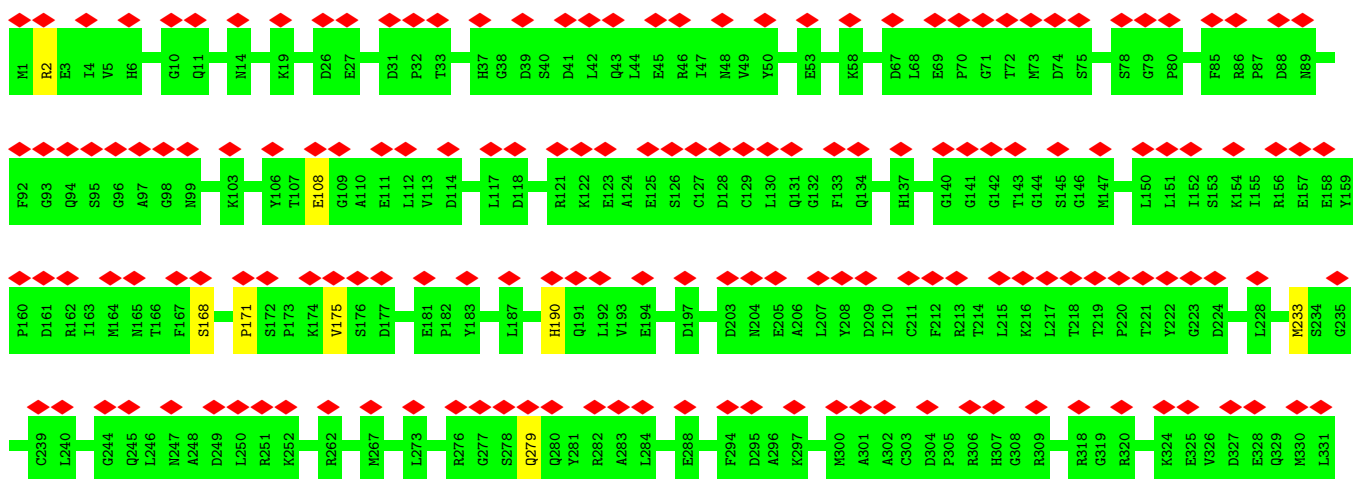


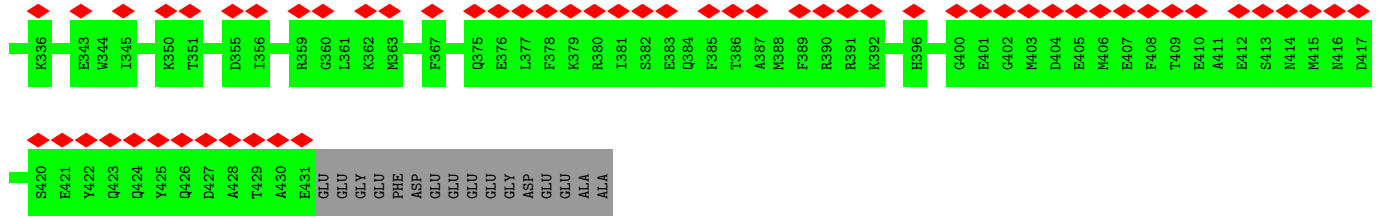


• Molecule 55: Tubulin beta chain

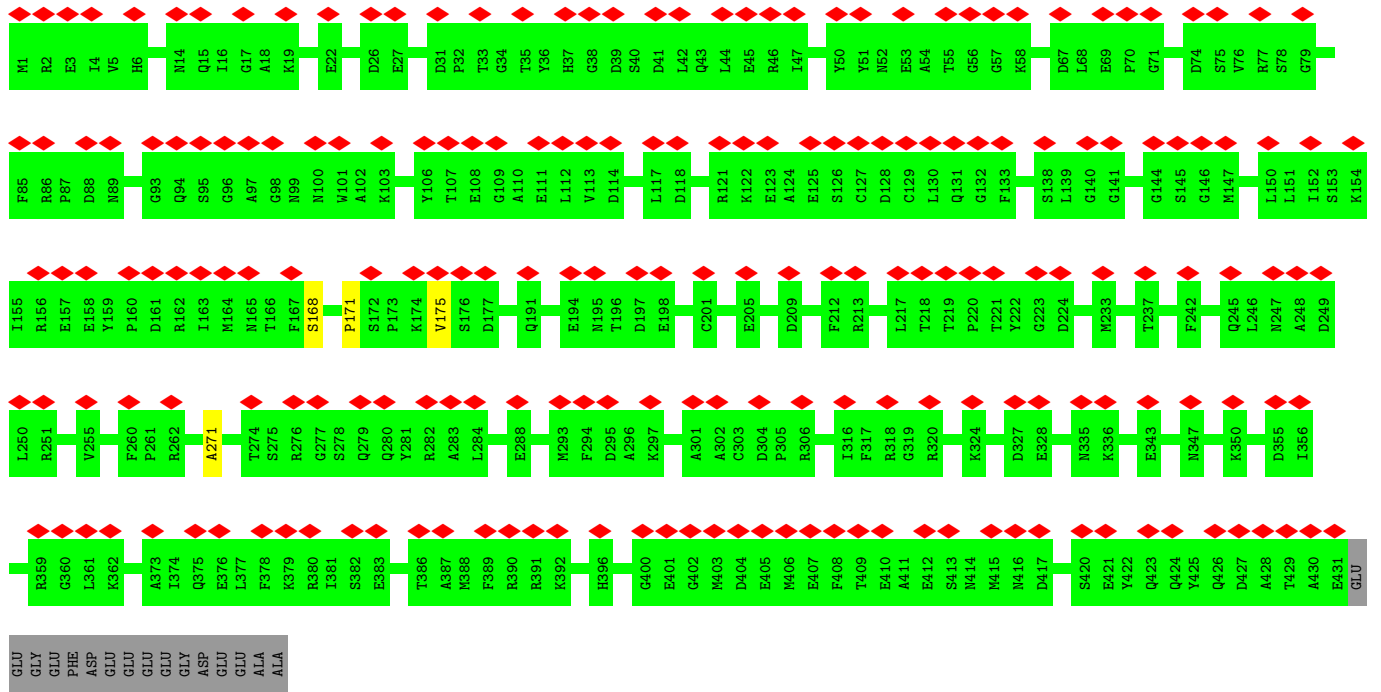


• Molecule 55: Tubulin beta chain

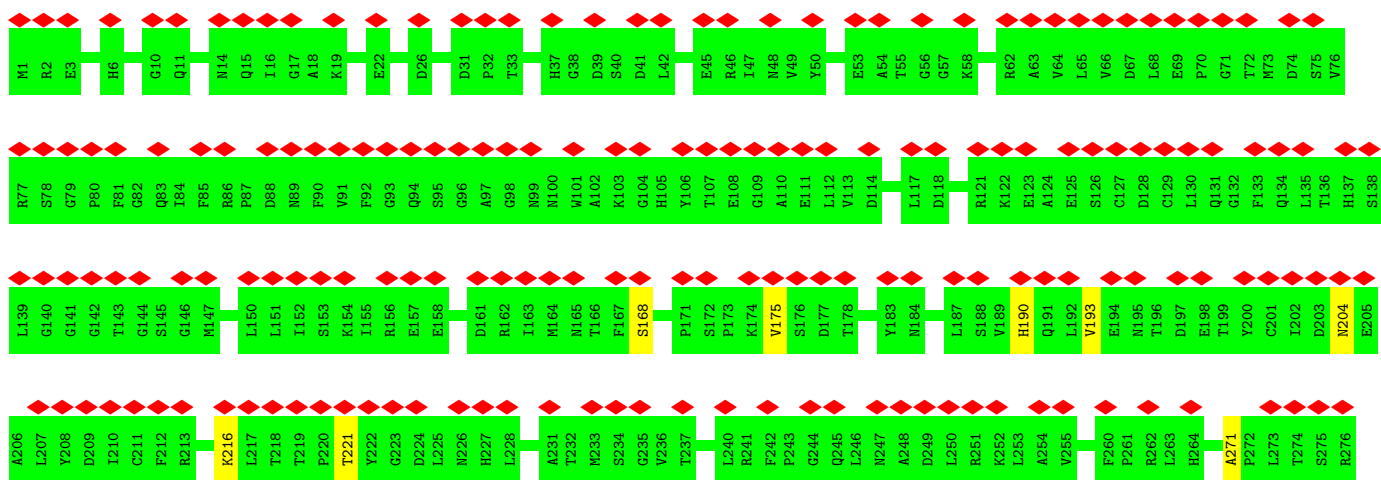


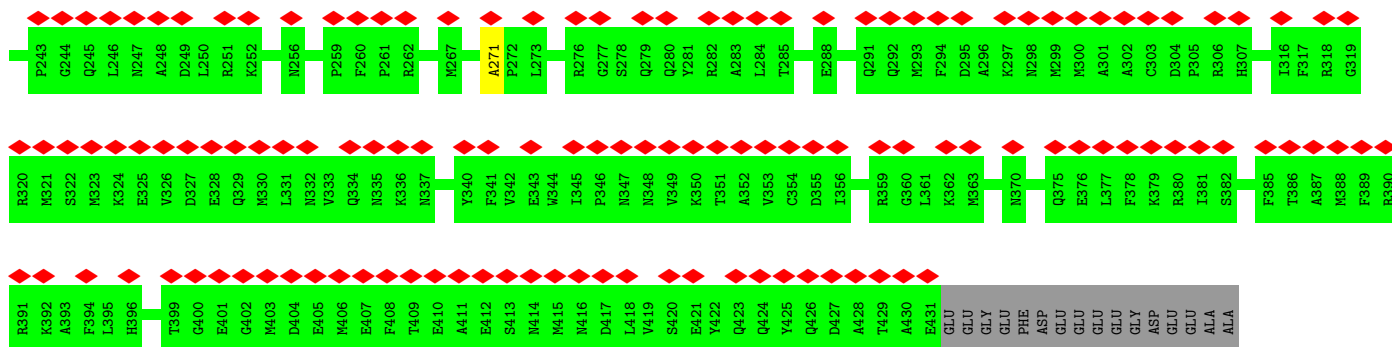


• Molecule 55: Tubulin beta chain

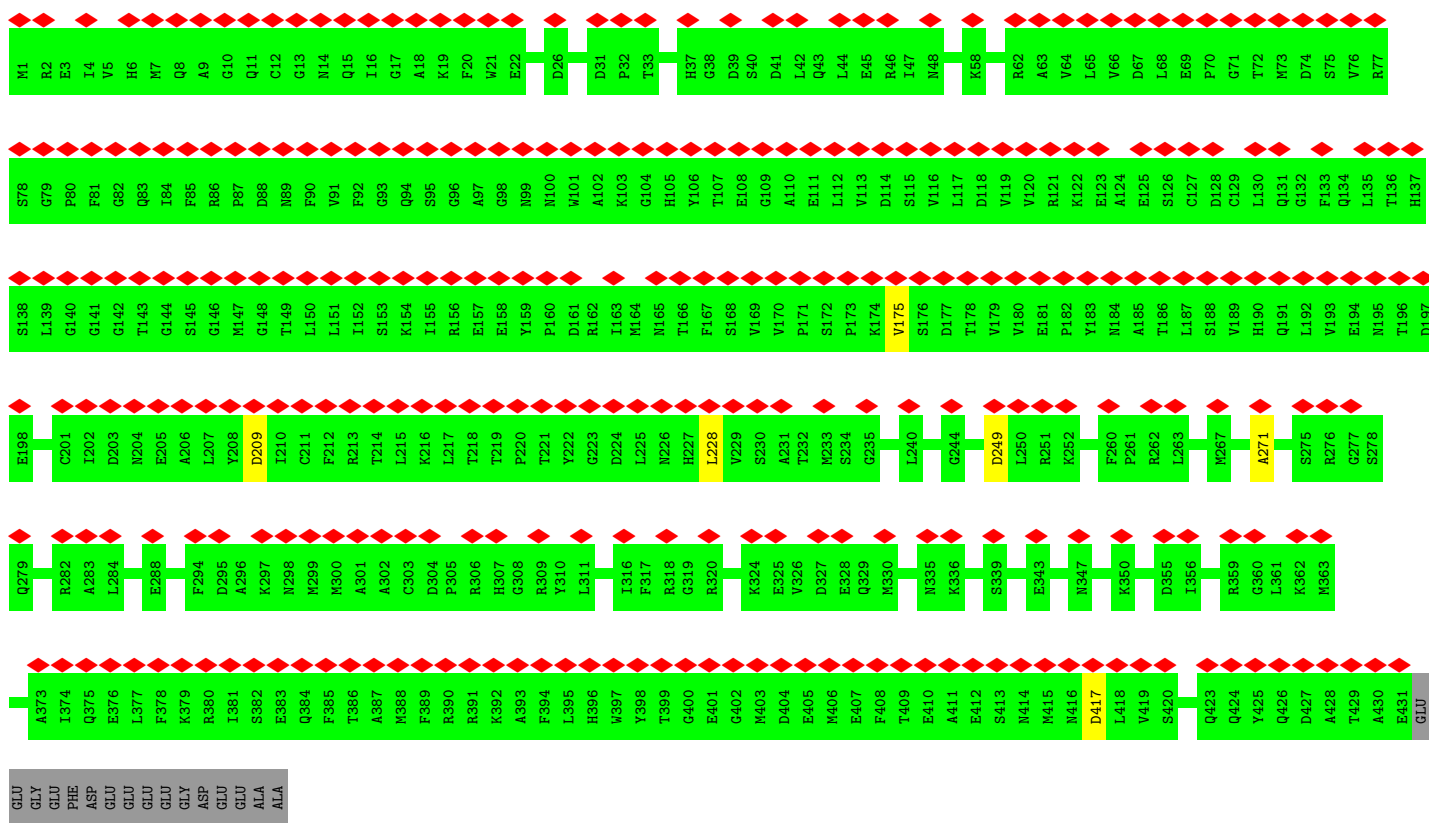


• Molecule 55: Tubulin beta chain

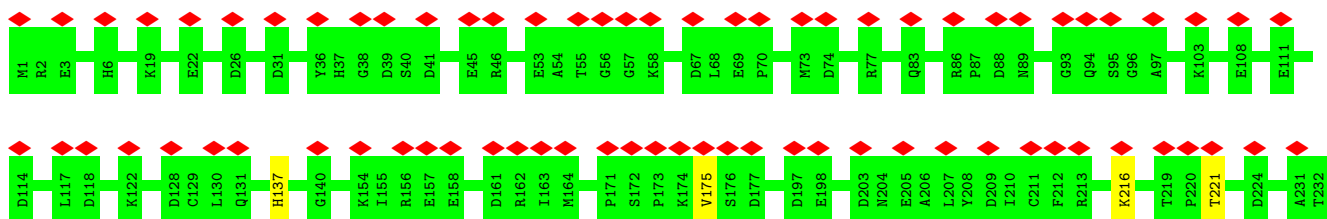


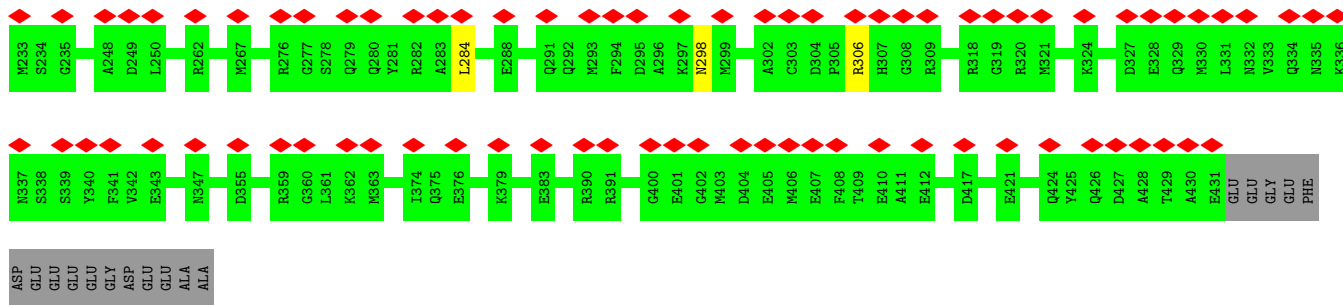


• Molecule 55: Tubulin beta chain

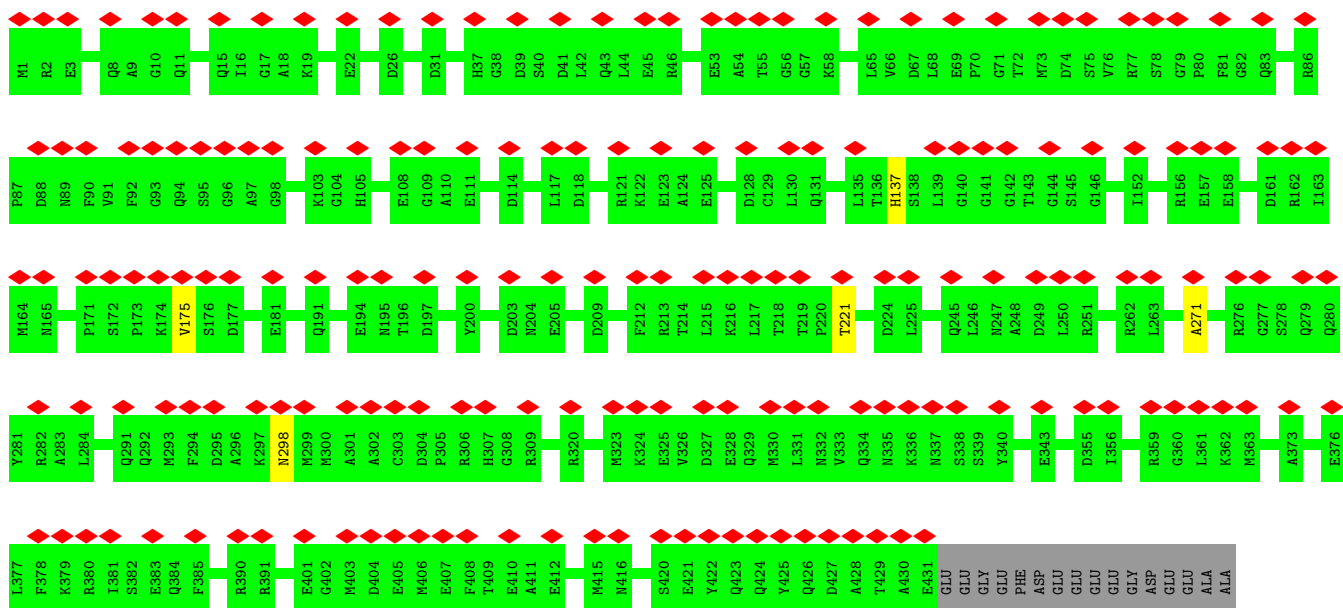
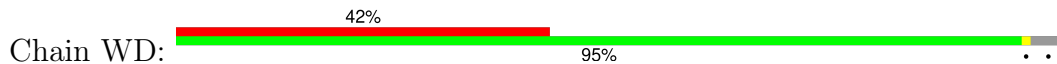


• Molecule 55: Tubulin beta chain

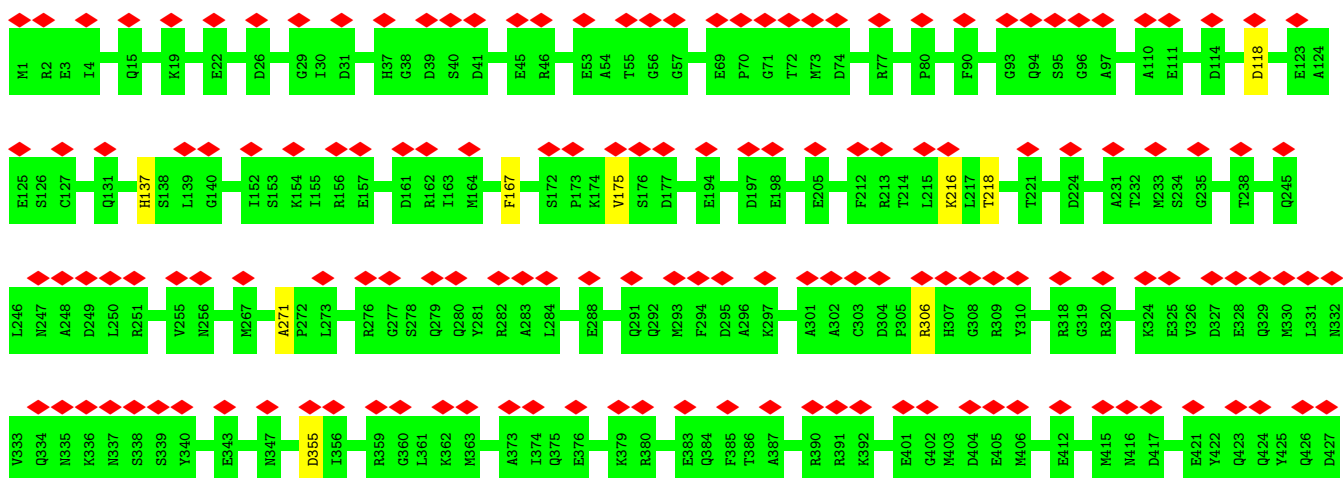


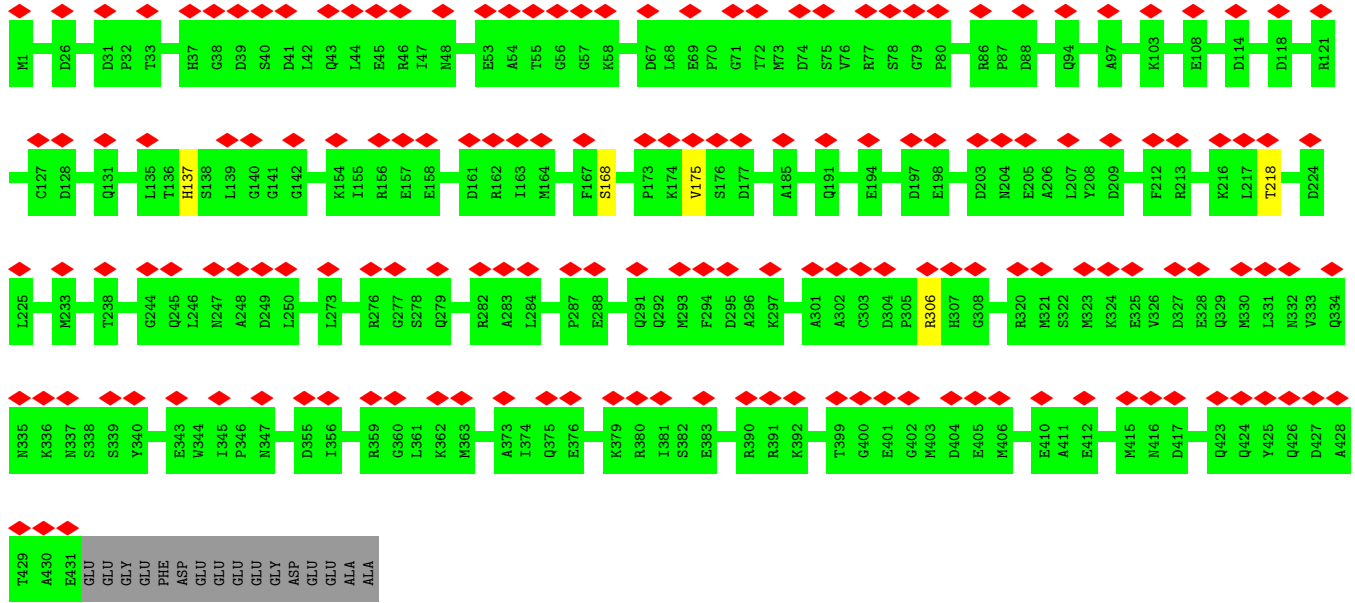


• Molecule 55: Tubulin beta chain



• Molecule 55: Tubulin beta chain





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127673	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	34	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	26.701	Depositor
Minimum map value	0.000	Depositor
Average map value	0.244	Depositor
Map value standard deviation	1.144	Depositor
Recommended contour level	6.63	Depositor
Map size (Å)	686.08, 686.08, 686.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GTP, 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	1A	0.32	0/330	0.83	1/440 (0.2%)
1	1B	0.30	0/2085	0.66	2/2806 (0.1%)
2	1E	0.31	0/3324	0.60	0/4478
2	1F	0.30	0/1298	0.57	0/1759
2	1G	0.28	0/2380	0.60	1/3191 (0.0%)
2	1H	0.30	0/3337	0.63	2/4495 (0.0%)
3	1K	0.28	0/1432	0.62	1/1926 (0.1%)
3	1L	0.30	0/1432	0.62	1/1926 (0.1%)
3	1M	0.29	0/1419	0.63	0/1910
3	1v	0.35	1/1737 (0.1%)	0.73	1/2324 (0.0%)
3	1w	0.31	0/736	0.69	1/981 (0.1%)
3	1x	0.30	0/2112	0.70	1/2824 (0.0%)
3	1y	0.35	1/1655 (0.1%)	0.68	0/2215
3	1z	0.31	0/736	0.68	1/981 (0.1%)
3	2a	0.24	0/457	0.61	0/609
4	1P	0.32	0/1665	0.64	0/2254
4	1Q	0.28	0/1154	0.63	0/1559
5	1T	0.29	0/1897	0.61	2/2561 (0.1%)
5	1U	0.30	0/927	0.61	0/1257
5	1V	0.32	0/1910	0.65	1/2578 (0.0%)
5	1W	0.29	0/889	0.62	0/1192
6	1Y	0.30	0/1033	0.66	0/1391
7	1a	0.32	0/1060	0.67	0/1434
7	1b	0.34	0/954	0.68	1/1297 (0.1%)
7	5E	0.30	0/1197	0.67	0/1627
7	5F	0.30	0/885	0.66	1/1197 (0.1%)
7	5G	0.31	0/1111	0.65	1/1512 (0.1%)
7	5H	0.31	0/922	0.70	1/1249 (0.1%)
7	5I	0.33	0/205	0.62	0/283
7	5J	0.30	0/1832	0.62	0/2482
7	5K	0.31	0/1046	0.66	0/1422
7	5L	0.30	0/985	0.62	0/1333

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	5M	0.26	0/115	0.51	0/157
7	5N	0.29	0/1915	0.63	0/2599
7	5O	0.32	0/122	0.62	0/169
8	1d	0.32	0/830	0.62	0/1125
9	1f	0.29	0/354	0.77	1/481 (0.2%)
9	1g	0.31	0/492	0.64	0/665
10	1i	0.27	0/314	0.64	0/422
10	1j	0.27	0/284	0.65	1/383 (0.3%)
10	9M	0.28	0/722	0.62	0/968
10	9N	0.27	0/722	0.58	0/968
10	9O	0.40	0/354	0.79	0/479
11	1l	0.29	0/307	0.63	0/415
11	1m	0.29	0/307	0.60	0/415
12	1o	0.33	0/255	0.80	0/338
12	1p	0.31	0/264	0.83	0/350
12	1q	0.27	0/387	0.77	0/515
12	1r	0.28	0/238	0.77	0/315
13	2A	0.30	0/2086	0.65	1/2797 (0.0%)
13	2B	0.31	0/2093	0.65	1/2807 (0.0%)
13	2C	0.31	0/2095	0.65	0/2809
13	2D	0.40	0/652	0.78	1/884 (0.1%)
14	2G	0.26	0/1920	0.59	0/2588
15	2J	0.29	0/884	0.61	0/1192
15	2K	0.29	0/884	0.60	0/1192
15	2L	0.28	0/884	0.62	0/1192
16	2O	0.35	0/989	0.63	0/1319
17	2R	0.32	0/1044	0.66	0/1382
17	2S	0.31	0/3277	0.62	0/4347
18	2V	0.28	0/2260	0.63	2/3067 (0.1%)
18	2W	0.28	0/2260	0.60	0/3067
19	3A	0.29	0/1582	0.63	1/2135 (0.0%)
19	3B	0.30	0/1582	0.66	1/2135 (0.0%)
19	3C	0.29	0/1526	0.69	1/2055 (0.0%)
19	3D	0.28	0/1492	0.66	1/2009 (0.0%)
19	3E	0.28	0/1574	0.65	0/2124
19	3F	0.29	0/1582	0.63	0/2135
19	3G	0.29	0/1574	0.61	0/2124
20	3J	0.29	0/4022	0.63	1/5441 (0.0%)
20	3K	0.31	0/559	0.74	1/752 (0.1%)
21	3N	0.40	0/2153	0.78	4/2863 (0.1%)
21	3O	0.34	0/2349	0.65	2/3126 (0.1%)
22	3R	0.30	0/1353	0.70	3/1833 (0.2%)
22	3S	0.30	0/1032	0.73	3/1397 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
22	3T	0.30	0/1353	0.68	2/1833 (0.1%)
23	3W	0.35	0/3244	0.72	3/4309 (0.1%)
23	3X	0.34	0/2677	0.63	0/3550
23	3Y	0.30	0/868	0.68	0/1153
23	3Z	0.28	0/1424	0.66	1/1897 (0.1%)
24	4A	0.28	0/4898	0.62	2/6616 (0.0%)
24	4B	0.28	0/4886	0.61	2/6600 (0.0%)
24	4C	0.29	0/4898	0.62	1/6616 (0.0%)
25	4F	0.33	0/2633	0.63	0/3500
25	4G	0.30	0/1775	0.66	1/2367 (0.0%)
26	4J	0.30	0/3050	0.63	2/4120 (0.0%)
26	4K	0.30	0/3039	0.65	0/4105
27	4N	0.31	0/1270	0.67	0/1714
27	4O	0.29	0/898	0.64	0/1212
27	4P	0.30	0/1252	0.65	0/1692
27	4Q	0.27	0/765	0.72	1/1035 (0.1%)
28	4T	0.26	0/1244	0.61	0/1666
28	4U	0.28	0/1244	0.66	1/1666 (0.1%)
28	4V	0.24	0/118	0.46	0/158
29	4Y	0.26	0/2480	0.56	0/3364
30	5A	0.28	0/274	0.59	0/369
30	5B	0.29	0/1705	0.62	0/2311
30	9Y	0.28	0/1118	0.68	1/1513 (0.1%)
30	9Z	0.32	0/811	0.66	0/1099
31	6A	0.29	0/1834	0.58	1/2479 (0.0%)
31	6B	0.33	0/1779	0.65	0/2406
31	6C	0.29	0/1811	0.58	1/2449 (0.0%)
31	6D	0.29	0/1826	0.56	0/2468
31	6E	0.28	0/1826	0.56	0/2468
31	6F	0.29	0/1826	0.57	0/2468
32	6I	0.28	0/653	0.60	0/887
32	6J	0.29	0/422	0.58	0/572
33	6M	0.27	0/3193	0.56	0/4326
33	6N	0.28	0/666	0.68	1/898 (0.1%)
34	6Q	0.29	0/1677	0.56	1/2275 (0.0%)
34	6R	0.33	0/624	0.58	0/853
35	6U	0.30	0/1260	0.63	1/1692 (0.1%)
35	6V	0.28	0/2304	0.57	0/3081
35	6W	0.29	0/2056	0.64	0/2743
35	6X	0.30	0/1041	0.65	0/1392
36	7A	0.29	0/6054	0.65	5/8189 (0.1%)
36	7B	0.28	0/3823	0.64	1/5163 (0.0%)
36	7C	0.28	0/4531	0.63	1/6118 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
36	7D	0.29	0/6046	0.65	4/8177 (0.0%)
37	7G	0.28	0/4421	0.61	0/5995
37	7H	0.30	0/4421	0.66	3/5995 (0.1%)
37	7I	0.29	0/5125	0.61	3/6942 (0.0%)
38	7M	0.28	0/2222	0.56	0/3012
38	7N	0.28	0/544	0.52	0/744
39	7Q	0.29	0/1234	0.67	1/1673 (0.1%)
39	7R	0.30	0/1167	0.67	1/1581 (0.1%)
40	7U	0.35	0/775	0.90	1/1052 (0.1%)
40	7V	0.35	0/472	0.78	0/645
41	7Y	0.29	0/1630	0.65	1/2209 (0.0%)
41	7Z	0.32	0/498	0.74	0/674
42	8A	0.28	0/1983	0.66	2/2694 (0.1%)
43	8D	0.25	0/3283	0.54	2/4406 (0.0%)
43	8E	0.29	0/1500	0.55	0/2013
43	8F	0.27	0/2155	0.54	0/2884
43	8G	0.28	0/3283	0.56	2/4406 (0.0%)
44	8J	0.26	0/3312	0.53	0/4461
44	8K	0.29	0/2646	0.55	0/3551
44	8L	0.27	0/3312	0.56	0/4461
44	8M	0.27	0/1064	0.55	0/1446
44	8N	0.29	0/145	0.63	0/195
45	8Q	0.24	0/182	0.50	0/245
45	8R	0.24	0/3268	0.54	1/4387 (0.0%)
45	8S	0.29	0/2497	0.58	2/3350 (0.1%)
45	8T	0.28	0/3268	0.58	0/4387
45	8U	0.29	0/962	0.58	0/1287
46	8X	0.28	0/902	0.68	0/1212
46	8Y	0.28	0/902	0.66	0/1212
46	8Z	0.28	0/902	0.71	2/1212 (0.2%)
47	9A	0.32	0/1747	0.71	3/2367 (0.1%)
48	9D	0.30	0/829	0.70	0/1110
49	9G	0.28	0/1270	0.57	0/1728
50	9J	0.26	0/847	0.60	0/1150
51	9R	0.26	0/1201	0.56	0/1631
52	9T	0.33	0/645	0.62	0/865
53	9V	0.34	0/196	0.74	0/266
53	9W	0.27	0/627	0.56	0/855
54	AA	0.29	0/3492	0.56	0/4742
54	AB	0.28	0/3492	0.54	0/4742
54	AE	0.29	0/3492	0.58	1/4742 (0.0%)
54	AG	0.28	0/3492	0.58	1/4742 (0.0%)
54	AI	0.29	0/3492	0.55	0/4742

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
54	AK	0.29	0/3492	0.58	0/4742
54	AM	0.28	0/3492	0.56	0/4742
54	BA	0.29	0/3492	0.60	2/4742 (0.0%)
54	BB	0.30	0/3492	0.59	0/4742
54	BE	0.30	0/3492	0.59	1/4742 (0.0%)
54	BG	0.29	0/3492	0.59	0/4742
54	BI	0.29	0/3492	0.59	1/4742 (0.0%)
54	BK	0.29	0/3492	0.60	1/4742 (0.0%)
54	BM	0.30	0/3492	0.59	0/4742
54	CA	0.29	0/3492	0.56	0/4742
54	CB	0.28	0/3492	0.59	1/4742 (0.0%)
54	CE	0.29	0/3492	0.59	1/4742 (0.0%)
54	CG	0.28	0/3492	0.58	0/4742
54	CI	0.30	0/3492	0.60	1/4742 (0.0%)
54	CK	0.29	0/3492	0.64	3/4742 (0.1%)
54	CM	0.31	0/3492	0.58	1/4742 (0.0%)
54	DA	0.29	0/3492	0.57	0/4742
54	DB	0.30	0/3492	0.58	0/4742
54	DE	0.29	0/3492	0.59	0/4742
54	DG	0.29	0/3492	0.63	3/4742 (0.1%)
54	DI	0.30	0/3492	0.58	1/4742 (0.0%)
54	DK	0.28	0/3492	0.56	0/4742
54	DM	0.29	0/3492	0.58	2/4742 (0.0%)
54	EA	0.39	0/3492	0.60	2/4742 (0.0%)
54	EC	0.29	0/3492	0.59	1/4742 (0.0%)
54	EE	0.28	0/3492	0.59	1/4742 (0.0%)
54	EG	0.30	0/3492	0.60	1/4742 (0.0%)
54	EI	0.30	0/3492	0.62	2/4742 (0.0%)
54	EK	0.30	0/3492	0.59	0/4742
54	FA	0.41	0/3492	0.60	1/4742 (0.0%)
54	FB	0.29	0/3492	0.61	2/4742 (0.0%)
54	FE	0.40	0/3492	0.62	1/4742 (0.0%)
54	FG	0.31	0/3492	0.62	3/4742 (0.1%)
54	FI	0.41	0/3492	0.63	0/4742
54	FK	0.29	0/3492	0.59	2/4742 (0.0%)
54	GA	0.30	0/3492	0.60	1/4742 (0.0%)
54	GB	0.30	0/3492	0.57	0/4742
54	GE	0.29	0/3492	0.57	0/4742
54	GG	0.29	0/3492	0.58	0/4742
54	GI	0.30	0/3492	0.59	1/4742 (0.0%)
54	GK	0.30	0/3492	0.61	2/4742 (0.0%)
54	HA	0.29	0/3492	0.59	1/4742 (0.0%)
54	HB	0.29	0/3492	0.57	1/4742 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
54	HE	0.28	0/3459	0.57	0/4697
54	HG	0.29	0/3483	0.57	2/4729 (0.0%)
54	HI	0.29	0/3492	0.56	0/4742
54	HK	0.29	0/3483	0.55	0/4729
54	IA	0.29	0/3492	0.58	1/4742 (0.0%)
54	IB	0.29	0/3475	0.56	0/4718
54	IE	0.31	0/3492	0.60	0/4742
54	IG	0.29	0/3492	0.57	1/4742 (0.0%)
54	II	0.29	0/3479	0.59	0/4723
54	IK	0.29	0/3492	0.56	0/4742
54	IM	0.28	0/3492	0.58	1/4742 (0.0%)
54	JA	0.29	0/3464	0.59	2/4703 (0.0%)
54	JB	0.28	0/3492	0.56	0/4742
54	JE	0.29	0/3492	0.57	1/4742 (0.0%)
54	JG	0.29	0/3492	0.57	0/4742
54	JI	0.30	0/3492	0.57	2/4742 (0.0%)
54	JK	0.28	0/3492	0.57	0/4742
54	KA	0.28	0/3492	0.55	0/4742
54	KB	0.31	0/3475	0.61	2/4718 (0.0%)
54	KE	0.30	0/3492	0.59	0/4742
54	KG	0.29	0/3492	0.60	1/4742 (0.0%)
54	KI	0.28	0/3492	0.56	0/4742
54	KK	0.29	0/3492	0.56	0/4742
54	LA	0.29	0/3492	0.54	1/4742 (0.0%)
54	LB	0.29	0/3492	0.59	1/4742 (0.0%)
54	LE	0.29	0/3492	0.57	2/4742 (0.0%)
54	LG	0.30	0/3492	0.58	1/4742 (0.0%)
54	LI	0.29	0/3492	0.55	0/4742
54	LK	0.29	0/3492	0.56	0/4742
54	MA	0.29	0/3492	0.56	0/4742
54	MB	0.29	0/3492	0.59	1/4742 (0.0%)
54	ME	0.29	0/3492	0.56	0/4742
54	MG	0.29	0/3492	0.57	0/4742
54	MI	0.30	0/3492	0.57	0/4742
54	MK	0.28	0/3492	0.57	1/4742 (0.0%)
54	ML	0.28	0/3492	0.55	0/4742
54	NA	0.30	0/3483	0.60	0/4729
54	NB	0.30	0/3492	0.60	0/4742
54	NE	0.29	0/3492	0.59	0/4742
54	NG	0.29	0/3492	0.60	2/4742 (0.0%)
54	NI	0.30	0/3475	0.61	1/4718 (0.0%)
54	NL	0.29	0/3468	0.59	0/4708
54	OA	0.30	0/3492	0.58	1/4742 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
54	OB	0.28	0/3475	0.57	0/4718
54	OE	0.30	0/3492	0.61	2/4742 (0.0%)
54	OG	0.30	0/3492	0.61	0/4742
54	OI	0.30	0/3492	0.59	0/4742
54	OK	0.29	0/3492	0.58	0/4742
54	OL	0.31	0/3492	0.59	0/4742
54	PA	0.29	0/3492	0.58	0/4742
54	PB	0.30	0/3492	0.58	1/4742 (0.0%)
54	PE	0.28	0/3492	0.55	0/4742
54	PG	0.30	0/3492	0.58	1/4742 (0.0%)
54	PI	0.30	0/3492	0.59	0/4742
54	PK	0.29	0/3492	0.61	1/4742 (0.0%)
54	PL	0.28	0/3492	0.59	0/4742
54	QA	0.29	0/3492	0.56	1/4742 (0.0%)
54	QB	0.29	0/3492	0.59	0/4742
54	QE	0.31	0/3492	0.58	0/4742
54	QG	0.31	0/3492	0.59	0/4742
54	QI	0.31	0/3492	0.60	0/4742
54	QK	0.29	0/3468	0.58	0/4708
54	QL	0.27	0/3487	0.58	1/4734 (0.0%)
54	RA	0.30	0/3492	0.59	2/4742 (0.0%)
54	RB	0.30	0/3492	0.61	2/4742 (0.0%)
54	RE	0.31	0/3492	0.65	5/4742 (0.1%)
54	RG	0.30	0/3492	0.59	1/4742 (0.0%)
54	RI	0.30	0/3492	0.61	0/4742
54	RK	0.30	0/3492	0.60	2/4742 (0.0%)
54	RL	0.29	0/3492	0.62	0/4742
54	SA	0.29	0/3492	0.62	4/4742 (0.1%)
54	SB	0.30	0/3492	0.59	1/4742 (0.0%)
54	SE	0.31	0/3492	0.59	1/4742 (0.0%)
54	SG	0.32	0/3492	0.62	0/4742
54	SI	0.31	0/3492	0.59	1/4742 (0.0%)
54	SK	0.29	0/3492	0.57	1/4742 (0.0%)
54	TA	0.29	0/3487	0.58	0/4734
54	TB	0.29	0/3487	0.58	0/4734
54	TE	0.31	0/3492	0.60	2/4742 (0.0%)
54	TG	0.30	0/3492	0.59	0/4742
54	TI	0.29	0/3492	0.60	2/4742 (0.0%)
54	TK	0.32	0/3492	0.64	1/4742 (0.0%)
54	UA	0.29	0/3487	0.60	1/4734 (0.0%)
54	UB	0.29	0/3472	0.59	2/4713 (0.0%)
54	UE	0.29	0/3492	0.59	0/4742
54	UG	0.28	0/3492	0.59	1/4742 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
54	UI	0.30	0/3492	0.62	2/4742 (0.0%)
54	UK	0.30	0/3492	0.61	1/4742 (0.0%)
54	VA	0.30	0/3492	0.62	1/4742 (0.0%)
54	VB	0.29	0/3492	0.59	0/4742
54	VE	0.30	0/3492	0.60	0/4742
54	VG	0.29	0/3483	0.63	2/4729 (0.0%)
54	VI	0.30	0/3492	0.60	1/4742 (0.0%)
54	VK	0.29	0/3492	0.60	2/4742 (0.0%)
54	WA	0.30	0/3492	0.62	1/4742 (0.0%)
54	WB	0.28	0/3487	0.58	0/4734
54	WE	0.30	0/3492	0.63	1/4742 (0.0%)
54	WG	0.30	0/3492	0.59	0/4742
54	WI	0.28	0/3492	0.59	1/4742 (0.0%)
54	WK	0.29	0/3492	0.56	1/4742 (0.0%)
55	AC	0.29	0/3458	0.60	2/4685 (0.0%)
55	AD	0.29	0/3458	0.60	1/4685 (0.0%)
55	AF	0.28	0/3458	0.59	1/4685 (0.0%)
55	AH	0.28	0/3458	0.59	0/4685
55	AJ	0.28	0/3458	0.58	1/4685 (0.0%)
55	AL	0.29	0/3458	0.58	0/4685
55	BC	0.30	0/3458	0.63	1/4685 (0.0%)
55	BD	0.30	0/3458	0.64	2/4685 (0.0%)
55	BF	0.30	0/3458	0.61	1/4685 (0.0%)
55	BH	0.33	0/3458	0.62	1/4685 (0.0%)
55	BJ	0.30	0/3458	0.62	1/4685 (0.0%)
55	BL	0.28	0/3458	0.60	0/4685
55	CC	0.30	0/3458	0.65	1/4685 (0.0%)
55	CD	0.30	0/3458	0.63	3/4685 (0.1%)
55	CF	0.29	0/3458	0.60	1/4685 (0.0%)
55	CH	0.30	0/3458	0.64	2/4685 (0.0%)
55	CJ	0.32	0/3458	0.67	4/4685 (0.1%)
55	CL	0.29	0/3458	0.62	4/4685 (0.1%)
55	DC	0.28	0/3458	0.61	3/4685 (0.1%)
55	DD	0.29	0/3458	0.60	1/4685 (0.0%)
55	DF	0.31	0/3458	0.61	1/4685 (0.0%)
55	DH	0.28	0/3458	0.61	2/4685 (0.0%)
55	DJ	0.28	0/3458	0.63	1/4685 (0.0%)
55	DL	0.30	0/3458	0.59	0/4685
55	EB	0.29	0/3458	0.62	2/4685 (0.0%)
55	ED	0.29	0/3458	0.65	6/4685 (0.1%)
55	EF	0.29	0/3458	0.62	3/4685 (0.1%)
55	EH	0.29	0/3458	0.65	2/4685 (0.0%)
55	EJ	0.29	0/3458	0.61	0/4685

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
55	EL	0.28	0/3458	0.63	2/4685 (0.0%)
55	EM	0.27	0/3458	0.60	2/4685 (0.0%)
55	FC	0.29	0/3458	0.64	1/4685 (0.0%)
55	FD	0.28	0/3458	0.59	1/4685 (0.0%)
55	FF	0.29	0/3458	0.62	2/4685 (0.0%)
55	FH	0.32	1/3458 (0.0%)	0.65	3/4685 (0.1%)
55	FJ	0.29	0/3458	0.64	4/4685 (0.1%)
55	FL	0.28	0/3458	0.63	3/4685 (0.1%)
55	FM	0.29	0/3458	0.60	1/4685 (0.0%)
55	GC	0.29	0/3458	0.60	1/4685 (0.0%)
55	GD	0.28	0/3458	0.58	0/4685
55	GF	0.28	0/3458	0.58	0/4685
55	GH	0.30	0/3458	0.59	1/4685 (0.0%)
55	GJ	0.31	0/3458	0.61	1/4685 (0.0%)
55	GL	0.28	0/3458	0.61	1/4685 (0.0%)
55	GM	0.28	0/3458	0.59	0/4685
55	HC	0.28	0/3458	0.57	0/4685
55	HD	0.29	0/3458	0.61	1/4685 (0.0%)
55	HF	0.28	0/3458	0.58	0/4685
55	HH	0.28	0/3458	0.57	0/4685
55	HJ	0.28	0/3458	0.57	0/4685
55	HL	0.29	0/3458	0.59	1/4685 (0.0%)
55	HM	0.27	0/3458	0.57	1/4685 (0.0%)
55	IC	0.28	0/3458	0.56	0/4685
55	ID	0.29	0/3458	0.60	1/4685 (0.0%)
55	IF	0.28	0/3458	0.56	0/4685
55	IH	0.28	0/3458	0.60	1/4685 (0.0%)
55	IJ	0.29	0/3458	0.59	1/4685 (0.0%)
55	IL	0.29	0/3458	0.61	0/4685
55	JC	0.29	0/3458	0.57	0/4685
55	JD	0.28	0/3458	0.60	1/4685 (0.0%)
55	JF	0.29	0/3458	0.62	3/4685 (0.1%)
55	JH	0.28	0/3458	0.59	1/4685 (0.0%)
55	JJ	0.28	0/3458	0.58	2/4685 (0.0%)
55	JL	0.29	0/3458	0.61	2/4685 (0.0%)
55	JM	0.29	0/3458	0.59	2/4685 (0.0%)
55	KC	0.29	0/3458	0.61	1/4685 (0.0%)
55	KD	0.29	0/3458	0.59	1/4685 (0.0%)
55	KF	0.28	0/3458	0.59	0/4685
55	KH	0.28	0/3458	0.60	2/4685 (0.0%)
55	KJ	0.28	0/3458	0.58	0/4685
55	KL	0.28	0/3458	0.61	0/4685
55	KM	0.28	0/3458	0.57	2/4685 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
55	LC	0.29	0/3458	0.59	2/4685 (0.0%)
55	LD	0.30	0/3458	0.57	0/4685
55	LF	0.29	0/3458	0.60	1/4685 (0.0%)
55	LH	0.28	0/3458	0.60	0/4685
55	LJ	0.30	0/3458	0.58	1/4685 (0.0%)
55	LL	0.30	0/3458	0.62	1/4685 (0.0%)
55	LM	0.28	0/3458	0.58	3/4685 (0.1%)
55	MC	0.29	0/3458	0.59	1/4685 (0.0%)
55	MD	0.29	0/3458	0.57	1/4685 (0.0%)
55	MF	0.28	0/3458	0.56	0/4685
55	MH	0.28	0/3458	0.58	2/4685 (0.0%)
55	MJ	0.28	0/3458	0.57	1/4685 (0.0%)
55	MM	0.29	0/3458	0.60	0/4685
55	NC	0.29	0/3458	0.63	3/4685 (0.1%)
55	ND	0.29	0/3458	0.59	0/4685
55	NF	0.29	0/3458	0.58	1/4685 (0.0%)
55	NH	0.28	0/3458	0.61	2/4685 (0.0%)
55	NJ	0.28	0/3458	0.60	2/4685 (0.0%)
55	NK	0.30	0/3458	0.65	3/4685 (0.1%)
55	NM	0.29	0/3458	0.61	0/4685
55	OC	0.29	0/3458	0.62	2/4685 (0.0%)
55	OD	0.29	0/3458	0.61	1/4685 (0.0%)
55	OF	0.30	0/3458	0.62	0/4685
55	OH	0.30	0/3458	0.63	2/4685 (0.0%)
55	OJ	0.29	0/3458	0.60	0/4685
55	OM	0.30	0/3458	0.61	1/4685 (0.0%)
55	PC	0.29	0/3458	0.63	1/4685 (0.0%)
55	PD	0.28	0/3458	0.59	1/4685 (0.0%)
55	PF	0.30	0/3458	0.63	2/4685 (0.0%)
55	PH	0.28	0/3458	0.57	0/4685
55	PJ	0.29	0/3458	0.60	1/4685 (0.0%)
55	PM	0.30	0/3458	0.58	0/4685
55	QC	0.30	0/3458	0.64	3/4685 (0.1%)
55	QD	0.30	0/3458	0.59	0/4685
55	QF	0.32	0/3458	0.66	3/4685 (0.1%)
55	QH	0.29	0/3458	0.64	2/4685 (0.0%)
55	QJ	0.31	0/3458	0.65	4/4685 (0.1%)
55	QM	0.29	0/3458	0.60	0/4685
55	RC	0.30	0/3458	0.64	1/4685 (0.0%)
55	RD	0.29	0/3458	0.63	2/4685 (0.0%)
55	RF	0.30	0/3458	0.62	3/4685 (0.1%)
55	RH	0.30	0/3458	0.63	0/4685
55	RJ	0.30	0/3458	0.63	2/4685 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
55	RM	0.31	0/3458	0.63	1/4685 (0.0%)
55	SC	0.30	0/3458	0.62	2/4685 (0.0%)
55	SD	0.30	0/3458	0.63	0/4685
55	SF	0.31	0/3458	0.63	2/4685 (0.0%)
55	SH	0.30	0/3458	0.61	0/4685
55	SJ	0.29	0/3458	0.62	1/4685 (0.0%)
55	SL	0.29	0/3458	0.63	1/4685 (0.0%)
55	SM	0.30	0/3458	0.64	3/4685 (0.1%)
55	TC	0.28	0/3458	0.59	1/4685 (0.0%)
55	TD	0.29	0/3458	0.62	1/4685 (0.0%)
55	TF	0.29	0/3458	0.62	0/4685
55	TH	0.29	0/3458	0.61	0/4685
55	TJ	0.30	0/3458	0.62	1/4685 (0.0%)
55	TL	0.28	0/3458	0.59	1/4685 (0.0%)
55	TM	0.30	1/3458 (0.0%)	0.61	1/4685 (0.0%)
55	UC	0.28	0/3458	0.61	2/4685 (0.0%)
55	UD	0.29	0/3458	0.61	1/4685 (0.0%)
55	UF	0.31	0/3458	0.67	0/4685
55	UH	0.31	0/3458	0.64	1/4685 (0.0%)
55	UJ	0.29	0/3458	0.62	0/4685
55	UL	0.30	0/3458	0.62	1/4685 (0.0%)
55	UM	0.30	0/3458	0.65	2/4685 (0.0%)
55	VC	0.30	0/3458	0.61	1/4685 (0.0%)
55	VD	0.30	0/3458	0.64	2/4685 (0.0%)
55	VF	0.31	0/3458	0.64	1/4685 (0.0%)
55	VH	0.31	0/3458	0.63	0/4685
55	VJ	0.29	0/3458	0.62	1/4685 (0.0%)
55	VL	0.29	0/3458	0.61	4/4685 (0.1%)
55	VM	0.30	0/3458	0.65	4/4685 (0.1%)
55	WC	0.30	0/3458	0.60	1/4685 (0.0%)
55	WD	0.30	0/3458	0.60	0/4685
55	WF	0.29	0/3458	0.60	1/4685 (0.0%)
55	WH	0.30	0/3458	0.62	0/4685
55	WJ	0.28	0/3458	0.59	0/4685
55	WL	0.29	0/3458	0.60	0/4685
All	All	0.29	4/1289690 (0.0%)	0.60	401/1747079 (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
1	1B	0	2
3	1v	0	1
3	1w	0	1
3	1y	0	1
3	2a	0	1
5	1V	0	1
6	1Y	0	1
7	1a	0	1
7	1b	0	2
7	5K	0	2
10	9O	0	1
12	1r	0	1
19	3B	0	1
20	3J	0	2
22	3S	0	1
23	3W	0	2
25	4G	0	1
26	4J	0	1
30	5B	0	1
30	9Z	0	2
31	6B	0	2
36	7A	0	1
36	7C	0	1
36	7D	0	1
37	7G	0	1
37	7H	0	1
37	7I	0	1
38	7M	0	2
40	7U	0	1
41	7Y	0	1
42	8A	0	1
43	8D	0	1
47	9A	0	1
48	9D	0	1
53	9V	0	2
54	AB	0	1
54	AE	0	1
54	AG	0	1
54	BA	0	1
54	BI	0	1
54	BK	0	1
54	CA	0	1
54	CB	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	CE	0	2
54	CI	0	1
54	CK	0	1
54	CM	0	1
54	DK	0	1
54	EG	0	2
54	EI	0	1
54	EK	0	1
54	FA	0	1
54	FB	0	2
54	FI	0	1
54	GB	0	1
54	HA	0	1
54	HB	0	1
54	HG	0	1
54	IA	0	1
54	IB	0	1
54	IG	0	2
54	II	0	1
54	IK	0	2
54	JA	0	1
54	JB	0	1
54	JE	0	1
54	JG	0	1
54	KB	0	1
54	KE	0	1
54	KG	0	1
54	KI	0	1
54	LA	0	1
54	MA	0	1
54	MB	0	1
54	MI	0	1
54	MK	0	1
54	NB	0	1
54	OE	0	2
54	OK	0	1
54	PA	0	1
54	PI	0	1
54	QB	0	2
54	QE	0	2
54	QI	0	1
54	QK	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	RA	0	1
54	RB	0	2
54	RE	0	1
54	RG	0	1
54	RI	0	1
54	RK	0	1
54	RL	0	2
54	SB	0	1
54	SE	0	1
54	SG	0	2
54	SI	0	1
54	TA	0	1
54	TB	0	2
54	TG	0	1
54	TI	0	1
54	TK	0	2
54	UB	0	1
54	UG	0	1
54	UI	0	1
54	UK	0	1
54	VB	0	1
54	VE	0	1
54	VG	0	1
54	WA	0	1
54	WB	0	1
54	WE	0	1
54	WI	0	1
54	WK	0	1
55	AC	0	1
55	AF	0	2
55	AH	0	2
55	AJ	0	1
55	AL	0	2
55	BC	0	3
55	CC	0	2
55	CD	0	1
55	CF	0	1
55	CH	0	1
55	CJ	0	2
55	CL	0	1
55	DC	0	1
55	DD	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	DF	0	2
55	DH	0	3
55	DJ	0	2
55	DL	0	1
55	EB	0	1
55	ED	0	1
55	EF	0	1
55	EH	0	1
55	EJ	0	1
55	EL	0	1
55	EM	0	2
55	FC	0	1
55	FD	0	1
55	FF	0	1
55	FJ	0	1
55	FL	0	1
55	FM	0	2
55	GF	0	1
55	GL	0	1
55	GM	0	1
55	HC	0	1
55	HD	0	2
55	HF	0	2
55	HH	0	1
55	HM	0	1
55	IC	0	2
55	ID	0	1
55	IF	0	1
55	IJ	0	1
55	IL	0	1
55	JC	0	2
55	JD	0	1
55	JF	0	2
55	JH	0	2
55	JJ	0	1
55	JL	0	1
55	JM	0	1
55	KC	0	1
55	KD	0	2
55	KF	0	1
55	KH	0	1
55	KJ	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	KL	0	1
55	LD	0	1
55	LF	0	3
55	LJ	0	1
55	LL	0	2
55	LM	0	1
55	MC	0	2
55	MD	0	1
55	MF	0	1
55	MH	0	1
55	MJ	0	2
55	MM	0	2
55	NC	0	1
55	ND	0	2
55	NH	0	4
55	NJ	0	2
55	NK	0	2
55	NM	0	3
55	OC	0	2
55	OF	0	2
55	OH	0	2
55	OJ	0	2
55	OM	0	1
55	PC	0	3
55	PD	0	1
55	PF	0	1
55	PH	0	2
55	PJ	0	1
55	QC	0	2
55	QD	0	2
55	QF	0	2
55	QH	0	1
55	QJ	0	2
55	QM	0	3
55	RC	0	1
55	RF	0	3
55	RH	0	1
55	RJ	0	2
55	SD	0	4
55	SF	0	1
55	SJ	0	1
55	SM	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	TD	0	2
55	TH	0	1
55	TJ	0	1
55	UC	0	2
55	UD	0	1
55	UF	0	1
55	UH	0	3
55	UJ	0	2
55	UL	0	1
55	UM	0	2
55	VC	0	1
55	VF	0	1
55	VH	0	3
55	VJ	0	2
55	VL	0	1
55	VM	0	1
55	WC	0	1
55	WD	0	2
55	WF	0	4
55	WH	0	1
55	WJ	0	1
55	WL	0	1
All	All	0	323

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	FH	171	PRO	CG-CD	-7.52	1.25	1.50
3	1v	670	CYS	CB-SG	-6.48	1.71	1.82
3	1y	670	CYS	CB-SG	-5.45	1.73	1.81
55	TM	194	GLU	CA-CB	5.39	1.65	1.53

The worst 5 of 401 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3J	312	TYR	C-N-CD	-10.17	98.22	120.60
55	FH	171	PRO	N-CD-CG	-9.84	88.45	103.20
55	VD	171	PRO	C-N-CA	9.69	145.92	121.70
55	ED	177	ASP	CB-CG-OD1	9.50	126.85	118.30
55	QC	187	LEU	CA-CB-CG	9.37	136.85	115.30

There are no chirality outliers.

5 of 323 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1B	189	ALA	Peptide
1	1B	296	MET	Peptide
5	1V	104	THR	Peptide
6	1Y	30	GLU	Peptide
7	1a	156	VAL	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1A	40/309 (13%)	29 (72%)	9 (22%)	2 (5%)	1	12
1	1B	265/309 (86%)	219 (83%)	42 (16%)	4 (2%)	8	33
2	1E	415/448 (93%)	390 (94%)	22 (5%)	3 (1%)	19	50
2	1F	164/448 (37%)	149 (91%)	14 (8%)	1 (1%)	22	53
2	1G	290/448 (65%)	279 (96%)	10 (3%)	1 (0%)	37	66
2	1H	416/448 (93%)	379 (91%)	33 (8%)	4 (1%)	13	42
3	1K	173/696 (25%)	154 (89%)	16 (9%)	3 (2%)	7	31
3	1L	173/696 (25%)	156 (90%)	15 (9%)	2 (1%)	11	38
3	1M	173/696 (25%)	160 (92%)	12 (7%)	1 (1%)	22	53
3	1v	203/696 (29%)	181 (89%)	22 (11%)	0	100	100
3	1w	85/696 (12%)	76 (89%)	9 (11%)	0	100	100
3	1x	244/696 (35%)	220 (90%)	20 (8%)	4 (2%)	8	32
3	1y	194/696 (28%)	181 (93%)	13 (7%)	0	100	100
3	1z	85/696 (12%)	83 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2a	52/696 (8%)	45 (86%)	6 (12%)	1 (2%)	6	29
4	1P	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
4	1Q	136/204 (67%)	122 (90%)	14 (10%)	0	100	100
5	1T	220/429 (51%)	193 (88%)	25 (11%)	2 (1%)	14	44
5	1U	107/429 (25%)	97 (91%)	10 (9%)	0	100	100
5	1V	221/429 (52%)	190 (86%)	28 (13%)	3 (1%)	9	34
5	1W	103/429 (24%)	91 (88%)	10 (10%)	2 (2%)	6	29
6	1Y	115/139 (83%)	98 (85%)	17 (15%)	0	100	100
7	1a	132/251 (53%)	106 (80%)	23 (17%)	3 (2%)	5	26
7	1b	120/251 (48%)	95 (79%)	22 (18%)	3 (2%)	4	24
7	5E	152/251 (61%)	115 (76%)	35 (23%)	2 (1%)	10	36
7	5F	110/251 (44%)	89 (81%)	19 (17%)	2 (2%)	7	30
7	5G	140/251 (56%)	109 (78%)	29 (21%)	2 (1%)	9	34
7	5H	115/251 (46%)	90 (78%)	21 (18%)	4 (4%)	3	19
7	5I	25/251 (10%)	20 (80%)	4 (16%)	1 (4%)	2	16
7	5J	231/251 (92%)	189 (82%)	37 (16%)	5 (2%)	5	26
7	5K	132/251 (53%)	99 (75%)	30 (23%)	3 (2%)	5	26
7	5L	123/251 (49%)	99 (80%)	21 (17%)	3 (2%)	5	25
7	5M	12/251 (5%)	11 (92%)	0	1 (8%)	0	5
7	5N	242/251 (96%)	194 (80%)	44 (18%)	4 (2%)	7	31
7	5O	13/251 (5%)	9 (69%)	4 (31%)	0	100	100
8	1d	99/359 (28%)	91 (92%)	8 (8%)	0	100	100
9	1f	34/206 (16%)	28 (82%)	6 (18%)	0	100	100
9	1g	49/206 (24%)	43 (88%)	6 (12%)	0	100	100
10	1i	32/188 (17%)	29 (91%)	2 (6%)	1 (3%)	3	21
10	1j	29/188 (15%)	24 (83%)	4 (14%)	1 (3%)	3	19
10	9M	82/188 (44%)	67 (82%)	15 (18%)	0	100	100
10	9N	82/188 (44%)	71 (87%)	10 (12%)	1 (1%)	11	38
10	9O	39/188 (21%)	25 (64%)	11 (28%)	3 (8%)	1	5
11	1l	37/176 (21%)	25 (68%)	12 (32%)	0	100	100
11	1m	37/176 (21%)	26 (70%)	11 (30%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	1o	27/142 (19%)	24 (89%)	1 (4%)	2 (7%)	1	6
12	1p	28/142 (20%)	27 (96%)	1 (4%)	0	100	100
12	1q	44/142 (31%)	40 (91%)	4 (9%)	0	100	100
12	1r	25/142 (18%)	23 (92%)	2 (8%)	0	100	100
13	2A	248/258 (96%)	216 (87%)	29 (12%)	3 (1%)	11	38
13	2B	249/258 (96%)	212 (85%)	30 (12%)	7 (3%)	4	22
13	2C	249/258 (96%)	209 (84%)	35 (14%)	5 (2%)	6	28
13	2D	77/258 (30%)	67 (87%)	8 (10%)	2 (3%)	4	23
14	2G	225/235 (96%)	187 (83%)	36 (16%)	2 (1%)	14	44
15	2J	105/141 (74%)	91 (87%)	14 (13%)	0	100	100
15	2K	105/141 (74%)	93 (89%)	10 (10%)	2 (2%)	6	29
15	2L	105/141 (74%)	95 (90%)	8 (8%)	2 (2%)	6	29
16	2O	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
17	2R	118/499 (24%)	112 (95%)	6 (5%)	0	100	100
17	2S	374/499 (75%)	366 (98%)	7 (2%)	1 (0%)	37	66
18	2V	282/292 (97%)	239 (85%)	38 (14%)	5 (2%)	7	30
18	2W	282/292 (97%)	243 (86%)	35 (12%)	4 (1%)	9	34
19	3A	185/195 (95%)	169 (91%)	16 (9%)	0	100	100
19	3B	185/195 (95%)	161 (87%)	24 (13%)	0	100	100
19	3C	176/195 (90%)	160 (91%)	16 (9%)	0	100	100
19	3D	170/195 (87%)	151 (89%)	18 (11%)	1 (1%)	22	53
19	3E	184/195 (94%)	163 (89%)	21 (11%)	0	100	100
19	3F	185/195 (95%)	170 (92%)	15 (8%)	0	100	100
19	3G	184/195 (94%)	168 (91%)	16 (9%)	0	100	100
20	3J	491/592 (83%)	400 (82%)	79 (16%)	12 (2%)	5	25
20	3K	68/592 (12%)	52 (76%)	14 (21%)	2 (3%)	3	22
21	3N	256/560 (46%)	245 (96%)	9 (4%)	2 (1%)	16	46
21	3O	276/560 (49%)	261 (95%)	12 (4%)	3 (1%)	12	40
22	3R	163/172 (95%)	130 (80%)	31 (19%)	2 (1%)	11	38
22	3S	125/172 (73%)	105 (84%)	19 (15%)	1 (1%)	16	46
22	3T	163/172 (95%)	137 (84%)	24 (15%)	2 (1%)	11	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	3W	382/541 (71%)	356 (93%)	22 (6%)	4 (1%)	13	42
23	3X	313/541 (58%)	311 (99%)	2 (1%)	0	100	100
23	3Y	102/541 (19%)	101 (99%)	1 (1%)	0	100	100
23	3Z	170/541 (31%)	160 (94%)	9 (5%)	1 (1%)	22	53
24	4A	615/635 (97%)	549 (89%)	65 (11%)	1 (0%)	44	71
24	4B	613/635 (96%)	564 (92%)	49 (8%)	0	100	100
24	4C	615/635 (97%)	551 (90%)	63 (10%)	1 (0%)	44	71
25	4F	311/516 (60%)	301 (97%)	10 (3%)	0	100	100
25	4G	204/516 (40%)	188 (92%)	12 (6%)	4 (2%)	6	28
26	4J	376/380 (99%)	319 (85%)	53 (14%)	4 (1%)	12	40
26	4K	374/380 (98%)	313 (84%)	56 (15%)	5 (1%)	10	36
27	4N	147/243 (60%)	130 (88%)	13 (9%)	4 (3%)	4	22
27	4O	104/243 (43%)	93 (89%)	9 (9%)	2 (2%)	6	29
27	4P	146/243 (60%)	131 (90%)	14 (10%)	1 (1%)	19	50
27	4Q	91/243 (37%)	74 (81%)	16 (18%)	1 (1%)	12	40
28	4T	141/231 (61%)	126 (89%)	11 (8%)	4 (3%)	4	22
28	4U	141/231 (61%)	128 (91%)	12 (8%)	1 (1%)	19	50
28	4V	12/231 (5%)	12 (100%)	0	0	100	100
29	4Y	298/302 (99%)	272 (91%)	23 (8%)	3 (1%)	13	42
30	5A	33/277 (12%)	28 (85%)	4 (12%)	1 (3%)	3	21
30	5B	209/277 (76%)	170 (81%)	34 (16%)	5 (2%)	5	25
30	9Y	136/277 (49%)	102 (75%)	28 (21%)	6 (4%)	2	14
30	9Z	97/277 (35%)	65 (67%)	29 (30%)	3 (3%)	3	21
31	6A	223/236 (94%)	213 (96%)	10 (4%)	0	100	100
31	6B	217/236 (92%)	194 (89%)	23 (11%)	0	100	100
31	6C	221/236 (94%)	208 (94%)	13 (6%)	0	100	100
31	6D	222/236 (94%)	204 (92%)	18 (8%)	0	100	100
31	6E	222/236 (94%)	213 (96%)	9 (4%)	0	100	100
31	6F	222/236 (94%)	204 (92%)	18 (8%)	0	100	100
32	6I	76/123 (62%)	65 (86%)	11 (14%)	0	100	100
32	6J	51/123 (42%)	46 (90%)	5 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	6M	389/469 (83%)	370 (95%)	18 (5%)	1 (0%)	37	66
33	6N	78/469 (17%)	69 (88%)	9 (12%)	0	100	100
34	6Q	195/310 (63%)	182 (93%)	13 (7%)	0	100	100
34	6R	70/310 (23%)	59 (84%)	11 (16%)	0	100	100
35	6U	147/379 (39%)	143 (97%)	4 (3%)	0	100	100
35	6V	272/379 (72%)	256 (94%)	14 (5%)	2 (1%)	19	50
35	6W	241/379 (64%)	229 (95%)	9 (4%)	3 (1%)	11	38
35	6X	119/379 (31%)	111 (93%)	7 (6%)	1 (1%)	16	46
36	7A	721/744 (97%)	612 (85%)	96 (13%)	13 (2%)	7	30
36	7B	445/744 (60%)	372 (84%)	68 (15%)	5 (1%)	12	40
36	7C	533/744 (72%)	441 (83%)	81 (15%)	11 (2%)	5	27
36	7D	720/744 (97%)	621 (86%)	87 (12%)	12 (2%)	7	31
37	7G	525/645 (81%)	437 (83%)	77 (15%)	11 (2%)	5	27
37	7H	525/645 (81%)	432 (82%)	80 (15%)	13 (2%)	4	24
37	7I	610/645 (95%)	519 (85%)	79 (13%)	12 (2%)	6	28
38	7M	261/322 (81%)	239 (92%)	21 (8%)	1 (0%)	30	61
38	7N	66/322 (20%)	64 (97%)	2 (3%)	0	100	100
39	7Q	141/185 (76%)	118 (84%)	21 (15%)	2 (1%)	9	34
39	7R	138/185 (75%)	122 (88%)	16 (12%)	0	100	100
40	7U	91/200 (46%)	61 (67%)	25 (28%)	5 (6%)	1	10
40	7V	51/200 (26%)	44 (86%)	6 (12%)	1 (2%)	6	28
41	7Y	198/204 (97%)	162 (82%)	31 (16%)	5 (2%)	4	24
41	7Z	62/204 (30%)	40 (64%)	20 (32%)	2 (3%)	3	20
42	8A	241/268 (90%)	203 (84%)	35 (14%)	3 (1%)	11	38
43	8D	395/462 (86%)	383 (97%)	11 (3%)	1 (0%)	37	66
43	8E	174/462 (38%)	170 (98%)	3 (2%)	1 (1%)	22	53
43	8F	261/462 (56%)	252 (97%)	9 (3%)	0	100	100
43	8G	395/462 (86%)	379 (96%)	15 (4%)	1 (0%)	37	66
44	8J	401/430 (93%)	380 (95%)	19 (5%)	2 (0%)	25	56
44	8K	318/430 (74%)	307 (96%)	10 (3%)	1 (0%)	37	66
44	8L	401/430 (93%)	383 (96%)	16 (4%)	2 (0%)	25	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	8M	124/430 (29%)	112 (90%)	11 (9%)	1 (1%)	16	46
44	8N	15/430 (4%)	12 (80%)	2 (13%)	1 (7%)	1	7
45	8Q	19/402 (5%)	19 (100%)	0	0	100	100
45	8R	398/402 (99%)	386 (97%)	10 (2%)	2 (0%)	25	56
45	8S	300/402 (75%)	290 (97%)	8 (3%)	2 (1%)	19	50
45	8T	398/402 (99%)	384 (96%)	13 (3%)	1 (0%)	37	66
45	8U	118/402 (29%)	116 (98%)	2 (2%)	0	100	100
46	8X	102/119 (86%)	82 (80%)	20 (20%)	0	100	100
46	8Y	102/119 (86%)	84 (82%)	16 (16%)	2 (2%)	6	28
46	8Z	102/119 (86%)	85 (83%)	15 (15%)	2 (2%)	6	28
47	9A	205/220 (93%)	163 (80%)	37 (18%)	5 (2%)	5	25
48	9D	94/171 (55%)	79 (84%)	15 (16%)	0	100	100
49	9G	148/150 (99%)	133 (90%)	12 (8%)	3 (2%)	6	28
50	9J	99/179 (55%)	95 (96%)	3 (3%)	1 (1%)	13	42
51	9R	140/153 (92%)	120 (86%)	20 (14%)	0	100	100
52	9T	71/83 (86%)	62 (87%)	9 (13%)	0	100	100
53	9V	22/294 (8%)	17 (77%)	2 (9%)	3 (14%)	0	1
53	9W	68/294 (23%)	62 (91%)	6 (9%)	0	100	100
54	AA	435/451 (96%)	407 (94%)	26 (6%)	2 (0%)	25	56
54	AB	435/451 (96%)	406 (93%)	29 (7%)	0	100	100
54	AE	435/451 (96%)	402 (92%)	33 (8%)	0	100	100
54	AG	435/451 (96%)	399 (92%)	35 (8%)	1 (0%)	44	71
54	AI	435/451 (96%)	410 (94%)	25 (6%)	0	100	100
54	AK	435/451 (96%)	400 (92%)	35 (8%)	0	100	100
54	AM	435/451 (96%)	407 (94%)	28 (6%)	0	100	100
54	BA	435/451 (96%)	407 (94%)	27 (6%)	1 (0%)	44	71
54	BB	435/451 (96%)	409 (94%)	24 (6%)	2 (0%)	25	56
54	BE	435/451 (96%)	406 (93%)	29 (7%)	0	100	100
54	BG	435/451 (96%)	409 (94%)	25 (6%)	1 (0%)	44	71
54	BI	435/451 (96%)	407 (94%)	28 (6%)	0	100	100
54	BK	435/451 (96%)	401 (92%)	33 (8%)	1 (0%)	44	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	BM	435/451 (96%)	403 (93%)	31 (7%)	1 (0%)	44	71
54	CA	435/451 (96%)	402 (92%)	32 (7%)	1 (0%)	44	71
54	CB	435/451 (96%)	397 (91%)	37 (8%)	1 (0%)	44	71
54	CE	435/451 (96%)	401 (92%)	32 (7%)	2 (0%)	25	56
54	CG	435/451 (96%)	409 (94%)	25 (6%)	1 (0%)	44	71
54	CI	435/451 (96%)	409 (94%)	26 (6%)	0	100	100
54	CK	435/451 (96%)	399 (92%)	36 (8%)	0	100	100
54	CM	435/451 (96%)	402 (92%)	31 (7%)	2 (0%)	25	56
54	DA	435/451 (96%)	406 (93%)	29 (7%)	0	100	100
54	DB	435/451 (96%)	403 (93%)	32 (7%)	0	100	100
54	DE	435/451 (96%)	395 (91%)	39 (9%)	1 (0%)	44	71
54	DG	435/451 (96%)	385 (88%)	48 (11%)	2 (0%)	25	56
54	DI	435/451 (96%)	395 (91%)	39 (9%)	1 (0%)	44	71
54	DK	435/451 (96%)	395 (91%)	39 (9%)	1 (0%)	44	71
54	DM	435/451 (96%)	398 (92%)	36 (8%)	1 (0%)	44	71
54	EA	435/451 (96%)	367 (84%)	56 (13%)	12 (3%)	4	22
54	EC	435/451 (96%)	411 (94%)	23 (5%)	1 (0%)	44	71
54	EE	435/451 (96%)	402 (92%)	32 (7%)	1 (0%)	44	71
54	EG	435/451 (96%)	408 (94%)	27 (6%)	0	100	100
54	EI	435/451 (96%)	398 (92%)	35 (8%)	2 (0%)	25	56
54	EK	435/451 (96%)	404 (93%)	31 (7%)	0	100	100
54	FA	435/451 (96%)	366 (84%)	57 (13%)	12 (3%)	4	22
54	FB	435/451 (96%)	409 (94%)	25 (6%)	1 (0%)	44	71
54	FE	435/451 (96%)	361 (83%)	60 (14%)	14 (3%)	3	20
54	FG	435/451 (96%)	397 (91%)	37 (8%)	1 (0%)	44	71
54	FI	435/451 (96%)	365 (84%)	59 (14%)	11 (2%)	4	24
54	FK	435/451 (96%)	392 (90%)	43 (10%)	0	100	100
54	GA	435/451 (96%)	393 (90%)	42 (10%)	0	100	100
54	GB	435/451 (96%)	400 (92%)	34 (8%)	1 (0%)	44	71
54	GE	435/451 (96%)	411 (94%)	23 (5%)	1 (0%)	44	71
54	GG	435/451 (96%)	408 (94%)	26 (6%)	1 (0%)	44	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	GI	435/451 (96%)	396 (91%)	39 (9%)	0	100	100
54	GK	435/451 (96%)	388 (89%)	45 (10%)	2 (0%)	25	56
54	HA	435/451 (96%)	402 (92%)	31 (7%)	2 (0%)	25	56
54	HB	435/451 (96%)	399 (92%)	36 (8%)	0	100	100
54	HE	428/451 (95%)	395 (92%)	31 (7%)	2 (0%)	25	56
54	HG	431/451 (96%)	400 (93%)	29 (7%)	2 (0%)	25	56
54	HI	435/451 (96%)	401 (92%)	33 (8%)	1 (0%)	44	71
54	HK	431/451 (96%)	404 (94%)	26 (6%)	1 (0%)	44	71
54	IA	435/451 (96%)	399 (92%)	35 (8%)	1 (0%)	44	71
54	IB	430/451 (95%)	400 (93%)	28 (6%)	2 (0%)	25	56
54	IE	435/451 (96%)	404 (93%)	31 (7%)	0	100	100
54	IG	435/451 (96%)	402 (92%)	33 (8%)	0	100	100
54	II	431/451 (96%)	403 (94%)	28 (6%)	0	100	100
54	IK	435/451 (96%)	401 (92%)	32 (7%)	2 (0%)	25	56
54	IM	435/451 (96%)	392 (90%)	43 (10%)	0	100	100
54	JA	428/451 (95%)	397 (93%)	30 (7%)	1 (0%)	44	71
54	JB	435/451 (96%)	406 (93%)	28 (6%)	1 (0%)	44	71
54	JE	435/451 (96%)	410 (94%)	24 (6%)	1 (0%)	44	71
54	JG	435/451 (96%)	404 (93%)	31 (7%)	0	100	100
54	JI	435/451 (96%)	401 (92%)	33 (8%)	1 (0%)	44	71
54	JK	435/451 (96%)	409 (94%)	25 (6%)	1 (0%)	44	71
54	KA	435/451 (96%)	416 (96%)	18 (4%)	1 (0%)	44	71
54	KB	430/451 (95%)	401 (93%)	29 (7%)	0	100	100
54	KE	435/451 (96%)	405 (93%)	29 (7%)	1 (0%)	44	71
54	KG	435/451 (96%)	404 (93%)	29 (7%)	2 (0%)	25	56
54	KI	435/451 (96%)	410 (94%)	25 (6%)	0	100	100
54	KK	435/451 (96%)	415 (95%)	20 (5%)	0	100	100
54	LA	435/451 (96%)	412 (95%)	23 (5%)	0	100	100
54	LB	435/451 (96%)	405 (93%)	29 (7%)	1 (0%)	44	71
54	LE	435/451 (96%)	414 (95%)	20 (5%)	1 (0%)	44	71
54	LG	435/451 (96%)	408 (94%)	25 (6%)	2 (0%)	25	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	LI	435/451 (96%)	414 (95%)	21 (5%)	0	100	100
54	LK	435/451 (96%)	416 (96%)	18 (4%)	1 (0%)	44	71
54	MA	435/451 (96%)	403 (93%)	30 (7%)	2 (0%)	25	56
54	MB	435/451 (96%)	412 (95%)	22 (5%)	1 (0%)	44	71
54	ME	435/451 (96%)	409 (94%)	25 (6%)	1 (0%)	44	71
54	MG	435/451 (96%)	412 (95%)	23 (5%)	0	100	100
54	MI	435/451 (96%)	401 (92%)	32 (7%)	2 (0%)	25	56
54	MK	435/451 (96%)	401 (92%)	34 (8%)	0	100	100
54	ML	435/451 (96%)	414 (95%)	21 (5%)	0	100	100
54	NA	431/451 (96%)	401 (93%)	28 (6%)	2 (0%)	25	56
54	NB	435/451 (96%)	387 (89%)	44 (10%)	4 (1%)	14	44
54	NE	435/451 (96%)	402 (92%)	32 (7%)	1 (0%)	44	71
54	NG	435/451 (96%)	401 (92%)	32 (7%)	2 (0%)	25	56
54	NI	430/451 (95%)	395 (92%)	34 (8%)	1 (0%)	44	71
54	NL	429/451 (95%)	389 (91%)	39 (9%)	1 (0%)	44	71
54	OA	435/451 (96%)	396 (91%)	38 (9%)	1 (0%)	44	71
54	OB	430/451 (95%)	405 (94%)	23 (5%)	2 (0%)	25	56
54	OE	435/451 (96%)	401 (92%)	32 (7%)	2 (0%)	25	56
54	OG	435/451 (96%)	404 (93%)	31 (7%)	0	100	100
54	OI	435/451 (96%)	405 (93%)	28 (6%)	2 (0%)	25	56
54	OK	435/451 (96%)	402 (92%)	32 (7%)	1 (0%)	44	71
54	OL	435/451 (96%)	393 (90%)	42 (10%)	0	100	100
54	PA	435/451 (96%)	403 (93%)	31 (7%)	1 (0%)	44	71
54	PB	435/451 (96%)	399 (92%)	35 (8%)	1 (0%)	44	71
54	PE	435/451 (96%)	400 (92%)	33 (8%)	2 (0%)	25	56
54	PG	435/451 (96%)	402 (92%)	33 (8%)	0	100	100
54	PI	435/451 (96%)	398 (92%)	36 (8%)	1 (0%)	44	71
54	PK	435/451 (96%)	392 (90%)	40 (9%)	3 (1%)	19	50
54	PL	435/451 (96%)	403 (93%)	32 (7%)	0	100	100
54	QA	435/451 (96%)	407 (94%)	25 (6%)	3 (1%)	19	50
54	QB	435/451 (96%)	392 (90%)	43 (10%)	0	100	100

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Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	QE	435/451 (96%)	390 (90%)	44 (10%)	1 (0%)	44	71
54	QG	435/451 (96%)	388 (89%)	45 (10%)	2 (0%)	25	56
54	QI	435/451 (96%)	398 (92%)	35 (8%)	2 (0%)	25	56
54	QK	429/451 (95%)	404 (94%)	24 (6%)	1 (0%)	44	71
54	QL	432/451 (96%)	389 (90%)	42 (10%)	1 (0%)	44	71
54	RA	435/451 (96%)	414 (95%)	18 (4%)	3 (1%)	19	50
54	RB	435/451 (96%)	391 (90%)	42 (10%)	2 (0%)	25	56
54	RE	435/451 (96%)	392 (90%)	41 (9%)	2 (0%)	25	56
54	RG	435/451 (96%)	395 (91%)	38 (9%)	2 (0%)	25	56
54	RI	435/451 (96%)	400 (92%)	35 (8%)	0	100	100
54	RK	435/451 (96%)	404 (93%)	30 (7%)	1 (0%)	44	71
54	RL	435/451 (96%)	399 (92%)	35 (8%)	1 (0%)	44	71
54	SA	435/451 (96%)	398 (92%)	37 (8%)	0	100	100
54	SB	435/451 (96%)	411 (94%)	23 (5%)	1 (0%)	44	71
54	SE	435/451 (96%)	402 (92%)	33 (8%)	0	100	100
54	SG	435/451 (96%)	409 (94%)	23 (5%)	3 (1%)	19	50
54	SI	435/451 (96%)	408 (94%)	26 (6%)	1 (0%)	44	71
54	SK	435/451 (96%)	399 (92%)	35 (8%)	1 (0%)	44	71
54	TA	432/451 (96%)	404 (94%)	28 (6%)	0	100	100
54	TB	432/451 (96%)	410 (95%)	21 (5%)	1 (0%)	44	71
54	TE	435/451 (96%)	406 (93%)	29 (7%)	0	100	100
54	TG	435/451 (96%)	402 (92%)	31 (7%)	2 (0%)	25	56
54	TI	435/451 (96%)	404 (93%)	31 (7%)	0	100	100
54	TK	435/451 (96%)	399 (92%)	34 (8%)	2 (0%)	25	56
54	UA	432/451 (96%)	395 (91%)	37 (9%)	0	100	100
54	UB	430/451 (95%)	398 (93%)	32 (7%)	0	100	100
54	UE	435/451 (96%)	409 (94%)	26 (6%)	0	100	100
54	UG	435/451 (96%)	397 (91%)	38 (9%)	0	100	100
54	UI	435/451 (96%)	395 (91%)	39 (9%)	1 (0%)	44	71
54	UK	435/451 (96%)	394 (91%)	41 (9%)	0	100	100
54	VA	435/451 (96%)	399 (92%)	33 (8%)	3 (1%)	19	50

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Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	VB	435/451 (96%)	401 (92%)	34 (8%)	0	100	100
54	VE	435/451 (96%)	407 (94%)	26 (6%)	2 (0%)	25	56
54	VG	431/451 (96%)	395 (92%)	36 (8%)	0	100	100
54	VI	435/451 (96%)	399 (92%)	36 (8%)	0	100	100
54	VK	435/451 (96%)	407 (94%)	27 (6%)	1 (0%)	44	71
54	WA	435/451 (96%)	408 (94%)	26 (6%)	1 (0%)	44	71
54	WB	432/451 (96%)	397 (92%)	33 (8%)	2 (0%)	25	56
54	WE	435/451 (96%)	394 (91%)	40 (9%)	1 (0%)	44	71
54	WG	435/451 (96%)	400 (92%)	33 (8%)	2 (0%)	25	56
54	WI	435/451 (96%)	389 (89%)	45 (10%)	1 (0%)	44	71
54	WK	435/451 (96%)	392 (90%)	39 (9%)	4 (1%)	14	44
55	AC	429/447 (96%)	396 (92%)	30 (7%)	3 (1%)	19	50
55	AD	429/447 (96%)	398 (93%)	29 (7%)	2 (0%)	25	56
55	AF	429/447 (96%)	396 (92%)	30 (7%)	3 (1%)	19	50
55	AH	429/447 (96%)	391 (91%)	32 (8%)	6 (1%)	9	34
55	AJ	429/447 (96%)	395 (92%)	31 (7%)	3 (1%)	19	50
55	AL	429/447 (96%)	398 (93%)	30 (7%)	1 (0%)	44	71
55	BC	429/447 (96%)	394 (92%)	32 (8%)	3 (1%)	19	50
55	BD	429/447 (96%)	385 (90%)	42 (10%)	2 (0%)	25	56
55	BF	429/447 (96%)	388 (90%)	38 (9%)	3 (1%)	19	50
55	BH	429/447 (96%)	393 (92%)	34 (8%)	2 (0%)	25	56
55	BJ	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	25	56
55	BL	429/447 (96%)	392 (91%)	33 (8%)	4 (1%)	14	44
55	CC	429/447 (96%)	371 (86%)	54 (13%)	4 (1%)	14	44
55	CD	429/447 (96%)	385 (90%)	40 (9%)	4 (1%)	14	44
55	CF	429/447 (96%)	390 (91%)	38 (9%)	1 (0%)	44	71
55	CH	429/447 (96%)	390 (91%)	37 (9%)	2 (0%)	25	56
55	CJ	429/447 (96%)	382 (89%)	45 (10%)	2 (0%)	25	56
55	CL	429/447 (96%)	386 (90%)	41 (10%)	2 (0%)	25	56
55	DC	429/447 (96%)	391 (91%)	35 (8%)	3 (1%)	19	50
55	DD	429/447 (96%)	386 (90%)	40 (9%)	3 (1%)	19	50

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Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	DF	429/447 (96%)	380 (89%)	44 (10%)	5 (1%)	11	38
55	DH	429/447 (96%)	393 (92%)	35 (8%)	1 (0%)	44	71
55	DJ	429/447 (96%)	389 (91%)	36 (8%)	4 (1%)	14	44
55	DL	429/447 (96%)	389 (91%)	36 (8%)	4 (1%)	14	44
55	EB	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	25	56
55	ED	429/447 (96%)	383 (89%)	42 (10%)	4 (1%)	14	44
55	EF	429/447 (96%)	394 (92%)	34 (8%)	1 (0%)	44	71
55	EH	429/447 (96%)	387 (90%)	36 (8%)	6 (1%)	9	34
55	EJ	429/447 (96%)	389 (91%)	39 (9%)	1 (0%)	44	71
55	EL	429/447 (96%)	389 (91%)	38 (9%)	2 (0%)	25	56
55	EM	429/447 (96%)	385 (90%)	40 (9%)	4 (1%)	14	44
55	FC	429/447 (96%)	386 (90%)	42 (10%)	1 (0%)	44	71
55	FD	429/447 (96%)	394 (92%)	32 (8%)	3 (1%)	19	50
55	FF	429/447 (96%)	403 (94%)	26 (6%)	0	100	100
55	FH	429/447 (96%)	384 (90%)	44 (10%)	1 (0%)	44	71
55	FJ	429/447 (96%)	390 (91%)	35 (8%)	4 (1%)	14	44
55	FL	429/447 (96%)	384 (90%)	40 (9%)	5 (1%)	11	38
55	FM	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	25	56
55	GC	429/447 (96%)	382 (89%)	44 (10%)	3 (1%)	19	50
55	GD	429/447 (96%)	376 (88%)	50 (12%)	3 (1%)	19	50
55	GF	429/447 (96%)	386 (90%)	39 (9%)	4 (1%)	14	44
55	GH	429/447 (96%)	391 (91%)	34 (8%)	4 (1%)	14	44
55	GJ	429/447 (96%)	393 (92%)	33 (8%)	3 (1%)	19	50
55	GL	429/447 (96%)	390 (91%)	37 (9%)	2 (0%)	25	56
55	GM	429/447 (96%)	399 (93%)	29 (7%)	1 (0%)	44	71
55	HC	429/447 (96%)	398 (93%)	28 (6%)	3 (1%)	19	50
55	HD	429/447 (96%)	382 (89%)	45 (10%)	2 (0%)	25	56
55	HF	429/447 (96%)	395 (92%)	32 (8%)	2 (0%)	25	56
55	HH	429/447 (96%)	393 (92%)	32 (8%)	4 (1%)	14	44
55	HJ	429/447 (96%)	398 (93%)	27 (6%)	4 (1%)	14	44
55	HL	429/447 (96%)	384 (90%)	40 (9%)	5 (1%)	11	38

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	HM	429/447 (96%)	393 (92%)	33 (8%)	3 (1%)	19	50
55	IC	429/447 (96%)	385 (90%)	42 (10%)	2 (0%)	25	56
55	ID	429/447 (96%)	390 (91%)	36 (8%)	3 (1%)	19	50
55	IF	429/447 (96%)	393 (92%)	34 (8%)	2 (0%)	25	56
55	IH	429/447 (96%)	396 (92%)	30 (7%)	3 (1%)	19	50
55	IJ	429/447 (96%)	386 (90%)	40 (9%)	3 (1%)	19	50
55	IL	429/447 (96%)	385 (90%)	39 (9%)	5 (1%)	11	38
55	JC	429/447 (96%)	407 (95%)	20 (5%)	2 (0%)	25	56
55	JD	429/447 (96%)	391 (91%)	36 (8%)	2 (0%)	25	56
55	JF	429/447 (96%)	385 (90%)	40 (9%)	4 (1%)	14	44
55	JH	429/447 (96%)	379 (88%)	45 (10%)	5 (1%)	11	38
55	JJ	429/447 (96%)	393 (92%)	32 (8%)	4 (1%)	14	44
55	JL	429/447 (96%)	382 (89%)	45 (10%)	2 (0%)	25	56
55	JM	429/447 (96%)	400 (93%)	27 (6%)	2 (0%)	25	56
55	KC	429/447 (96%)	389 (91%)	36 (8%)	4 (1%)	14	44
55	KD	429/447 (96%)	388 (90%)	38 (9%)	3 (1%)	19	50
55	KF	429/447 (96%)	399 (93%)	27 (6%)	3 (1%)	19	50
55	KH	429/447 (96%)	398 (93%)	28 (6%)	3 (1%)	19	50
55	KJ	429/447 (96%)	390 (91%)	37 (9%)	2 (0%)	25	56
55	KL	429/447 (96%)	386 (90%)	42 (10%)	1 (0%)	44	71
55	KM	429/447 (96%)	409 (95%)	19 (4%)	1 (0%)	44	71
55	LC	429/447 (96%)	396 (92%)	30 (7%)	3 (1%)	19	50
55	LD	429/447 (96%)	397 (92%)	30 (7%)	2 (0%)	25	56
55	LF	429/447 (96%)	395 (92%)	32 (8%)	2 (0%)	25	56
55	LH	429/447 (96%)	388 (90%)	37 (9%)	4 (1%)	14	44
55	LJ	429/447 (96%)	397 (92%)	30 (7%)	2 (0%)	25	56
55	LL	429/447 (96%)	392 (91%)	34 (8%)	3 (1%)	19	50
55	LM	429/447 (96%)	397 (92%)	31 (7%)	1 (0%)	44	71
55	MC	429/447 (96%)	392 (91%)	35 (8%)	2 (0%)	25	56
55	MD	429/447 (96%)	402 (94%)	23 (5%)	4 (1%)	14	44
55	MF	429/447 (96%)	407 (95%)	21 (5%)	1 (0%)	44	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	MH	429/447 (96%)	385 (90%)	40 (9%)	4 (1%)	14	44
55	MJ	429/447 (96%)	395 (92%)	30 (7%)	4 (1%)	14	44
55	MM	429/447 (96%)	389 (91%)	38 (9%)	2 (0%)	25	56
55	NC	429/447 (96%)	383 (89%)	44 (10%)	2 (0%)	25	56
55	ND	429/447 (96%)	391 (91%)	33 (8%)	5 (1%)	11	38
55	NF	429/447 (96%)	388 (90%)	36 (8%)	5 (1%)	11	38
55	NH	429/447 (96%)	386 (90%)	42 (10%)	1 (0%)	44	71
55	NJ	429/447 (96%)	381 (89%)	44 (10%)	4 (1%)	14	44
55	NK	429/447 (96%)	388 (90%)	40 (9%)	1 (0%)	44	71
55	NM	429/447 (96%)	381 (89%)	45 (10%)	3 (1%)	19	50
55	OC	429/447 (96%)	391 (91%)	36 (8%)	2 (0%)	25	56
55	OD	429/447 (96%)	386 (90%)	41 (10%)	2 (0%)	25	56
55	OF	429/447 (96%)	395 (92%)	32 (8%)	2 (0%)	25	56
55	OH	429/447 (96%)	391 (91%)	38 (9%)	0	100	100
55	OJ	429/447 (96%)	392 (91%)	34 (8%)	3 (1%)	19	50
55	OM	429/447 (96%)	393 (92%)	33 (8%)	3 (1%)	19	50
55	PC	429/447 (96%)	389 (91%)	36 (8%)	4 (1%)	14	44
55	PD	429/447 (96%)	396 (92%)	31 (7%)	2 (0%)	25	56
55	PF	429/447 (96%)	389 (91%)	38 (9%)	2 (0%)	25	56
55	PH	429/447 (96%)	391 (91%)	36 (8%)	2 (0%)	25	56
55	PJ	429/447 (96%)	377 (88%)	49 (11%)	3 (1%)	19	50
55	PM	429/447 (96%)	387 (90%)	38 (9%)	4 (1%)	14	44
55	QC	429/447 (96%)	386 (90%)	39 (9%)	4 (1%)	14	44
55	QD	429/447 (96%)	391 (91%)	37 (9%)	1 (0%)	44	71
55	QF	429/447 (96%)	383 (89%)	43 (10%)	3 (1%)	19	50
55	QH	429/447 (96%)	388 (90%)	38 (9%)	3 (1%)	19	50
55	QJ	429/447 (96%)	379 (88%)	49 (11%)	1 (0%)	44	71
55	QM	429/447 (96%)	393 (92%)	35 (8%)	1 (0%)	44	71
55	RC	429/447 (96%)	383 (89%)	44 (10%)	2 (0%)	25	56
55	RD	429/447 (96%)	395 (92%)	30 (7%)	4 (1%)	14	44
55	RF	429/447 (96%)	391 (91%)	36 (8%)	2 (0%)	25	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	RH	429/447 (96%)	388 (90%)	38 (9%)	3 (1%)	19	50
55	RJ	429/447 (96%)	381 (89%)	46 (11%)	2 (0%)	25	56
55	RM	429/447 (96%)	396 (92%)	29 (7%)	4 (1%)	14	44
55	SC	429/447 (96%)	396 (92%)	31 (7%)	2 (0%)	25	56
55	SD	429/447 (96%)	380 (89%)	48 (11%)	1 (0%)	44	71
55	SF	429/447 (96%)	405 (94%)	21 (5%)	3 (1%)	19	50
55	SH	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	25	56
55	SJ	429/447 (96%)	389 (91%)	38 (9%)	2 (0%)	25	56
55	SL	429/447 (96%)	384 (90%)	42 (10%)	3 (1%)	19	50
55	SM	429/447 (96%)	390 (91%)	36 (8%)	3 (1%)	19	50
55	TC	429/447 (96%)	386 (90%)	40 (9%)	3 (1%)	19	50
55	TD	429/447 (96%)	384 (90%)	42 (10%)	3 (1%)	19	50
55	TF	429/447 (96%)	395 (92%)	32 (8%)	2 (0%)	25	56
55	TH	429/447 (96%)	385 (90%)	41 (10%)	3 (1%)	19	50
55	TJ	429/447 (96%)	386 (90%)	39 (9%)	4 (1%)	14	44
55	TL	429/447 (96%)	381 (89%)	47 (11%)	1 (0%)	44	71
55	TM	429/447 (96%)	384 (90%)	42 (10%)	3 (1%)	19	50
55	UC	429/447 (96%)	380 (89%)	46 (11%)	3 (1%)	19	50
55	UD	429/447 (96%)	392 (91%)	33 (8%)	4 (1%)	14	44
55	UF	429/447 (96%)	379 (88%)	46 (11%)	4 (1%)	14	44
55	UH	429/447 (96%)	380 (89%)	45 (10%)	4 (1%)	14	44
55	UJ	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	25	56
55	UL	429/447 (96%)	381 (89%)	45 (10%)	3 (1%)	19	50
55	UM	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	25	56
55	VC	429/447 (96%)	378 (88%)	48 (11%)	3 (1%)	19	50
55	VD	429/447 (96%)	386 (90%)	39 (9%)	4 (1%)	14	44
55	VF	429/447 (96%)	388 (90%)	39 (9%)	2 (0%)	25	56
55	VH	429/447 (96%)	372 (87%)	53 (12%)	4 (1%)	14	44
55	VJ	429/447 (96%)	384 (90%)	44 (10%)	1 (0%)	44	71
55	VL	429/447 (96%)	377 (88%)	48 (11%)	4 (1%)	14	44
55	VM	429/447 (96%)	397 (92%)	31 (7%)	1 (0%)	44	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	WC	429/447 (96%)	396 (92%)	30 (7%)	3 (1%)	19	50
55	WD	429/447 (96%)	392 (91%)	35 (8%)	2 (0%)	25	56
55	WF	429/447 (96%)	390 (91%)	36 (8%)	3 (1%)	19	50
55	WH	429/447 (96%)	394 (92%)	34 (8%)	1 (0%)	44	71
55	WJ	429/447 (96%)	405 (94%)	23 (5%)	1 (0%)	44	71
55	WL	429/447 (96%)	390 (91%)	36 (8%)	3 (1%)	19	50
All	All	159050/186788 (85%)	144743 (91%)	13391 (8%)	916 (1%)	24	53

5 of 916 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	1E	132	ARG
2	1E	359	GLU
2	1F	51	ASP
2	1H	222	MET
3	1L	68	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1A	34/253 (13%)	34 (100%)	0	100	100
1	1B	221/253 (87%)	221 (100%)	0	100	100
2	1E	350/374 (94%)	349 (100%)	1 (0%)	91	94
2	1F	140/374 (37%)	139 (99%)	1 (1%)	81	88
2	1G	248/374 (66%)	247 (100%)	1 (0%)	89	93
2	1H	352/374 (94%)	350 (99%)	2 (1%)	84	90
3	1K	159/612 (26%)	159 (100%)	0	100	100
3	1L	159/612 (26%)	158 (99%)	1 (1%)	84	90
3	1M	155/612 (25%)	155 (100%)	0	100	100
3	1v	187/612 (31%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1w	81/612 (13%)	81 (100%)	0	100	100
3	1x	226/612 (37%)	225 (100%)	1 (0%)	89	93
3	1y	178/612 (29%)	178 (100%)	0	100	100
3	1z	81/612 (13%)	80 (99%)	1 (1%)	67	80
3	2a	50/612 (8%)	50 (100%)	0	100	100
4	1P	175/183 (96%)	175 (100%)	0	100	100
4	1Q	121/183 (66%)	120 (99%)	1 (1%)	79	87
5	1T	199/383 (52%)	198 (100%)	1 (0%)	86	91
5	1U	97/383 (25%)	97 (100%)	0	100	100
5	1V	201/383 (52%)	201 (100%)	0	100	100
5	1W	95/383 (25%)	95 (100%)	0	100	100
6	1Y	112/126 (89%)	112 (100%)	0	100	100
7	1a	118/213 (55%)	118 (100%)	0	100	100
7	1b	99/213 (46%)	99 (100%)	0	100	100
7	5E	127/213 (60%)	127 (100%)	0	100	100
7	5F	99/213 (46%)	99 (100%)	0	100	100
7	5G	117/213 (55%)	117 (100%)	0	100	100
7	5H	103/213 (48%)	103 (100%)	0	100	100
7	5I	22/213 (10%)	21 (96%)	1 (4%)	23	52
7	5J	197/213 (92%)	197 (100%)	0	100	100
7	5K	109/213 (51%)	108 (99%)	1 (1%)	75	85
7	5L	110/213 (52%)	109 (99%)	1 (1%)	75	85
7	5M	14/213 (7%)	14 (100%)	0	100	100
7	5N	206/213 (97%)	206 (100%)	0	100	100
7	5O	12/213 (6%)	12 (100%)	0	100	100
8	1d	92/311 (30%)	90 (98%)	2 (2%)	47	69
9	1f	33/180 (18%)	33 (100%)	0	100	100
9	1g	48/180 (27%)	48 (100%)	0	100	100
10	1i	31/164 (19%)	31 (100%)	0	100	100
10	1j	28/164 (17%)	28 (100%)	0	100	100
10	9M	76/164 (46%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	9N	76/164 (46%)	76 (100%)	0	100	100
10	9O	37/164 (23%)	37 (100%)	0	100	100
11	1l	33/153 (22%)	33 (100%)	0	100	100
11	1m	33/153 (22%)	32 (97%)	1 (3%)	36	62
12	1o	26/129 (20%)	26 (100%)	0	100	100
12	1p	27/129 (21%)	27 (100%)	0	100	100
12	1q	41/129 (32%)	40 (98%)	1 (2%)	44	68
12	1r	24/129 (19%)	24 (100%)	0	100	100
13	2A	226/233 (97%)	226 (100%)	0	100	100
13	2B	226/233 (97%)	224 (99%)	2 (1%)	75	85
13	2C	227/233 (97%)	227 (100%)	0	100	100
13	2D	69/233 (30%)	69 (100%)	0	100	100
14	2G	199/205 (97%)	199 (100%)	0	100	100
15	2J	93/122 (76%)	93 (100%)	0	100	100
15	2K	93/122 (76%)	93 (100%)	0	100	100
15	2L	93/122 (76%)	93 (100%)	0	100	100
16	2O	99/100 (99%)	99 (100%)	0	100	100
17	2R	108/457 (24%)	108 (100%)	0	100	100
17	2S	347/457 (76%)	346 (100%)	1 (0%)	91	94
18	2V	252/259 (97%)	251 (100%)	1 (0%)	89	93
18	2W	252/259 (97%)	252 (100%)	0	100	100
19	3A	174/180 (97%)	174 (100%)	0	100	100
19	3B	174/180 (97%)	173 (99%)	1 (1%)	84	90
19	3C	167/180 (93%)	167 (100%)	0	100	100
19	3D	164/180 (91%)	164 (100%)	0	100	100
19	3E	173/180 (96%)	173 (100%)	0	100	100
19	3F	174/180 (97%)	174 (100%)	0	100	100
19	3G	173/180 (96%)	172 (99%)	1 (1%)	84	90
20	3J	429/509 (84%)	421 (98%)	8 (2%)	52	72
20	3K	61/509 (12%)	60 (98%)	1 (2%)	58	76
21	3N	222/478 (46%)	219 (99%)	3 (1%)	62	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	3O	240/478 (50%)	234 (98%)	6 (2%)	42	67
22	3R	147/154 (96%)	146 (99%)	1 (1%)	81	88
22	3S	112/154 (73%)	112 (100%)	0	100	100
22	3T	147/154 (96%)	147 (100%)	0	100	100
23	3W	342/480 (71%)	337 (98%)	5 (2%)	60	77
23	3X	278/480 (58%)	276 (99%)	2 (1%)	81	88
23	3Y	89/480 (18%)	89 (100%)	0	100	100
23	3Z	153/480 (32%)	152 (99%)	1 (1%)	81	88
24	4A	532/546 (97%)	532 (100%)	0	100	100
24	4B	530/546 (97%)	528 (100%)	2 (0%)	89	93
24	4C	532/546 (97%)	531 (100%)	1 (0%)	92	95
25	4F	266/454 (59%)	266 (100%)	0	100	100
25	4G	191/454 (42%)	191 (100%)	0	100	100
26	4J	325/327 (99%)	324 (100%)	1 (0%)	91	94
26	4K	324/327 (99%)	324 (100%)	0	100	100
27	4N	132/212 (62%)	132 (100%)	0	100	100
27	4O	92/212 (43%)	92 (100%)	0	100	100
27	4P	129/212 (61%)	129 (100%)	0	100	100
27	4Q	75/212 (35%)	74 (99%)	1 (1%)	65	79
28	4T	133/209 (64%)	133 (100%)	0	100	100
28	4U	133/209 (64%)	132 (99%)	1 (1%)	79	87
28	4V	12/209 (6%)	12 (100%)	0	100	100
29	4Y	265/267 (99%)	265 (100%)	0	100	100
30	5A	26/237 (11%)	26 (100%)	0	100	100
30	5B	182/237 (77%)	180 (99%)	2 (1%)	70	82
30	9Y	122/237 (52%)	120 (98%)	2 (2%)	58	76
30	9Z	82/237 (35%)	82 (100%)	0	100	100
31	6A	195/204 (96%)	194 (100%)	1 (0%)	86	91
31	6B	188/204 (92%)	187 (100%)	1 (0%)	86	91
31	6C	192/204 (94%)	192 (100%)	0	100	100
31	6D	194/204 (95%)	194 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	6E	194/204 (95%)	193 (100%)	1 (0%)	86	91
31	6F	194/204 (95%)	194 (100%)	0	100	100
32	6I	70/106 (66%)	69 (99%)	1 (1%)	62	78
32	6J	46/106 (43%)	46 (100%)	0	100	100
33	6M	343/410 (84%)	343 (100%)	0	100	100
33	6N	69/410 (17%)	69 (100%)	0	100	100
34	6Q	183/275 (66%)	183 (100%)	0	100	100
34	6R	67/275 (24%)	67 (100%)	0	100	100
35	6U	132/338 (39%)	131 (99%)	1 (1%)	79	87
35	6V	240/338 (71%)	238 (99%)	2 (1%)	79	87
35	6W	219/338 (65%)	219 (100%)	0	100	100
35	6X	112/338 (33%)	112 (100%)	0	100	100
36	7A	644/660 (98%)	642 (100%)	2 (0%)	91	94
36	7B	410/660 (62%)	408 (100%)	2 (0%)	86	91
36	7C	480/660 (73%)	478 (100%)	2 (0%)	89	93
36	7D	643/660 (97%)	643 (100%)	0	100	100
37	7G	477/577 (83%)	476 (100%)	1 (0%)	92	95
37	7H	477/577 (83%)	474 (99%)	3 (1%)	84	90
37	7I	553/577 (96%)	550 (100%)	3 (0%)	86	91
38	7M	230/283 (81%)	229 (100%)	1 (0%)	89	93
38	7N	62/283 (22%)	62 (100%)	0	100	100
39	7Q	127/160 (79%)	127 (100%)	0	100	100
39	7R	119/160 (74%)	119 (100%)	0	100	100
40	7U	87/183 (48%)	86 (99%)	1 (1%)	70	82
40	7V	49/183 (27%)	48 (98%)	1 (2%)	50	71
41	7Y	179/183 (98%)	179 (100%)	0	100	100
41	7Z	55/183 (30%)	55 (100%)	0	100	100
42	8A	210/231 (91%)	209 (100%)	1 (0%)	86	91
43	8D	364/412 (88%)	364 (100%)	0	100	100
43	8E	164/412 (40%)	164 (100%)	0	100	100
43	8F	242/412 (59%)	241 (100%)	1 (0%)	89	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	8G	364/412 (88%)	364 (100%)	0	100	100
44	8J	364/389 (94%)	364 (100%)	0	100	100
44	8K	287/389 (74%)	287 (100%)	0	100	100
44	8L	364/389 (94%)	364 (100%)	0	100	100
44	8M	122/389 (31%)	122 (100%)	0	100	100
44	8N	16/389 (4%)	16 (100%)	0	100	100
45	8Q	18/365 (5%)	18 (100%)	0	100	100
45	8R	363/365 (100%)	361 (99%)	2 (1%)	84	90
45	8S	278/365 (76%)	277 (100%)	1 (0%)	89	93
45	8T	363/365 (100%)	362 (100%)	1 (0%)	91	94
45	8U	108/365 (30%)	108 (100%)	0	100	100
46	8X	99/111 (89%)	99 (100%)	0	100	100
46	8Y	99/111 (89%)	99 (100%)	0	100	100
46	8Z	99/111 (89%)	98 (99%)	1 (1%)	73	84
47	9A	187/200 (94%)	187 (100%)	0	100	100
48	9D	87/149 (58%)	87 (100%)	0	100	100
49	9G	138/139 (99%)	137 (99%)	1 (1%)	81	88
50	9J	91/157 (58%)	91 (100%)	0	100	100
51	9R	130/139 (94%)	130 (100%)	0	100	100
52	9T	70/77 (91%)	70 (100%)	0	100	100
53	9V	19/250 (8%)	19 (100%)	0	100	100
53	9W	64/250 (26%)	64 (100%)	0	100	100
54	AA	365/376 (97%)	365 (100%)	0	100	100
54	AB	365/376 (97%)	365 (100%)	0	100	100
54	AE	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	AG	365/376 (97%)	365 (100%)	0	100	100
54	AI	365/376 (97%)	365 (100%)	0	100	100
54	AK	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	AM	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	BA	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	BB	365/376 (97%)	365 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	BE	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	BG	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	BI	365/376 (97%)	365 (100%)	0	100	100
54	BK	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	BM	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	CA	365/376 (97%)	365 (100%)	0	100	100
54	CB	365/376 (97%)	365 (100%)	0	100	100
54	CE	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	CG	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	CI	365/376 (97%)	365 (100%)	0	100	100
54	CK	365/376 (97%)	365 (100%)	0	100	100
54	CM	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	DA	365/376 (97%)	365 (100%)	0	100	100
54	DB	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	DE	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	DG	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	DI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	DK	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	DM	365/376 (97%)	365 (100%)	0	100	100
54	EA	365/376 (97%)	332 (91%)	33 (9%)	8	27
54	EC	365/376 (97%)	365 (100%)	0	100	100
54	EE	365/376 (97%)	365 (100%)	0	100	100
54	EG	365/376 (97%)	365 (100%)	0	100	100
54	EI	365/376 (97%)	365 (100%)	0	100	100
54	EK	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	FA	365/376 (97%)	329 (90%)	36 (10%)	6	24
54	FB	365/376 (97%)	365 (100%)	0	100	100
54	FE	365/376 (97%)	322 (88%)	43 (12%)	4	17
54	FG	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	FI	365/376 (97%)	339 (93%)	26 (7%)	12	37
54	FK	365/376 (97%)	365 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	GA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	GB	365/376 (97%)	365 (100%)	0	100	100
54	GE	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	GG	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	GI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	GK	365/376 (97%)	365 (100%)	0	100	100
54	HA	365/376 (97%)	365 (100%)	0	100	100
54	HB	365/376 (97%)	365 (100%)	0	100	100
54	HE	362/376 (96%)	361 (100%)	1 (0%)	91	94
54	HG	365/376 (97%)	362 (99%)	3 (1%)	79	87
54	HI	365/376 (97%)	365 (100%)	0	100	100
54	HK	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	IA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	IB	364/376 (97%)	364 (100%)	0	100	100
54	IE	365/376 (97%)	365 (100%)	0	100	100
54	IG	365/376 (97%)	365 (100%)	0	100	100
54	II	364/376 (97%)	364 (100%)	0	100	100
54	IK	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	IM	365/376 (97%)	362 (99%)	3 (1%)	79	87
54	JA	363/376 (96%)	363 (100%)	0	100	100
54	JB	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	JE	365/376 (97%)	365 (100%)	0	100	100
54	JG	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	JI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	JK	365/376 (97%)	365 (100%)	0	100	100
54	KA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	KB	364/376 (97%)	362 (100%)	2 (0%)	86	91
54	KE	365/376 (97%)	365 (100%)	0	100	100
54	KG	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	KI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	KK	365/376 (97%)	364 (100%)	1 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	LA	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	LB	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	LE	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	LG	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	LI	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	LK	365/376 (97%)	365 (100%)	0	100	100
54	MA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	MB	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	ME	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	MG	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	MI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	MK	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	ML	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	NA	365/376 (97%)	365 (100%)	0	100	100
54	NB	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	NE	365/376 (97%)	365 (100%)	0	100	100
54	NG	365/376 (97%)	365 (100%)	0	100	100
54	NI	364/376 (97%)	363 (100%)	1 (0%)	91	94
54	NL	363/376 (96%)	363 (100%)	0	100	100
54	OA	365/376 (97%)	365 (100%)	0	100	100
54	OB	364/376 (97%)	362 (100%)	2 (0%)	86	91
54	OE	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	OG	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	OI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	OK	365/376 (97%)	365 (100%)	0	100	100
54	OL	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	PA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	PB	365/376 (97%)	365 (100%)	0	100	100
54	PE	365/376 (97%)	365 (100%)	0	100	100
54	PG	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	PI	365/376 (97%)	365 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	PK	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	PL	365/376 (97%)	365 (100%)	0	100	100
54	QA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	QB	365/376 (97%)	365 (100%)	0	100	100
54	QE	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	QG	365/376 (97%)	361 (99%)	4 (1%)	70	82
54	QI	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	QK	363/376 (96%)	362 (100%)	1 (0%)	91	94
54	QL	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	RA	365/376 (97%)	365 (100%)	0	100	100
54	RB	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	RE	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	RG	365/376 (97%)	365 (100%)	0	100	100
54	RI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	RK	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	RL	365/376 (97%)	365 (100%)	0	100	100
54	SA	365/376 (97%)	365 (100%)	0	100	100
54	SB	365/376 (97%)	365 (100%)	0	100	100
54	SE	365/376 (97%)	365 (100%)	0	100	100
54	SG	365/376 (97%)	365 (100%)	0	100	100
54	SI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	SK	365/376 (97%)	365 (100%)	0	100	100
54	TA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	TB	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	TE	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	TG	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	TI	365/376 (97%)	365 (100%)	0	100	100
54	TK	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	UA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	UB	363/376 (96%)	362 (100%)	1 (0%)	91	94
54	UE	365/376 (97%)	363 (100%)	2 (0%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	UG	365/376 (97%)	365 (100%)	0	100	100
54	UI	365/376 (97%)	365 (100%)	0	100	100
54	UK	365/376 (97%)	365 (100%)	0	100	100
54	VA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	VB	365/376 (97%)	365 (100%)	0	100	100
54	VE	365/376 (97%)	365 (100%)	0	100	100
54	VG	365/376 (97%)	365 (100%)	0	100	100
54	VI	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	VK	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	WA	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	WB	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	WE	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	WG	365/376 (97%)	363 (100%)	2 (0%)	86	91
54	WI	365/376 (97%)	364 (100%)	1 (0%)	91	94
54	WK	365/376 (97%)	364 (100%)	1 (0%)	91	94
55	AC	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	AD	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	AF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	AH	369/381 (97%)	369 (100%)	0	100	100
55	AJ	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	AL	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	BC	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	BD	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	BF	369/381 (97%)	366 (99%)	3 (1%)	79	87
55	BH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	BJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	BL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	CC	369/381 (97%)	369 (100%)	0	100	100
55	CD	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	CF	369/381 (97%)	369 (100%)	0	100	100
55	CH	369/381 (97%)	369 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	CJ	369/381 (97%)	369 (100%)	0	100	100
55	CL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	DC	369/381 (97%)	369 (100%)	0	100	100
55	DD	369/381 (97%)	369 (100%)	0	100	100
55	DF	369/381 (97%)	369 (100%)	0	100	100
55	DH	369/381 (97%)	369 (100%)	0	100	100
55	DJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	DL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	EB	369/381 (97%)	369 (100%)	0	100	100
55	ED	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	EF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	EH	369/381 (97%)	369 (100%)	0	100	100
55	EJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	EL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	EM	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	FC	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	FD	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	FF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	FH	369/381 (97%)	369 (100%)	0	100	100
55	FJ	369/381 (97%)	369 (100%)	0	100	100
55	FL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	FM	369/381 (97%)	369 (100%)	0	100	100
55	GC	369/381 (97%)	369 (100%)	0	100	100
55	GD	369/381 (97%)	369 (100%)	0	100	100
55	GF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	GH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	GJ	369/381 (97%)	369 (100%)	0	100	100
55	GL	369/381 (97%)	369 (100%)	0	100	100
55	GM	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	HC	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	HD	369/381 (97%)	366 (99%)	3 (1%)	79	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	HF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	HH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	HJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	HL	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	HM	369/381 (97%)	369 (100%)	0	100	100
55	IC	369/381 (97%)	369 (100%)	0	100	100
55	ID	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	IF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	IH	369/381 (97%)	369 (100%)	0	100	100
55	IJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	IL	369/381 (97%)	369 (100%)	0	100	100
55	JC	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	JD	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	JF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	JH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	JJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	JL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	JM	369/381 (97%)	369 (100%)	0	100	100
55	KC	369/381 (97%)	369 (100%)	0	100	100
55	KD	369/381 (97%)	369 (100%)	0	100	100
55	KF	369/381 (97%)	369 (100%)	0	100	100
55	KH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	KJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	KL	369/381 (97%)	369 (100%)	0	100	100
55	KM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	LC	369/381 (97%)	369 (100%)	0	100	100
55	LD	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	LF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	LH	369/381 (97%)	369 (100%)	0	100	100
55	LJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	LL	369/381 (97%)	367 (100%)	2 (0%)	86	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	LM	369/381 (97%)	369 (100%)	0	100	100
55	MC	369/381 (97%)	369 (100%)	0	100	100
55	MD	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	MF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	MH	369/381 (97%)	369 (100%)	0	100	100
55	MJ	369/381 (97%)	369 (100%)	0	100	100
55	MM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	NC	369/381 (97%)	366 (99%)	3 (1%)	79	87
55	ND	369/381 (97%)	369 (100%)	0	100	100
55	NF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	NH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	NJ	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	NK	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	NM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	OC	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	OD	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	OF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	OH	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	OJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	OM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	PC	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	PD	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	PF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	PH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	PJ	369/381 (97%)	369 (100%)	0	100	100
55	PM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	QC	369/381 (97%)	366 (99%)	3 (1%)	79	87
55	QD	369/381 (97%)	369 (100%)	0	100	100
55	QF	369/381 (97%)	369 (100%)	0	100	100
55	QH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	QJ	369/381 (97%)	369 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	QM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	RC	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	RD	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	RF	369/381 (97%)	369 (100%)	0	100	100
55	RH	369/381 (97%)	369 (100%)	0	100	100
55	RJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	RM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	SC	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	SD	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	SF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	SH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	SJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	SL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	SM	369/381 (97%)	369 (100%)	0	100	100
55	TC	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	TD	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	TF	369/381 (97%)	369 (100%)	0	100	100
55	TH	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	TJ	369/381 (97%)	369 (100%)	0	100	100
55	TL	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	TM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	UC	369/381 (97%)	366 (99%)	3 (1%)	79	87
55	UD	369/381 (97%)	369 (100%)	0	100	100
55	UF	369/381 (97%)	369 (100%)	0	100	100
55	UH	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	UJ	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	UL	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	UM	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	VC	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	VD	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	VF	369/381 (97%)	369 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	VH	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	VJ	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	VL	369/381 (97%)	369 (100%)	0	100	100
55	VM	369/381 (97%)	369 (100%)	0	100	100
55	WC	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	WD	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	WF	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	WH	369/381 (97%)	368 (100%)	1 (0%)	91	94
55	WJ	369/381 (97%)	367 (100%)	2 (0%)	86	91
55	WL	369/381 (97%)	368 (100%)	1 (0%)	91	94
All	All	136639/159445 (86%)	136150 (100%)	489 (0%)	88	93

5 of 489 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	FE	257	THR
55	TH	2	ARG
54	FI	338	LYS
55	TC	2	ARG
54	WA	308	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 400 such sidechains are listed below:

Mol	Chain	Res	Type
55	MF	190	HIS
54	QA	128	GLN
55	WL	14	ASN
54	MK	329	ASN
55	OD	347	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 446 ligands modelled in this entry, 148 are monoatomic - leaving 298 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
56	GTP	AA	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	FL	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	RI	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.31	5 (14%)
58	GDP	MM	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	2 (6%)
56	GTP	BB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.25	3 (8%)
56	GTP	OI	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.25	4 (11%)
56	GTP	WK	501	57	29,34,34	1.19	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	RD	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	SJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	EK	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	MB	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.31	4 (11%)
58	GDP	CL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	IG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	PK	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	AL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	QD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.13	2 (6%)
56	GTP	GK	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	IL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	GDP	PC	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
56	GTP	GI	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	3 (8%)
58	GDP	JH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.05	2 (6%)
58	GDP	TD	501	-	25,30,30	0.92	0	30,47,47	1.10	2 (6%)
58	GDP	WF	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	QH	501	-	25,30,30	1.03	1 (4%)	30,47,47	1.05	2 (6%)
58	GDP	OJ	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	RM	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.18	3 (10%)
58	GDP	BC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	UE	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.32	4 (11%)
56	GTP	CB	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.31	4 (11%)
56	GTP	DE	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	EH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	3 (10%)
56	GTP	JG	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	NK	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	HH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
58	GDP	GF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	VM	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.13	2 (6%)
56	GTP	TE	501	57	29,34,34	1.19	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	GD	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	BI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	SB	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	DJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.19	3 (10%)
58	GDP	CF	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	FD	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	UJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
56	GTP	KB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	BK	501	57	29,34,34	1.26	3 (10%)	35,54,54	1.31	6 (17%)
56	GTP	IB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.31	5 (14%)
56	GTP	NE	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	DH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	3 (10%)
58	GDP	UM	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.14	3 (10%)
56	GTP	PA	501	57	29,34,34	1.27	2 (6%)	35,54,54	1.30	5 (14%)
58	GDP	KF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	JJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	GTP	FA	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)
56	GTP	AE	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	OB	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	MF	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	1 (3%)
56	GTP	IE	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)
56	GTP	HE	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.32	4 (11%)
56	GTP	JE	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	VC	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	SI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.26	4 (11%)
58	GDP	AF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
56	GTP	WI	501	57	29,34,34	1.25	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	HI	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	GM	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	TA	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.30	4 (11%)
56	GTP	EC	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	BM	501	57	29,34,34	1.25	2 (6%)	35,54,54	1.30	5 (14%)
56	GTP	LG	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	5 (14%)
56	GTP	MK	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	3 (8%)
58	GDP	EF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
56	GTP	LA	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	IC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.15	3 (10%)
58	GDP	LL	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
58	GDP	NF	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.10	2 (6%)
56	GTP	LB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	MI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.25	3 (8%)
56	GTP	EG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	TB	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	UF	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	UH	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.05	2 (6%)
58	GDP	LF	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.11	2 (6%)
56	GTP	VA	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	AC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	DB	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	BF	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
58	GDP	EB	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.08	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	GDP	ED	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.15	2 (6%)
56	GTP	OE	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	PE	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	3 (8%)
56	GTP	VI	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	OA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	PJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	QJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.05	3 (10%)
56	GTP	KA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	ME	501	57	29,34,34	1.25	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	KL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	MD	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	UD	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.21	3 (10%)
56	GTP	AB	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	FG	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.31	4 (11%)
58	GDP	TC	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	OF	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	CE	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	3 (8%)
58	GDP	HD	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	RH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.14	3 (10%)
56	GTP	VE	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	HF	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
56	GTP	CG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.25	4 (11%)
58	GDP	WJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
58	GDP	DC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	SH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	CA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	3 (8%)
58	GDP	RF	501	-	25,30,30	0.92	1 (4%)	30,47,47	1.04	1 (3%)
56	GTP	HB	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	IF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	1 (3%)
56	GTP	QL	501	57	29,34,34	1.28	5 (17%)	35,54,54	1.31	4 (11%)
56	GTP	VB	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	RL	501	57	29,34,34	1.26	3 (10%)	35,54,54	1.33	5 (14%)
58	GDP	OM	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	3 (10%)
58	GDP	TL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	VJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	GTP	NG	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	RA	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	JI	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	UK	501	57	29,34,34	1.19	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	GL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	2 (6%)
58	GDP	PH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	NC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.14	2 (6%)
58	GDP	KM	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	PM	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	DF	501	-	25,30,30	0.95	2 (8%)	30,47,47	1.00	1 (3%)
56	GTP	FE	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	QM	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
56	GTP	LK	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	CJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
56	GTP	SE	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	HJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	HK	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)
56	GTP	DI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	3 (8%)
58	GDP	DD	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.04	1 (3%)
58	GDP	RJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	FF	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.12	2 (6%)
58	GDP	NJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
56	GTP	KK	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	TM	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.11	2 (6%)
58	GDP	KJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.11	2 (6%)
56	GTP	QE	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	BH	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	JB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	OD	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.19	3 (10%)
56	GTP	NI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	BL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	HL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	1 (3%)
56	GTP	UG	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	GG	501	57	29,34,34	1.19	2 (6%)	35,54,54	1.29	3 (8%)
58	GDP	FH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.11	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	GTP	QI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.31	5 (14%)
58	GDP	FJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	AG	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.25	4 (11%)
56	GTP	WA	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	5 (14%)
56	GTP	AK	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
56	GTP	NL	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	TJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.06	2 (6%)
58	GDP	KD	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
56	GTP	JK	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	ML	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.31	5 (14%)
56	GTP	OG	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	FB	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.32	4 (11%)
58	GDP	VH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.18	3 (10%)
56	GTP	RK	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	JD	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	LD	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	QC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	VF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.07	2 (6%)
56	GTP	BG	501	57	29,34,34	1.28	3 (10%)	35,54,54	1.32	5 (14%)
56	GTP	QG	501	57	29,34,34	1.25	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	MH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	SK	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	TK	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.25	4 (11%)
56	GTP	DM	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	SM	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	IK	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	UC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
58	GDP	CC	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	UB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	PB	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	3 (8%)
56	GTP	II	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
56	GTP	LE	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.31	3 (8%)
56	GTP	GE	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.26	4 (11%)
58	GDP	AJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
56	GTP	KG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.31	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	GDP	FC	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	2 (6%)
58	GDP	AD	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.10	3 (10%)
58	GDP	MC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
56	GTP	VK	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	OL	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	CM	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.26	4 (11%)
58	GDP	UL	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.13	3 (10%)
58	GDP	EJ	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
56	GTP	PI	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	LM	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	OH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	DG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.25	4 (11%)
58	GDP	DL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.11	1 (3%)
56	GTP	TG	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	WC	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	SF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.16	3 (10%)
56	GTP	TI	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.23	4 (11%)
58	GDP	LC	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	GC	501	-	25,30,30	0.94	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	IJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	MJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	SD	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	1 (3%)
56	GTP	KI	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	EA	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.35	5 (14%)
56	GTP	OK	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	WL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	JC	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.10	3 (10%)
56	GTP	GA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.25	3 (8%)
56	GTP	WB	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	3 (8%)
58	GDP	VL	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.03	1 (3%)
56	GTP	RG	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	BJ	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
56	GTP	RB	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	LH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	KH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	GDP	JF	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	3 (10%)
56	GTP	HG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	NH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	3 (10%)
56	GTP	FI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.33	4 (11%)
56	GTP	UA	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	SL	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
56	GTP	SG	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.30	4 (11%)
56	GTP	PL	501	57	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	CI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	BD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.11	3 (10%)
58	GDP	TH	501	-	25,30,30	1.00	1 (4%)	30,47,47	1.12	2 (6%)
58	GDP	FM	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.13	2 (6%)
56	GTP	EI	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	IM	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	KE	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	5 (14%)
56	GTP	DK	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.32	5 (14%)
56	GTP	MG	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.30	4 (11%)
56	GTP	PG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	WD	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.13	3 (10%)
56	GTP	FK	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	4 (11%)
56	GTP	BE	501	57	29,34,34	1.17	2 (6%)	35,54,54	1.36	5 (14%)
56	GTP	WE	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.26	4 (11%)
58	GDP	IH	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	QF	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.12	3 (10%)
56	GTP	CK	501	-	29,34,34	1.28	4 (13%)	35,54,54	1.27	5 (14%)
56	GTP	JA	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.30	4 (11%)
56	GTP	MA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.33	5 (14%)
58	GDP	KC	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	LJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	NA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	CD	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	EL	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.11	2 (6%)
58	GDP	HM	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	CH	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
58	GDP	WH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	GTP	NB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	JL	501	-	25,30,30	0.98	1 (4%)	30,47,47	0.98	1 (3%)
56	GTP	VG	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.31	5 (14%)
56	GTP	QK	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.31	4 (11%)
56	GTP	WG	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.30	5 (14%)
58	GDP	ND	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.06	2 (6%)
56	GTP	DA	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	PF	501	-	25,30,30	0.86	0	30,47,47	1.51	5 (16%)
58	GDP	PD	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.12	2 (6%)
56	GTP	BA	501	57	29,34,34	1.25	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	AH	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.10	2 (6%)
56	GTP	HA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.30	4 (11%)
56	GTP	UI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.30	5 (14%)
58	GDP	EM	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	ID	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.08	2 (6%)
58	GDP	JM	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.07	2 (6%)
58	GDP	RC	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.06	2 (6%)
56	GTP	AI	501	57	29,34,34	1.20	2 (6%)	35,54,54	1.31	5 (14%)
56	GTP	QA	501	57	29,34,34	1.23	2 (6%)	35,54,54	1.28	4 (11%)
56	GTP	RE	501	57	29,34,34	1.25	2 (6%)	35,54,54	1.27	4 (11%)
58	GDP	SC	501	-	25,30,30	0.98	1 (4%)	30,47,47	1.13	3 (10%)
56	GTP	SA	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.31	4 (11%)
56	GTP	QB	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.31	4 (11%)
58	GDP	VD	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.17	4 (13%)
56	GTP	IA	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.28	4 (11%)
58	GDP	HC	501	-	25,30,30	1.01	1 (4%)	30,47,47	1.06	2 (6%)
58	GDP	GJ	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.10	2 (6%)
56	GTP	AM	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.26	4 (11%)
58	GDP	NM	501	-	25,30,30	0.97	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	EE	501	57	29,34,34	1.24	2 (6%)	35,54,54	1.30	4 (11%)
58	GDP	GH	501	-	25,30,30	0.99	1 (4%)	30,47,47	1.16	3 (10%)
56	GTP	GB	501	57	29,34,34	1.21	2 (6%)	35,54,54	1.29	4 (11%)
58	GDP	TF	501	-	25,30,30	0.95	1 (4%)	30,47,47	1.09	2 (6%)
58	GDP	OC	501	-	25,30,30	0.96	1 (4%)	30,47,47	1.09	2 (6%)
56	GTP	LI	501	57	29,34,34	1.22	2 (6%)	35,54,54	1.28	4 (11%)

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
56	GTP	AA	501	57	-	7/18/38/38	0/3/3/3
58	GDP	FL	501	-	-	2/12/32/32	0/3/3/3
56	GTP	RI	501	57	-	5/18/38/38	0/3/3/3
58	GDP	MM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	BB	501	57	-	4/18/38/38	0/3/3/3
56	GTP	OI	501	57	-	4/18/38/38	0/3/3/3
56	GTP	WK	501	57	-	6/18/38/38	0/3/3/3
58	GDP	RD	501	-	-	2/12/32/32	0/3/3/3
58	GDP	SJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	EK	501	57	-	2/18/38/38	0/3/3/3
56	GTP	MB	501	57	-	5/18/38/38	0/3/3/3
58	GDP	CL	501	-	-	2/12/32/32	0/3/3/3
56	GTP	IG	501	57	-	6/18/38/38	0/3/3/3
56	GTP	PK	501	57	-	1/18/38/38	0/3/3/3
58	GDP	AL	501	-	-	2/12/32/32	0/3/3/3
58	GDP	QD	501	-	-	1/12/32/32	0/3/3/3
56	GTP	GK	501	57	-	4/18/38/38	0/3/3/3
58	GDP	IL	501	-	-	2/12/32/32	0/3/3/3
58	GDP	PC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	GI	501	57	-	3/18/38/38	0/3/3/3
58	GDP	JH	501	-	-	1/12/32/32	0/3/3/3
58	GDP	TD	501	-	-	3/12/32/32	0/3/3/3
58	GDP	WF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	QH	501	-	-	5/12/32/32	0/3/3/3
58	GDP	OJ	501	-	-	1/12/32/32	0/3/3/3
58	GDP	RM	501	-	-	2/12/32/32	0/3/3/3
58	GDP	BC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	UE	501	57	-	4/18/38/38	0/3/3/3
56	GTP	CB	501	57	-	2/18/38/38	0/3/3/3
56	GTP	DE	501	57	-	3/18/38/38	0/3/3/3
58	GDP	EH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	JG	501	57	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	NK	501	-	-	1/12/32/32	0/3/3/3
58	GDP	HH	501	-	-	1/12/32/32	0/3/3/3
58	GDP	GF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	VM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	TE	501	57	-	4/18/38/38	0/3/3/3
58	GDP	GD	501	-	-	1/12/32/32	0/3/3/3
56	GTP	BI	501	57	-	7/18/38/38	0/3/3/3
56	GTP	SB	501	57	-	1/18/38/38	0/3/3/3
58	GDP	DJ	501	-	-	4/12/32/32	0/3/3/3
58	GDP	CF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	FD	501	-	-	1/12/32/32	0/3/3/3
58	GDP	UJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	KB	501	57	-	2/18/38/38	0/3/3/3
56	GTP	BK	501	57	-	5/18/38/38	0/3/3/3
56	GTP	IB	501	57	-	5/18/38/38	0/3/3/3
56	GTP	NE	501	57	-	3/18/38/38	0/3/3/3
58	GDP	DH	501	-	-	1/12/32/32	0/3/3/3
58	GDP	UM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	PA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	KF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	JJ	501	-	-	3/12/32/32	0/3/3/3
56	GTP	FA	501	57	-	4/18/38/38	0/3/3/3
56	GTP	AE	501	57	-	6/18/38/38	0/3/3/3
56	GTP	OB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	MF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	IE	501	57	-	6/18/38/38	0/3/3/3
56	GTP	HE	501	57	-	6/18/38/38	0/3/3/3
56	GTP	JE	501	57	-	3/18/38/38	0/3/3/3
58	GDP	VC	501	-	-	1/12/32/32	0/3/3/3
56	GTP	SI	501	57	-	2/18/38/38	0/3/3/3
58	GDP	AF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	WI	501	57	-	6/18/38/38	0/3/3/3
56	GTP	HI	501	57	-	6/18/38/38	0/3/3/3
58	GDP	GM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	TA	501	57	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	EC	501	57	-	3/18/38/38	0/3/3/3
56	GTP	BM	501	57	-	9/18/38/38	0/3/3/3
56	GTP	LG	501	57	-	3/18/38/38	0/3/3/3
56	GTP	MK	501	57	-	6/18/38/38	0/3/3/3
58	GDP	EF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	LA	501	57	-	7/18/38/38	0/3/3/3
58	GDP	IC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	LL	501	-	-	1/12/32/32	0/3/3/3
58	GDP	NF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	LB	501	57	-	3/18/38/38	0/3/3/3
56	GTP	MI	501	57	-	3/18/38/38	0/3/3/3
56	GTP	EG	501	57	-	3/18/38/38	0/3/3/3
56	GTP	TB	501	57	-	8/18/38/38	0/3/3/3
58	GDP	UF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	UH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	LF	501	-	-	3/12/32/32	0/3/3/3
56	GTP	VA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	AC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	DB	501	57	-	1/18/38/38	0/3/3/3
58	GDP	BF	501	-	-	1/12/32/32	0/3/3/3
58	GDP	EB	501	-	-	1/12/32/32	0/3/3/3
58	GDP	ED	501	-	-	2/12/32/32	0/3/3/3
56	GTP	OE	501	57	-	7/18/38/38	0/3/3/3
56	GTP	PE	501	57	-	3/18/38/38	0/3/3/3
56	GTP	VI	501	57	-	3/18/38/38	0/3/3/3
56	GTP	OA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	PJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	QJ	501	-	-	1/12/32/32	0/3/3/3
56	GTP	KA	501	57	-	2/18/38/38	0/3/3/3
56	GTP	ME	501	57	-	6/18/38/38	0/3/3/3
58	GDP	KL	501	-	-	2/12/32/32	0/3/3/3
58	GDP	MD	501	-	-	1/12/32/32	0/3/3/3
58	GDP	UD	501	-	-	3/12/32/32	0/3/3/3
56	GTP	AB	501	57	-	3/18/38/38	0/3/3/3
56	GTP	FG	501	57	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	TC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	OF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	CE	501	57	-	3/18/38/38	0/3/3/3
58	GDP	HD	501	-	-	2/12/32/32	0/3/3/3
58	GDP	RH	501	-	-	1/12/32/32	0/3/3/3
56	GTP	VE	501	57	-	4/18/38/38	0/3/3/3
58	GDP	HF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	CG	501	57	-	4/18/38/38	0/3/3/3
58	GDP	WJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	DC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	SH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	CA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	RF	501	-	-	5/12/32/32	0/3/3/3
56	GTP	HB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	IF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	QL	501	57	-	9/18/38/38	0/3/3/3
56	GTP	VB	501	57	-	6/18/38/38	0/3/3/3
56	GTP	RL	501	57	-	8/18/38/38	0/3/3/3
58	GDP	OM	501	-	-	2/12/32/32	0/3/3/3
58	GDP	TL	501	-	-	2/12/32/32	0/3/3/3
58	GDP	VJ	501	-	-	1/12/32/32	0/3/3/3
56	GTP	NG	501	57	-	7/18/38/38	0/3/3/3
56	GTP	RA	501	57	-	3/18/38/38	0/3/3/3
56	GTP	JI	501	57	-	2/18/38/38	0/3/3/3
56	GTP	UK	501	57	-	9/18/38/38	0/3/3/3
58	GDP	GL	501	-	-	1/12/32/32	0/3/3/3
58	GDP	PH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	NC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	KM	501	-	-	1/12/32/32	0/3/3/3
58	GDP	PM	501	-	-	2/12/32/32	0/3/3/3
58	GDP	DF	501	-	-	1/12/32/32	0/3/3/3
56	GTP	FE	501	57	-	8/18/38/38	0/3/3/3
58	GDP	QM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	LK	501	57	-	8/18/38/38	0/3/3/3
58	GDP	CJ	501	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	SE	501	57	-	6/18/38/38	0/3/3/3
58	GDP	HJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	HK	501	57	-	10/18/38/38	0/3/3/3
56	GTP	DI	501	57	-	2/18/38/38	0/3/3/3
58	GDP	DD	501	-	-	3/12/32/32	0/3/3/3
58	GDP	RJ	501	-	-	1/12/32/32	0/3/3/3
58	GDP	FF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	NJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	KK	501	57	-	4/18/38/38	0/3/3/3
58	GDP	TM	501	-	-	1/12/32/32	0/3/3/3
58	GDP	KJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	QE	501	57	-	2/18/38/38	0/3/3/3
58	GDP	BH	501	-	-	1/12/32/32	0/3/3/3
56	GTP	JB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	OD	501	-	-	4/12/32/32	0/3/3/3
56	GTP	NI	501	57	-	6/18/38/38	0/3/3/3
58	GDP	BL	501	-	-	2/12/32/32	0/3/3/3
58	GDP	HL	501	-	-	3/12/32/32	0/3/3/3
56	GTP	UG	501	57	-	6/18/38/38	0/3/3/3
56	GTP	GG	501	57	-	3/18/38/38	0/3/3/3
58	GDP	FH	501	-	-	3/12/32/32	0/3/3/3
56	GTP	QI	501	57	-	2/18/38/38	0/3/3/3
58	GDP	FJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	AG	501	57	-	4/18/38/38	0/3/3/3
56	GTP	WA	501	57	-	1/18/38/38	0/3/3/3
56	GTP	AK	501	57	-	5/18/38/38	0/3/3/3
56	GTP	NL	501	57	-	4/18/38/38	0/3/3/3
58	GDP	TJ	501	-	-	1/12/32/32	0/3/3/3
58	GDP	KD	501	-	-	2/12/32/32	0/3/3/3
56	GTP	JK	501	57	-	8/18/38/38	0/3/3/3
56	GTP	ML	501	57	-	3/18/38/38	0/3/3/3
56	GTP	OG	501	57	-	3/18/38/38	0/3/3/3
56	GTP	FB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	VH	501	-	-	3/12/32/32	0/3/3/3
56	GTP	RK	501	57	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	JD	501	-	-	2/12/32/32	0/3/3/3
58	GDP	LD	501	-	-	2/12/32/32	0/3/3/3
58	GDP	QC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	VF	501	-	-	1/12/32/32	0/3/3/3
56	GTP	BG	501	57	-	8/18/38/38	0/3/3/3
56	GTP	QG	501	57	-	6/18/38/38	0/3/3/3
58	GDP	MH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	SK	501	57	-	3/18/38/38	0/3/3/3
56	GTP	TK	501	57	-	4/18/38/38	0/3/3/3
56	GTP	DM	501	57	-	3/18/38/38	0/3/3/3
58	GDP	SM	501	-	-	1/12/32/32	0/3/3/3
56	GTP	IK	501	57	-	4/18/38/38	0/3/3/3
58	GDP	UC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	CC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	UB	501	57	-	3/18/38/38	0/3/3/3
56	GTP	PB	501	57	-	3/18/38/38	0/3/3/3
56	GTP	II	501	57	-	8/18/38/38	0/3/3/3
56	GTP	LE	501	57	-	3/18/38/38	0/3/3/3
56	GTP	GE	501	57	-	2/18/38/38	0/3/3/3
58	GDP	AJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	KG	501	57	-	3/18/38/38	0/3/3/3
58	GDP	FC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	AD	501	-	-	5/12/32/32	0/3/3/3
58	GDP	MC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	VK	501	57	-	7/18/38/38	0/3/3/3
56	GTP	OL	501	57	-	7/18/38/38	0/3/3/3
56	GTP	CM	501	57	-	4/18/38/38	0/3/3/3
58	GDP	UL	501	-	-	3/12/32/32	0/3/3/3
58	GDP	EJ	501	-	-	1/12/32/32	0/3/3/3
56	GTP	PI	501	57	-	3/18/38/38	0/3/3/3
58	GDP	LM	501	-	-	1/12/32/32	0/3/3/3
58	GDP	OH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	DG	501	57	-	5/18/38/38	0/3/3/3
58	GDP	DL	501	-	-	1/12/32/32	0/3/3/3
56	GTP	TG	501	57	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	WC	501	-	-	1/12/32/32	0/3/3/3
58	GDP	SF	501	-	-	3/12/32/32	0/3/3/3
56	GTP	TI	501	57	-	7/18/38/38	0/3/3/3
58	GDP	LC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	GC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	IJ	501	-	-	1/12/32/32	0/3/3/3
58	GDP	MJ	501	-	-	3/12/32/32	0/3/3/3
58	GDP	SD	501	-	-	4/12/32/32	0/3/3/3
56	GTP	KI	501	57	-	1/18/38/38	0/3/3/3
56	GTP	EA	501	57	-	2/18/38/38	0/3/3/3
56	GTP	OK	501	57	-	6/18/38/38	0/3/3/3
58	GDP	WL	501	-	-	1/12/32/32	0/3/3/3
58	GDP	JC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	GA	501	57	-	6/18/38/38	0/3/3/3
56	GTP	WB	501	57	-	7/18/38/38	0/3/3/3
58	GDP	VL	501	-	-	5/12/32/32	0/3/3/3
56	GTP	RG	501	57	-	2/18/38/38	0/3/3/3
58	GDP	BJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	RB	501	57	-	6/18/38/38	0/3/3/3
58	GDP	LH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	KH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	JF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	HG	501	57	-	3/18/38/38	0/3/3/3
58	GDP	NH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	FI	501	57	-	3/18/38/38	0/3/3/3
56	GTP	UA	501	57	-	8/18/38/38	0/3/3/3
58	GDP	SL	501	-	-	2/12/32/32	0/3/3/3
56	GTP	SG	501	57	-	7/18/38/38	0/3/3/3
56	GTP	PL	501	57	-	3/18/38/38	0/3/3/3
56	GTP	CI	501	57	-	2/18/38/38	0/3/3/3
58	GDP	BD	501	-	-	3/12/32/32	0/3/3/3
58	GDP	TH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	FM	501	-	-	1/12/32/32	0/3/3/3
56	GTP	EI	501	57	-	2/18/38/38	0/3/3/3
56	GTP	IM	501	57	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	KE	501	57	-	2/18/38/38	0/3/3/3
56	GTP	DK	501	57	-	5/18/38/38	0/3/3/3
56	GTP	MG	501	57	-	3/18/38/38	0/3/3/3
56	GTP	PG	501	57	-	7/18/38/38	0/3/3/3
58	GDP	WD	501	-	-	1/12/32/32	0/3/3/3
56	GTP	FK	501	57	-	7/18/38/38	0/3/3/3
56	GTP	BE	501	57	-	3/18/38/38	0/3/3/3
56	GTP	WE	501	57	-	4/18/38/38	0/3/3/3
58	GDP	IH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	QF	501	-	-	4/12/32/32	0/3/3/3
56	GTP	CK	501	-	-	7/18/38/38	0/3/3/3
56	GTP	JA	501	57	-	3/18/38/38	0/3/3/3
56	GTP	MA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	KC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	LJ	501	-	-	4/12/32/32	0/3/3/3
56	GTP	NA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	CD	501	-	-	3/12/32/32	0/3/3/3
58	GDP	EL	501	-	-	1/12/32/32	0/3/3/3
58	GDP	HM	501	-	-	1/12/32/32	0/3/3/3
58	GDP	CH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	WH	501	-	-	1/12/32/32	0/3/3/3
56	GTP	NB	501	57	-	10/18/38/38	0/3/3/3
58	GDP	JL	501	-	-	3/12/32/32	0/3/3/3
56	GTP	VG	501	57	-	4/18/38/38	0/3/3/3
56	GTP	QK	501	57	-	3/18/38/38	0/3/3/3
56	GTP	WG	501	57	-	2/18/38/38	0/3/3/3
58	GDP	ND	501	-	-	1/12/32/32	0/3/3/3
56	GTP	DA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	PF	501	-	-	1/12/32/32	0/3/3/3
58	GDP	PD	501	-	-	1/12/32/32	0/3/3/3
56	GTP	BA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	AH	501	-	-	3/12/32/32	0/3/3/3
56	GTP	HA	501	57	-	3/18/38/38	0/3/3/3
56	GTP	UI	501	57	-	3/18/38/38	0/3/3/3
58	GDP	EM	501	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	ID	501	-	-	2/12/32/32	0/3/3/3
58	GDP	JM	501	-	-	1/12/32/32	0/3/3/3
58	GDP	RC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	AI	501	57	-	3/18/38/38	0/3/3/3
56	GTP	QA	501	57	-	6/18/38/38	0/3/3/3
56	GTP	RE	501	57	-	3/18/38/38	0/3/3/3
58	GDP	SC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	SA	501	57	-	4/18/38/38	0/3/3/3
56	GTP	QB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	VD	501	-	-	1/12/32/32	0/3/3/3
56	GTP	IA	501	57	-	2/18/38/38	0/3/3/3
58	GDP	HC	501	-	-	5/12/32/32	0/3/3/3
58	GDP	GJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	AM	501	57	-	6/18/38/38	0/3/3/3
58	GDP	NM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	EE	501	57	-	1/18/38/38	0/3/3/3
58	GDP	GH	501	-	-	1/12/32/32	0/3/3/3
56	GTP	GB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	TF	501	-	-	1/12/32/32	0/3/3/3
58	GDP	OC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	LI	501	57	-	2/18/38/38	0/3/3/3

The worst 5 of 453 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	PA	501	GTP	C5-C6	-4.53	1.38	1.47
56	RE	501	GTP	C5-C6	-4.42	1.38	1.47
56	RG	501	GTP	C5-C6	-4.31	1.38	1.47
56	EE	501	GTP	C5-C6	-4.30	1.38	1.47
56	KG	501	GTP	C5-C6	-4.30	1.38	1.47

The worst 5 of 919 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	PF	501	GDP	O6-C6-C5	-3.81	116.77	124.32
56	TG	501	GTP	C8-N7-C5	3.74	108.92	102.55
56	SE	501	GTP	C8-N7-C5	3.73	108.89	102.55
56	GK	501	GTP	C8-N7-C5	3.72	108.88	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	CE	501	GTP	C8-N7-C5	3.72	108.88	102.55

There are no chirality outliers.

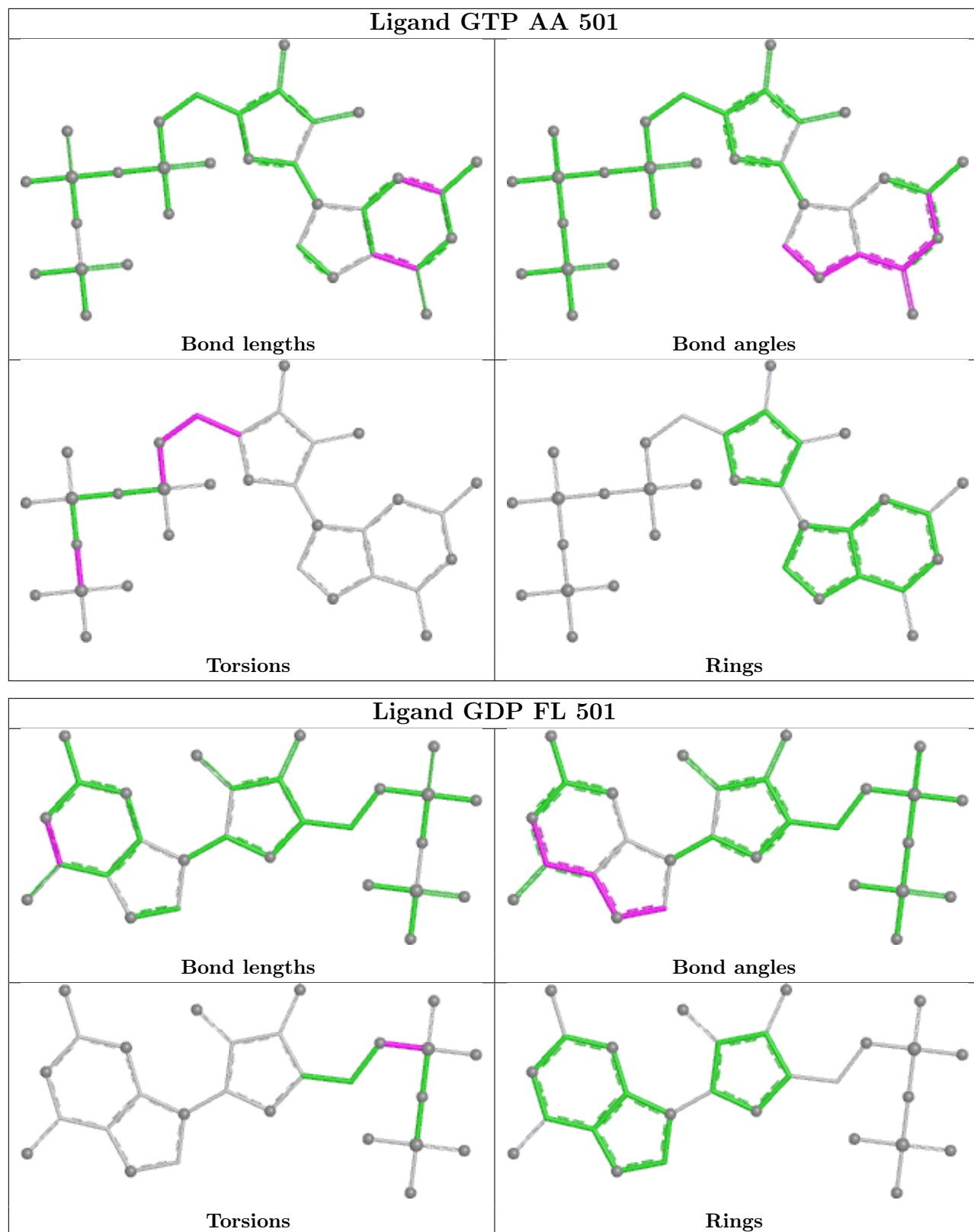
5 of 937 torsion outliers are listed below:

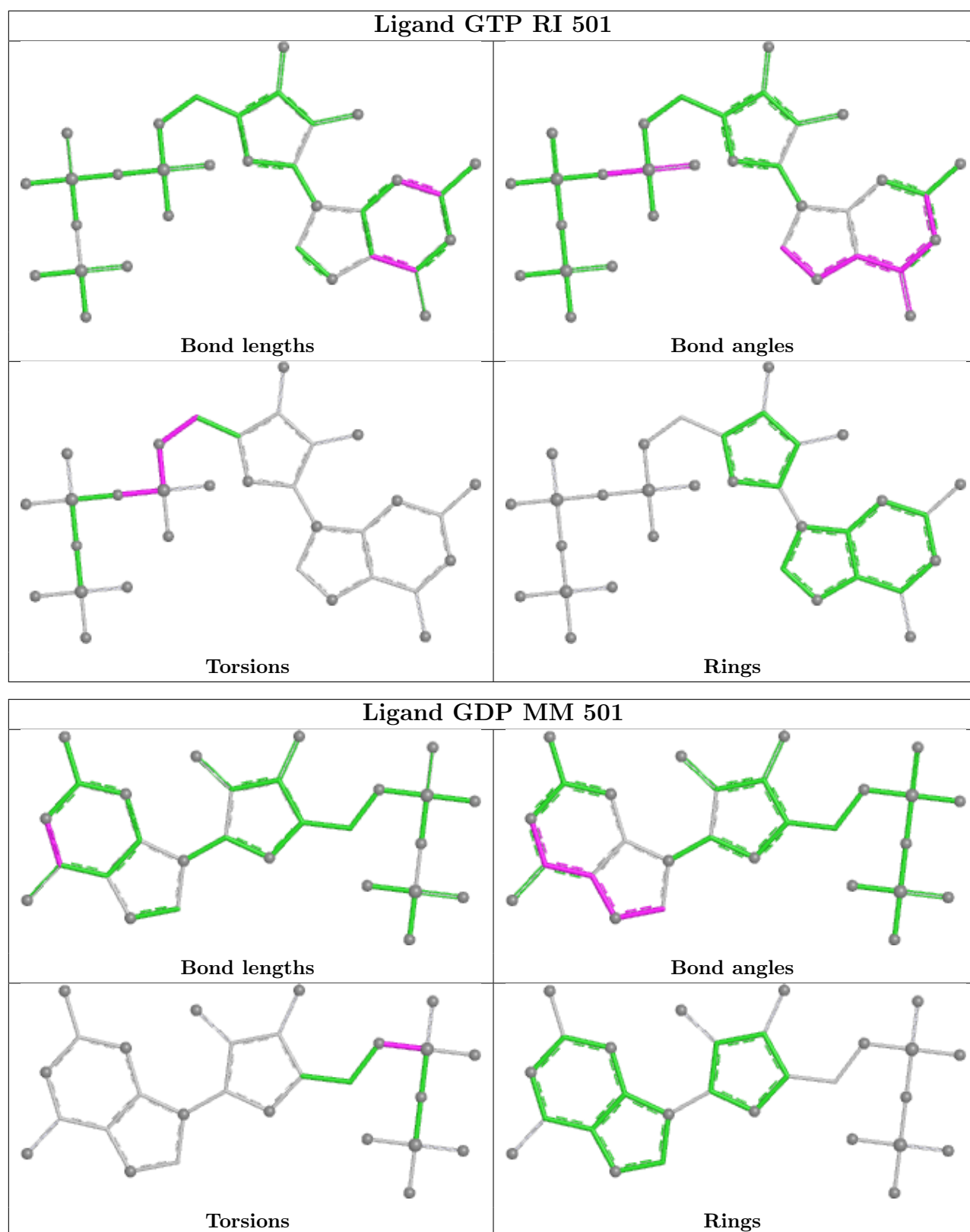
Mol	Chain	Res	Type	Atoms
56	AA	501	GTP	C5'-O5'-PA-O3A
56	AA	501	GTP	C5'-O5'-PA-O1A
56	AA	501	GTP	C5'-O5'-PA-O2A
56	AB	501	GTP	C5'-O5'-PA-O3A
56	AE	501	GTP	C5'-O5'-PA-O3A

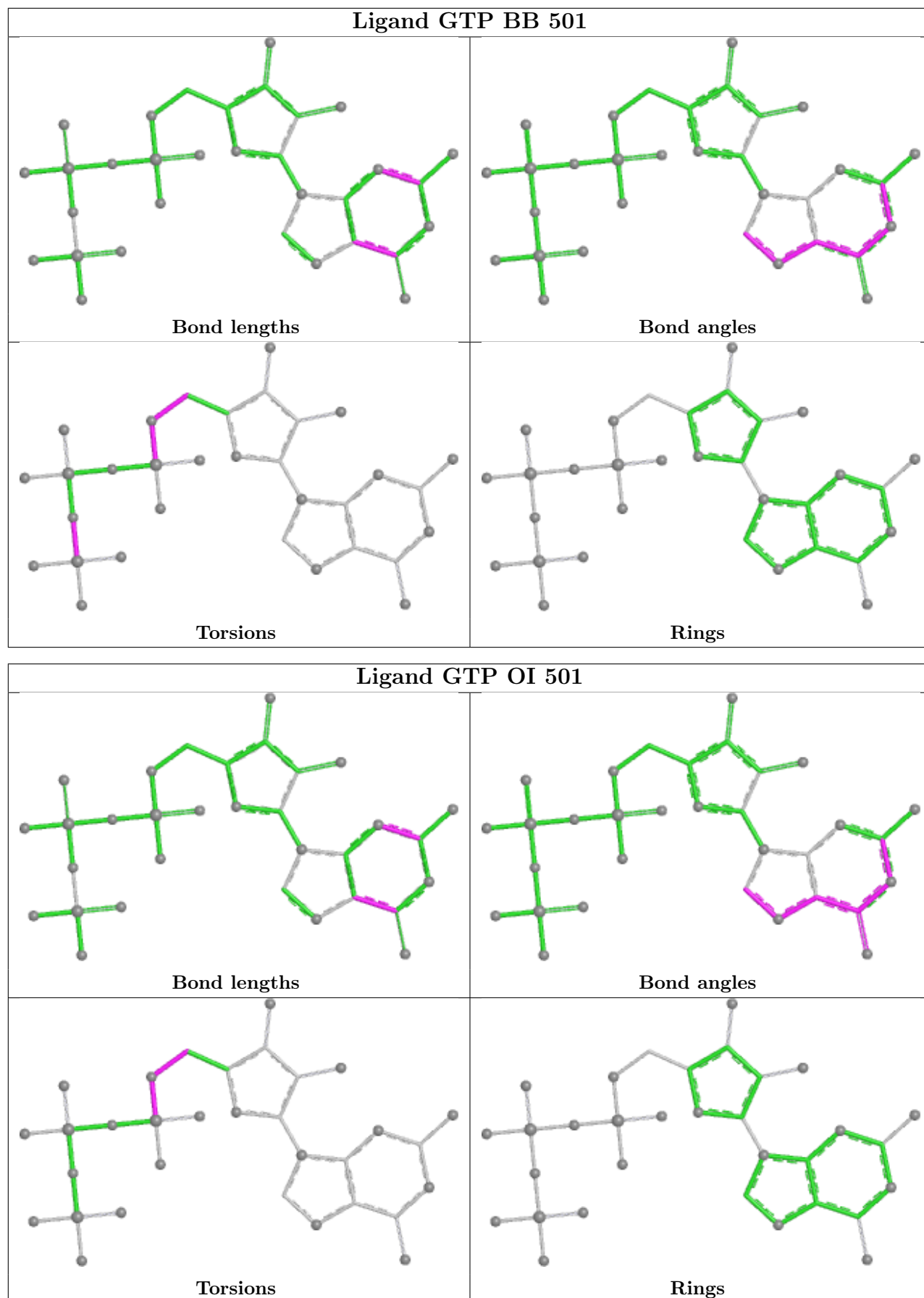
There are no ring outliers.

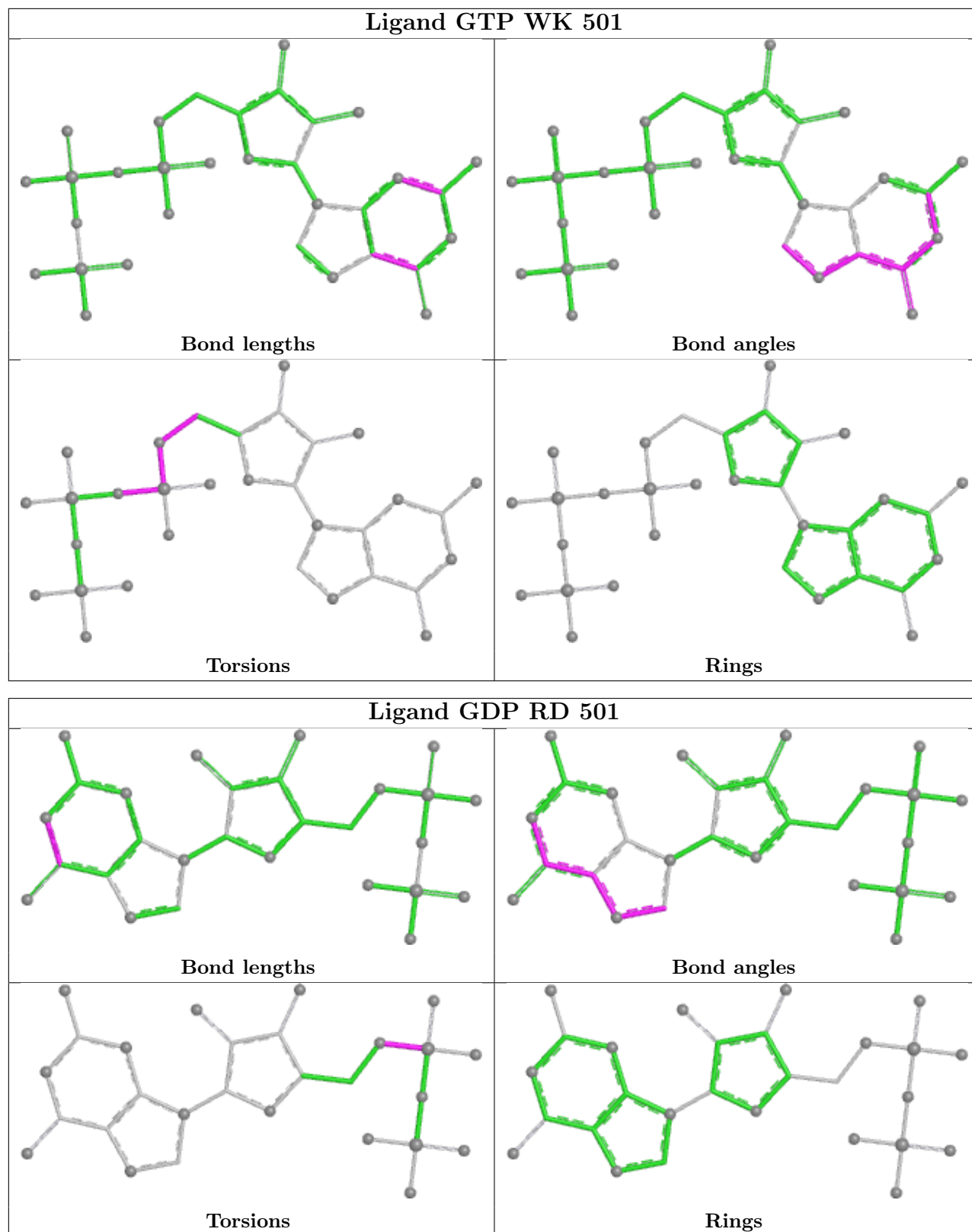
No monomer is involved in short contacts.

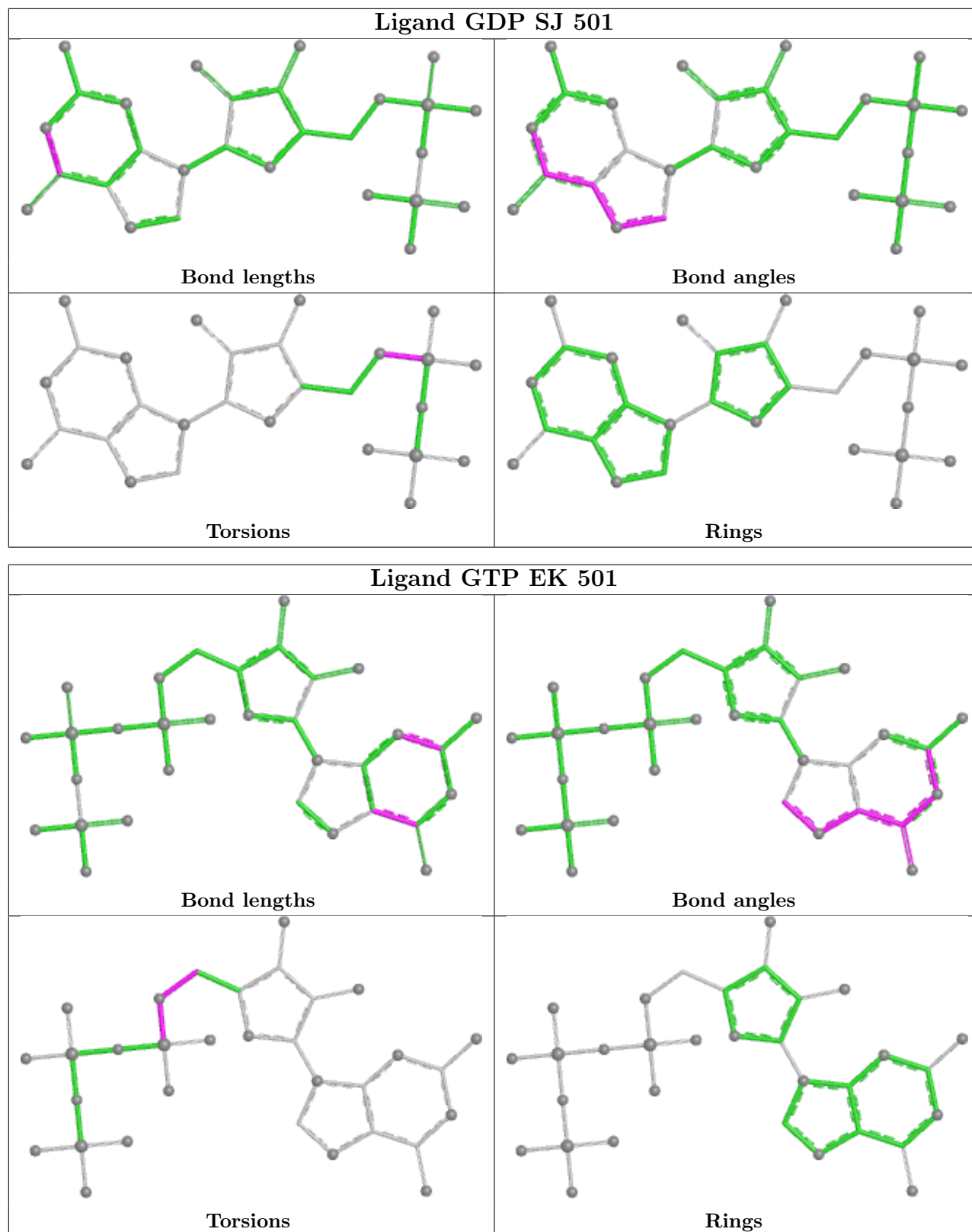
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

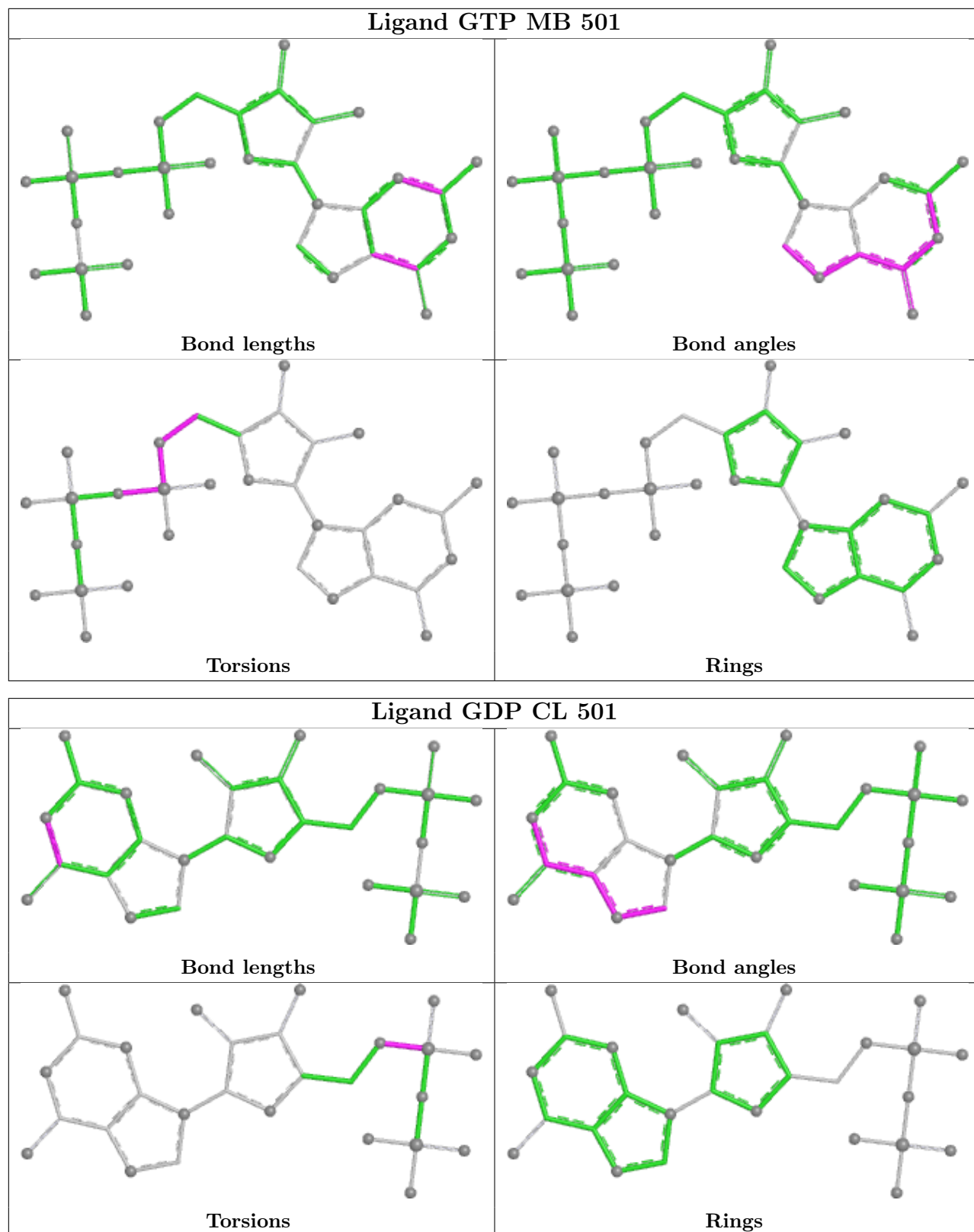


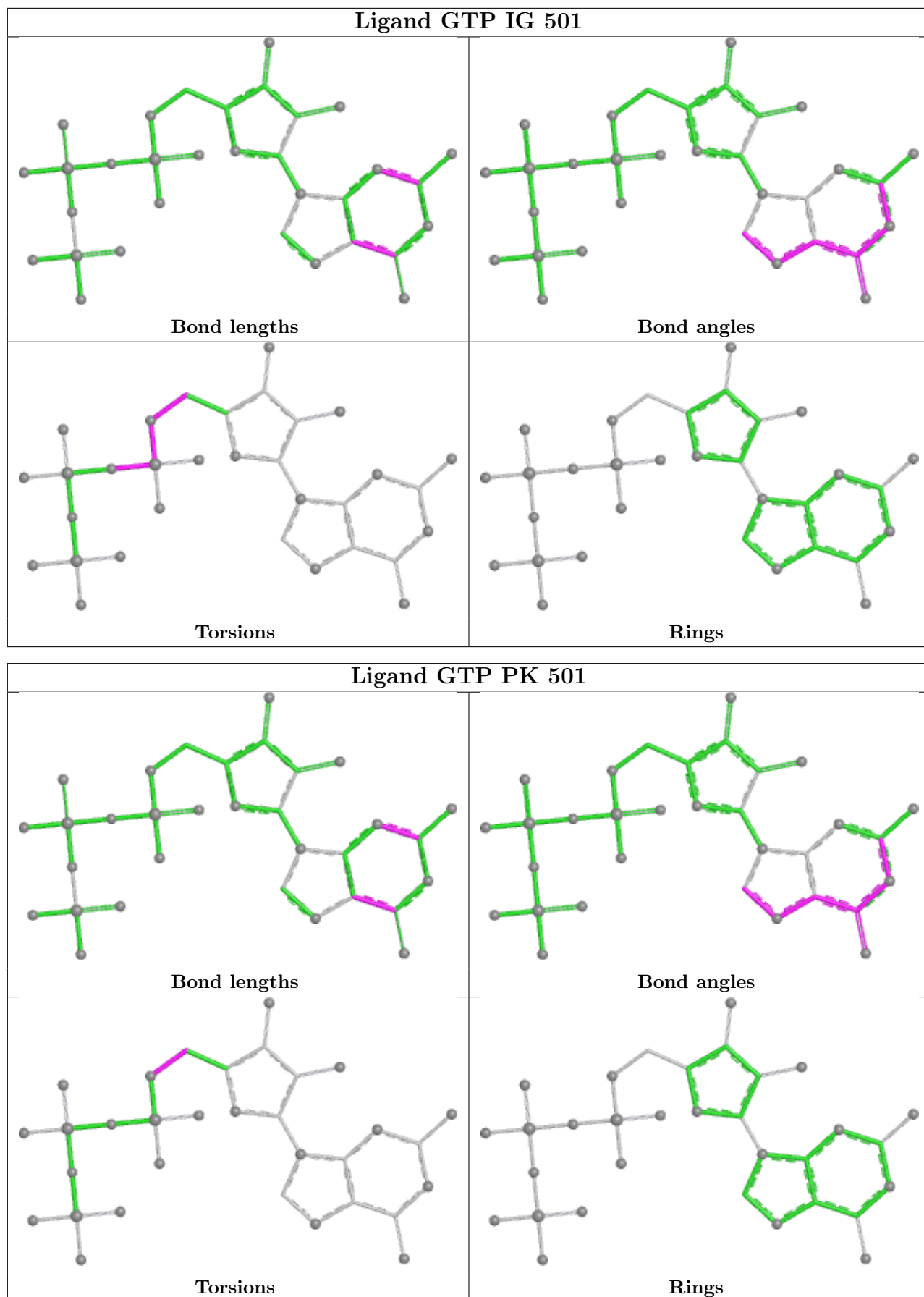


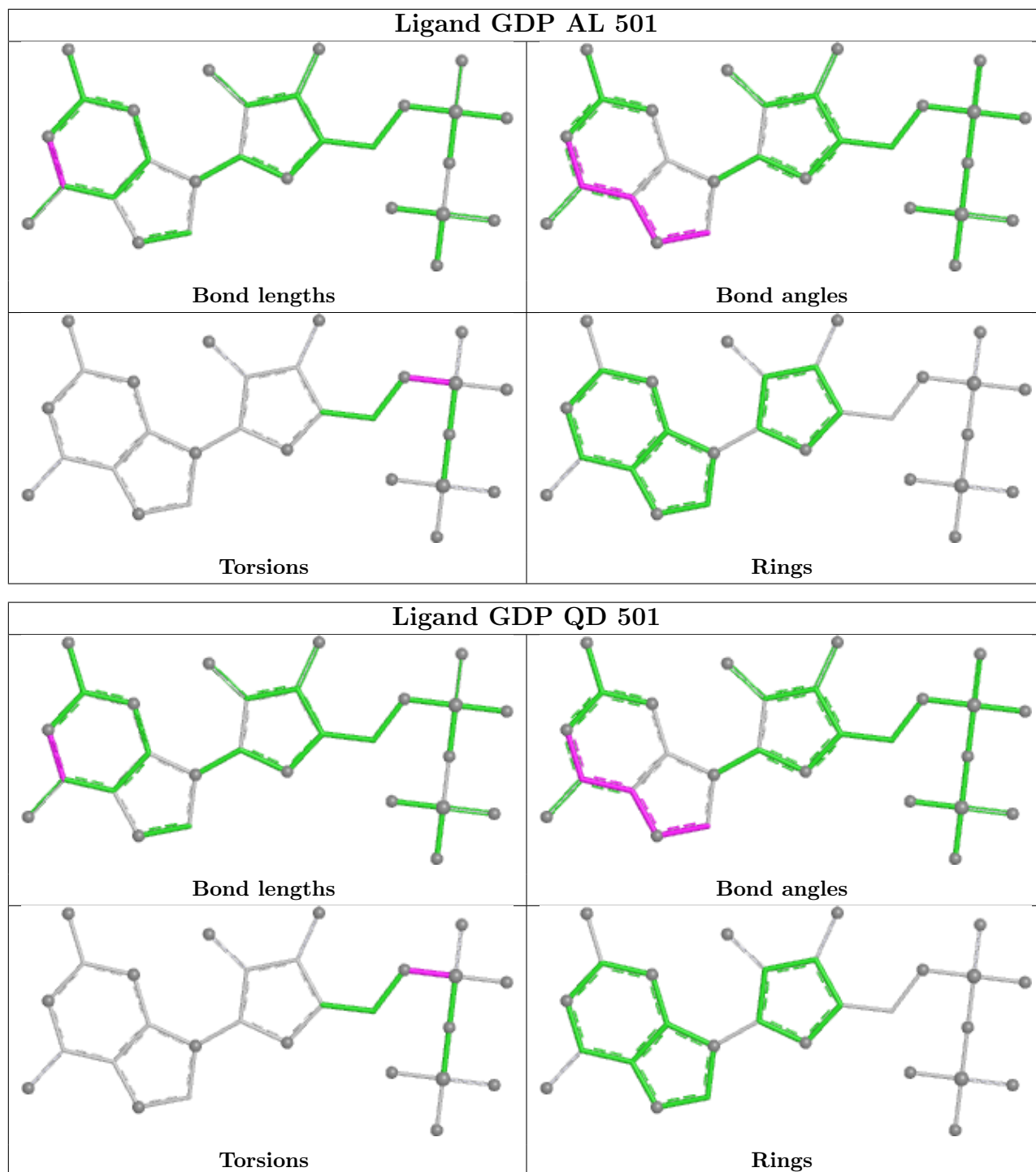


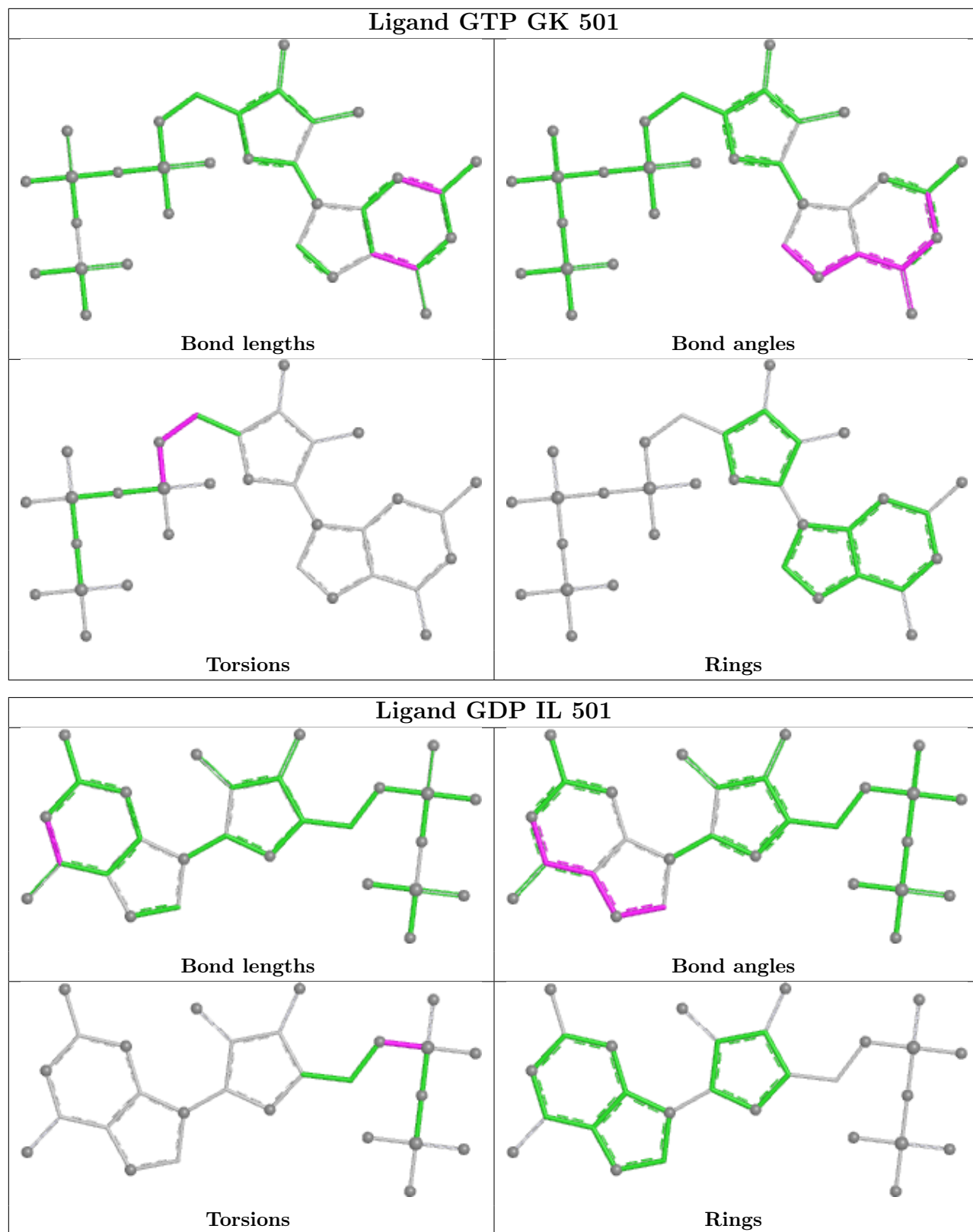


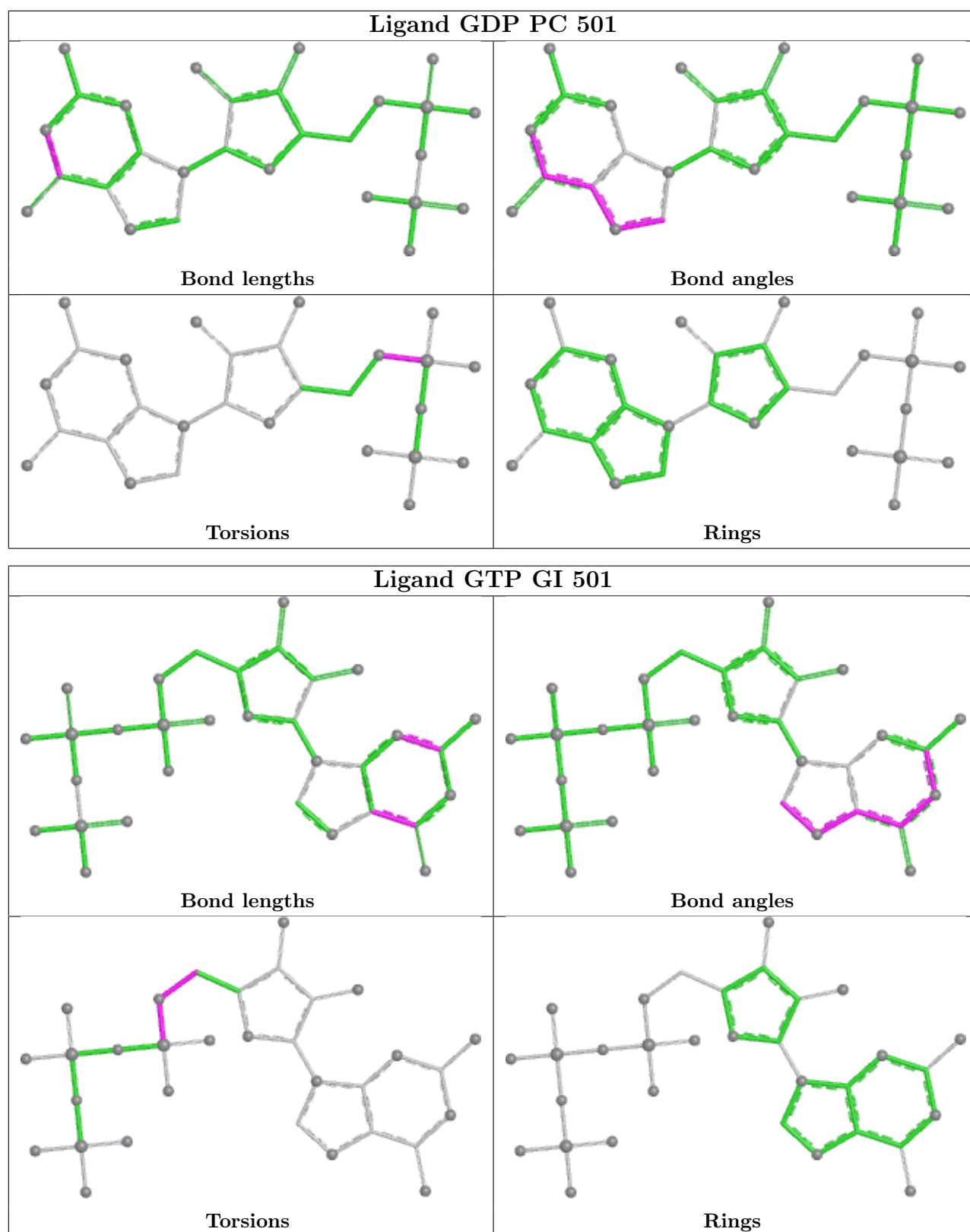


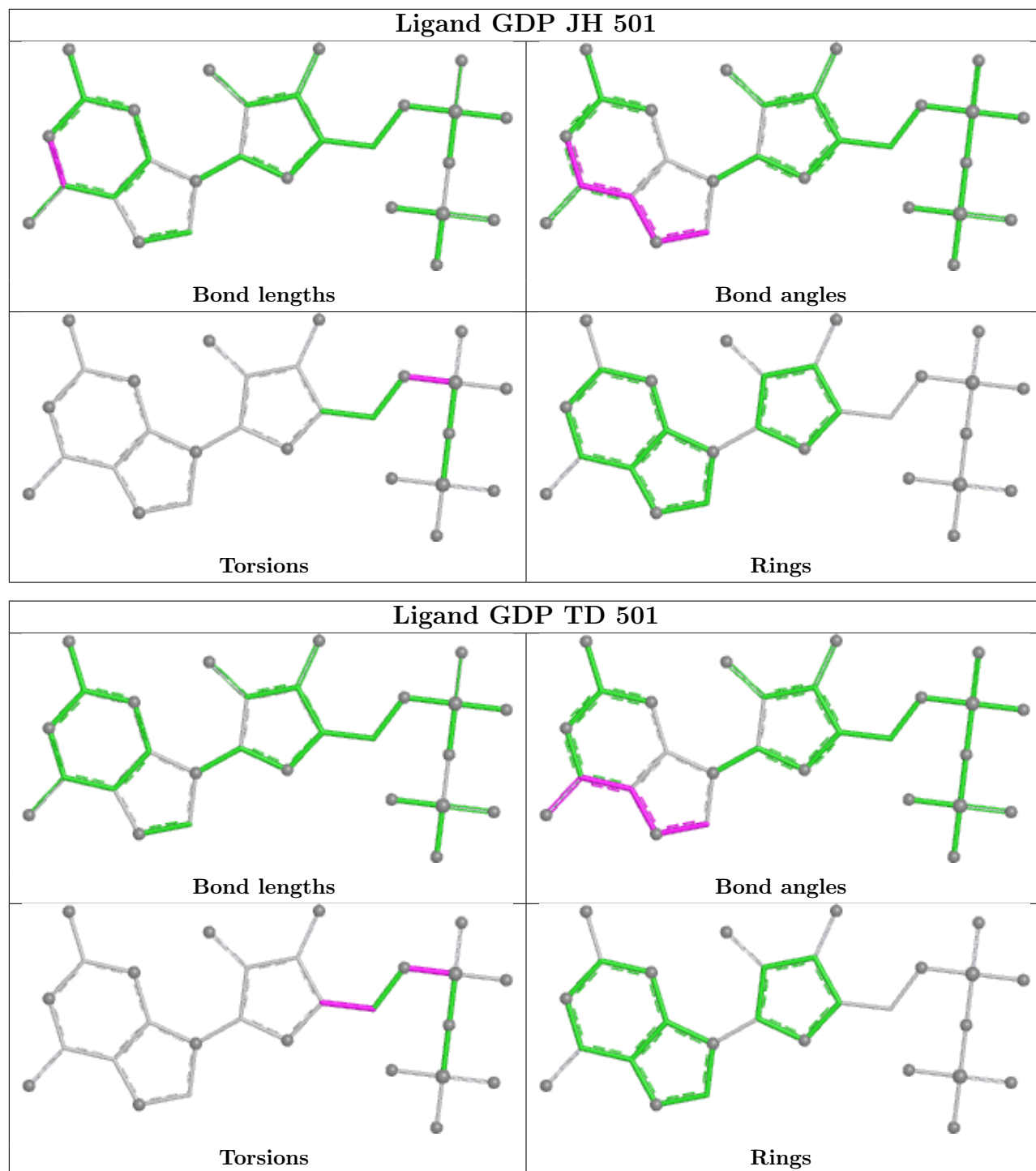


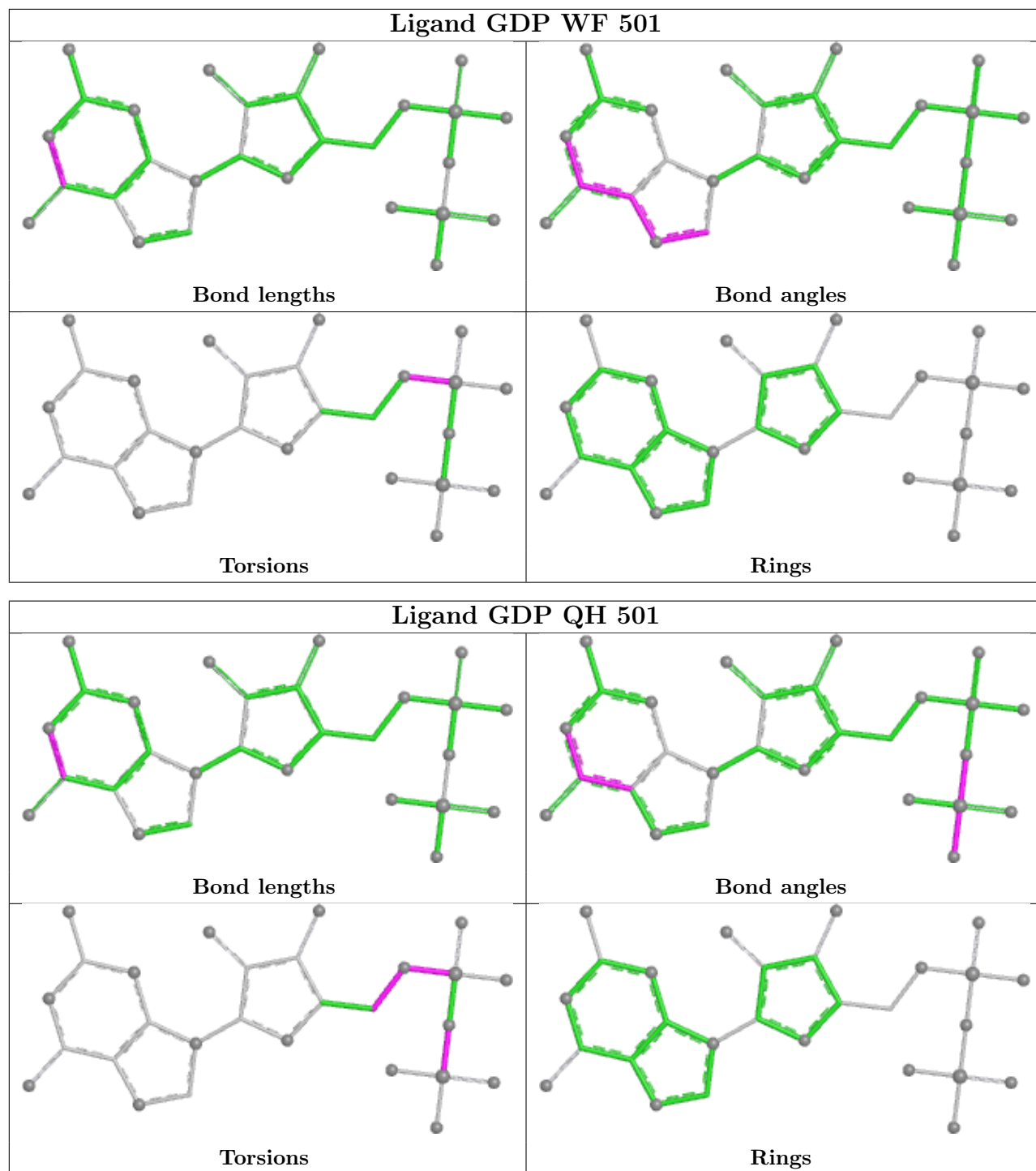


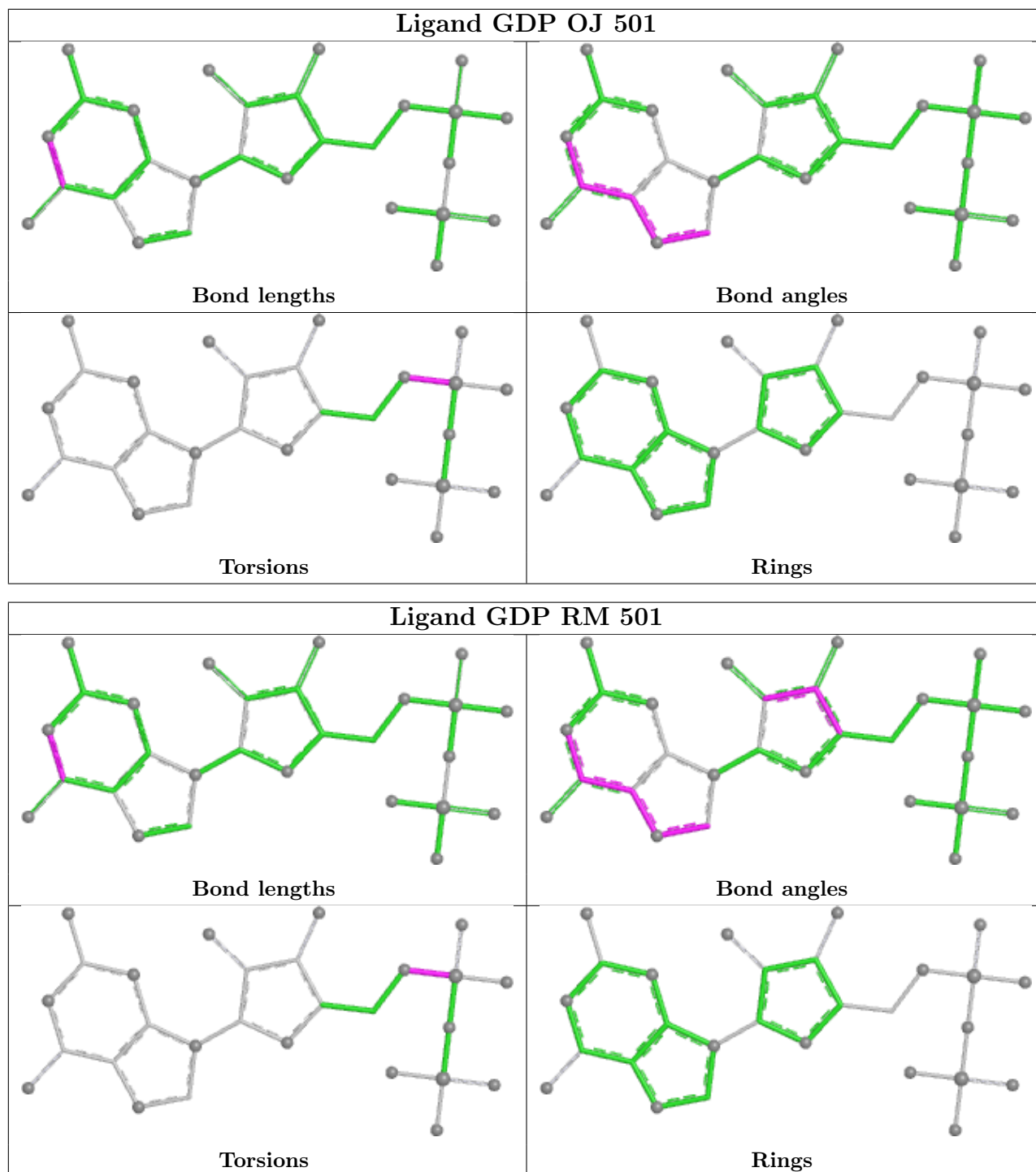


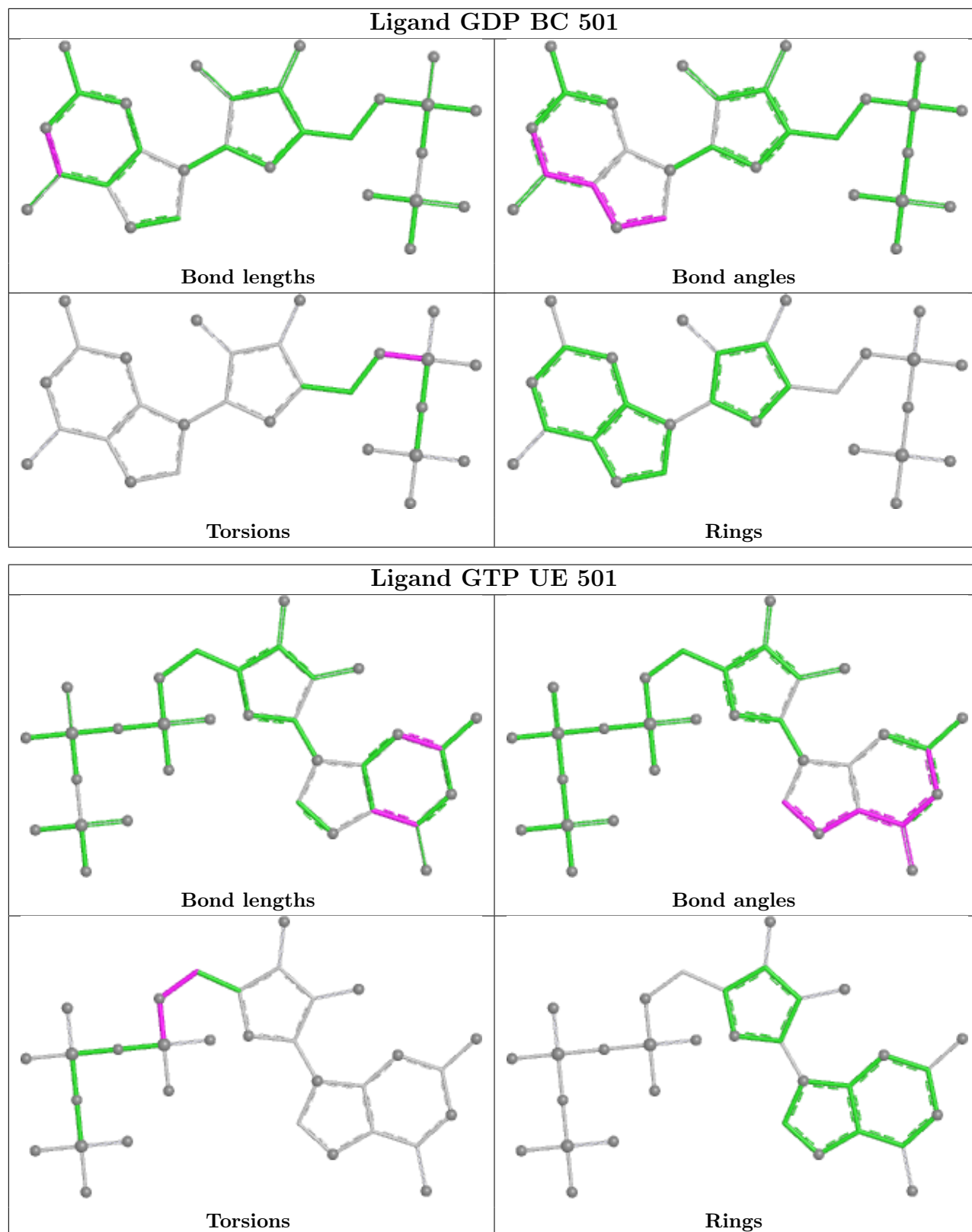


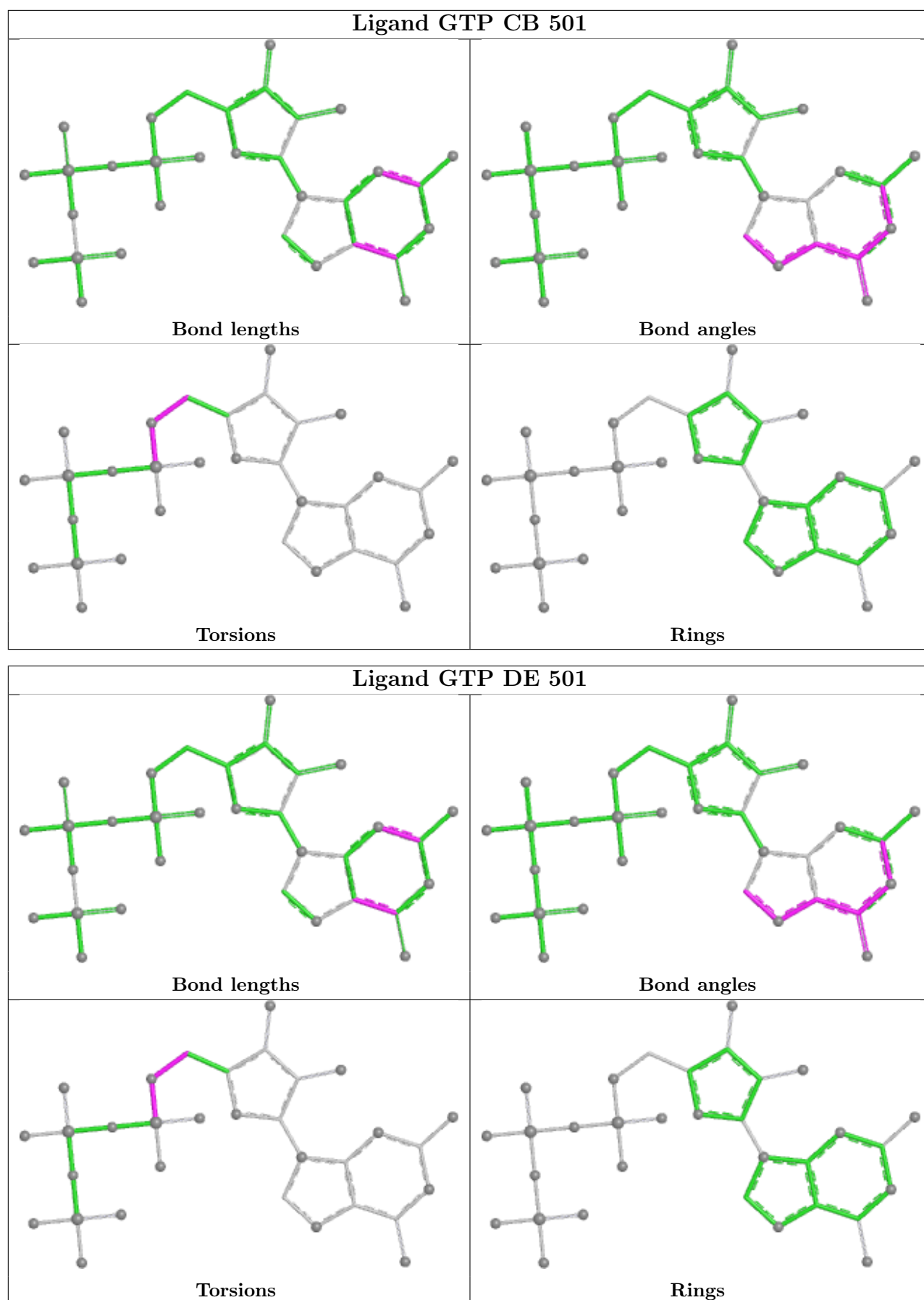


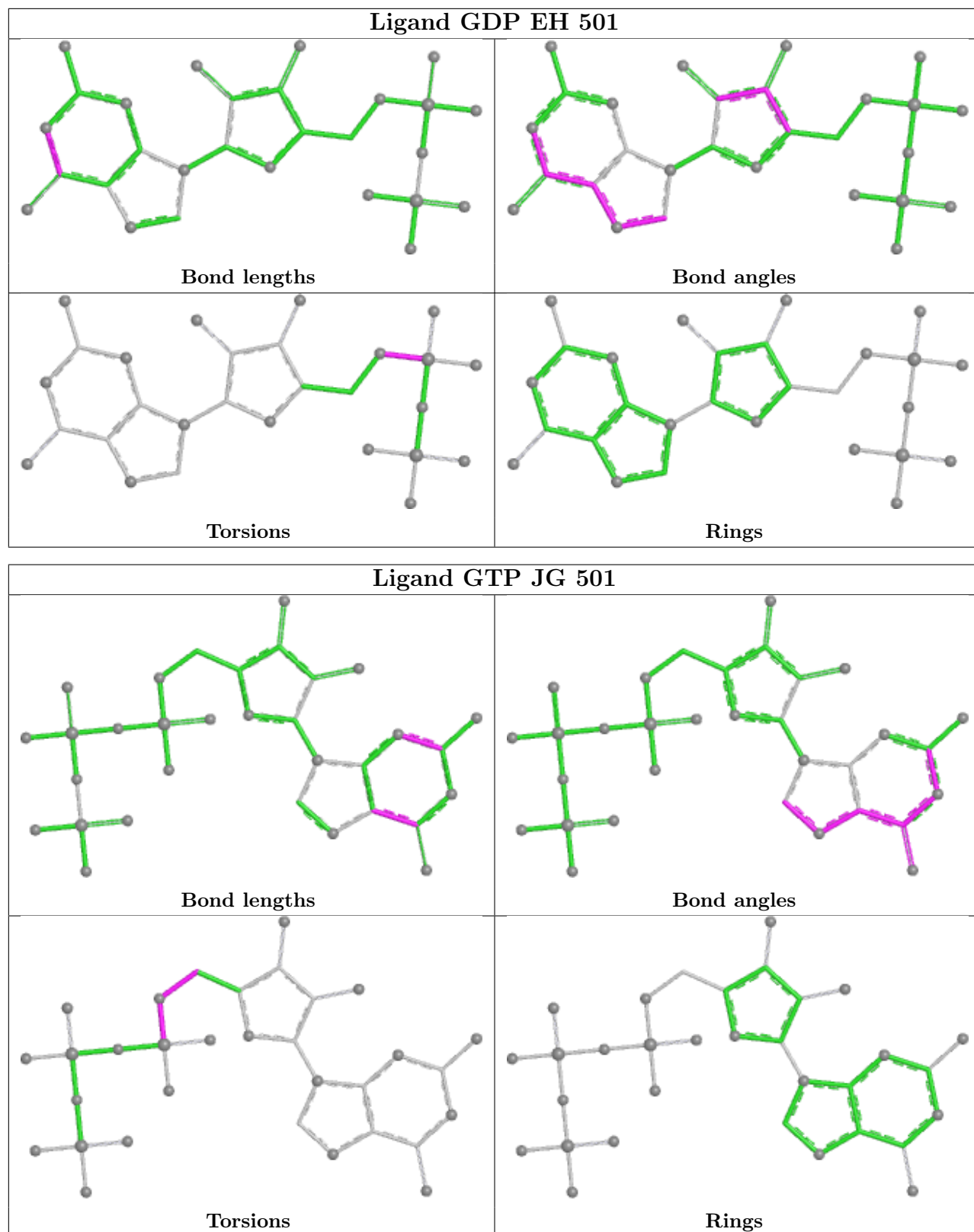


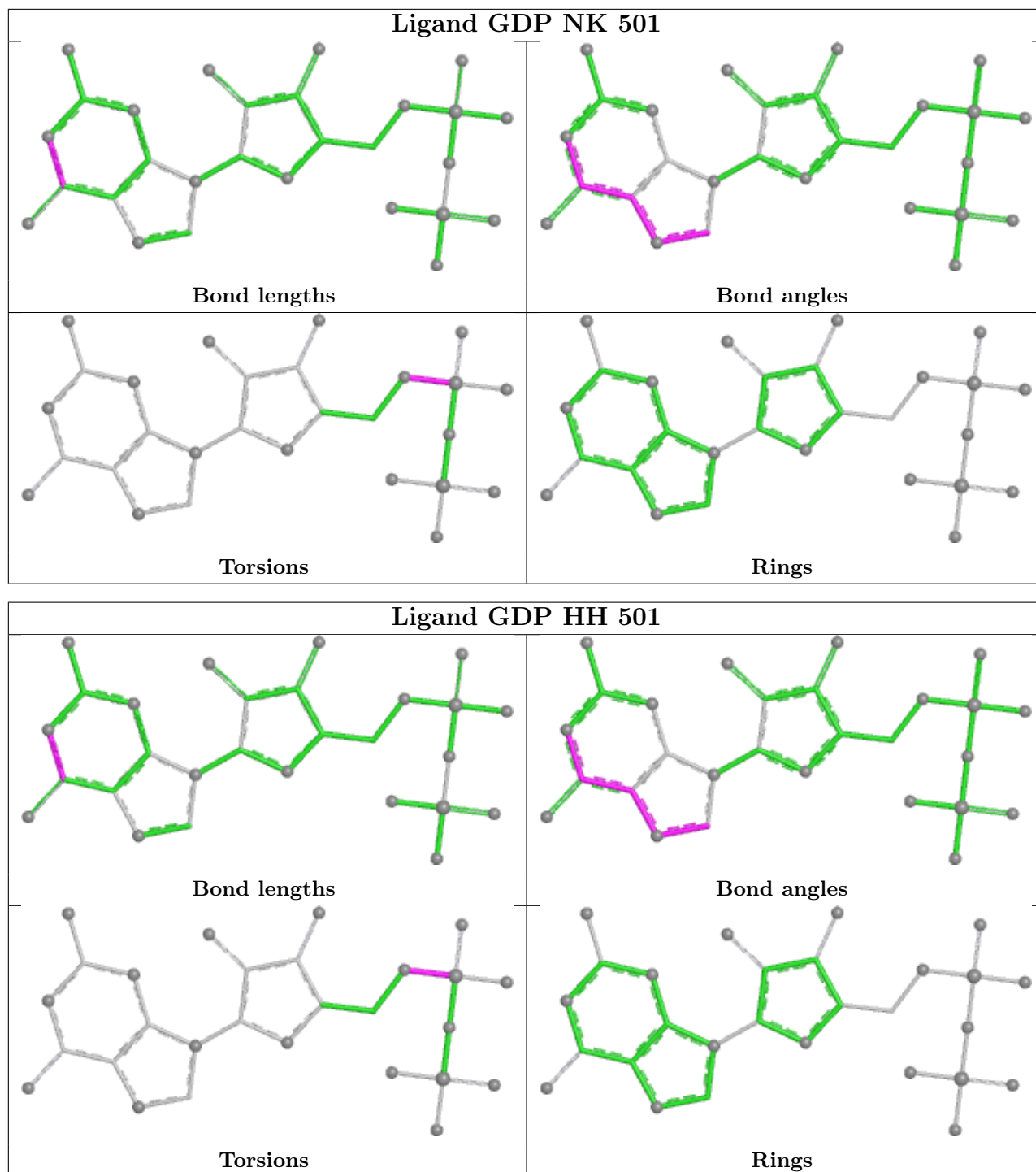


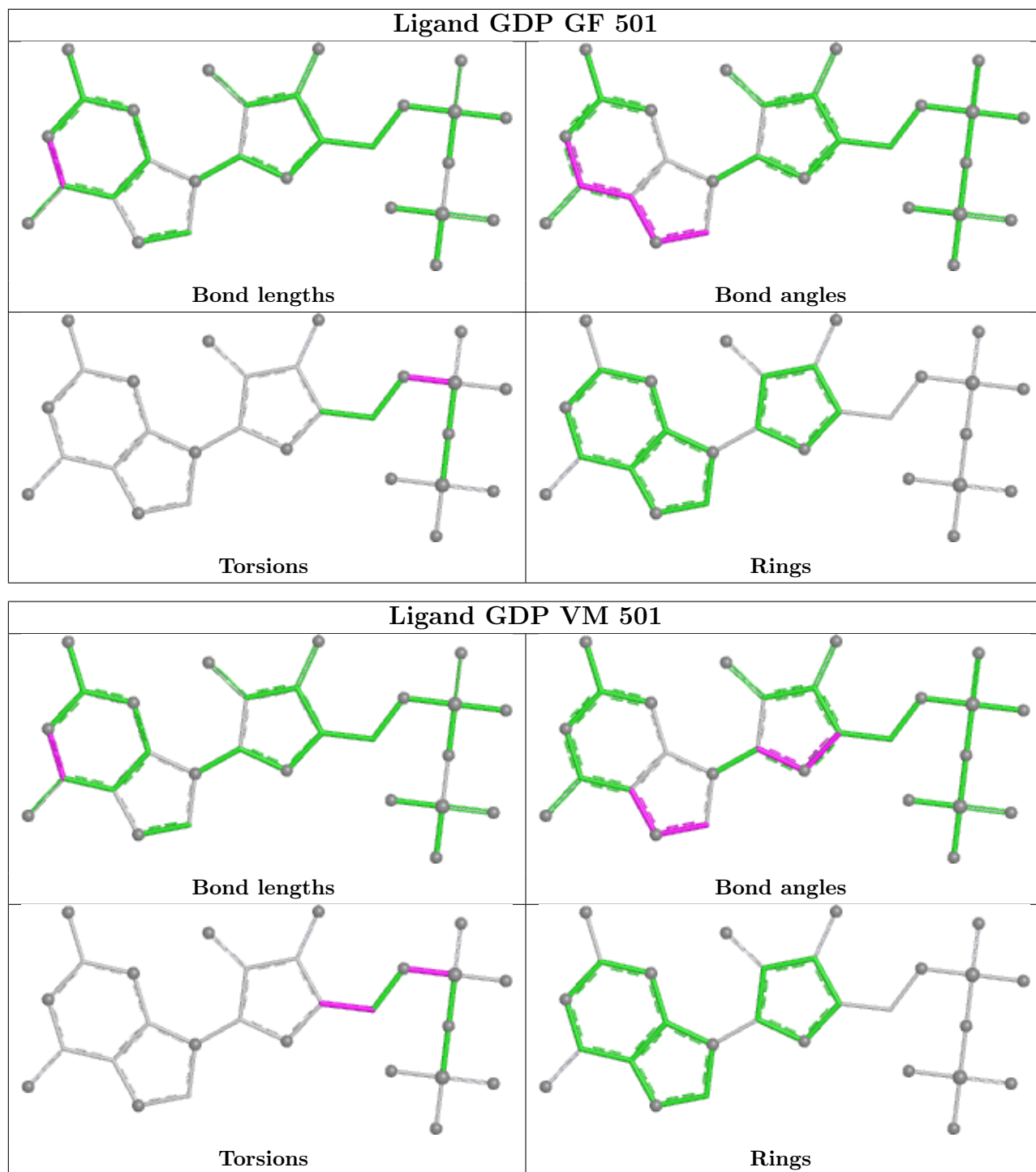


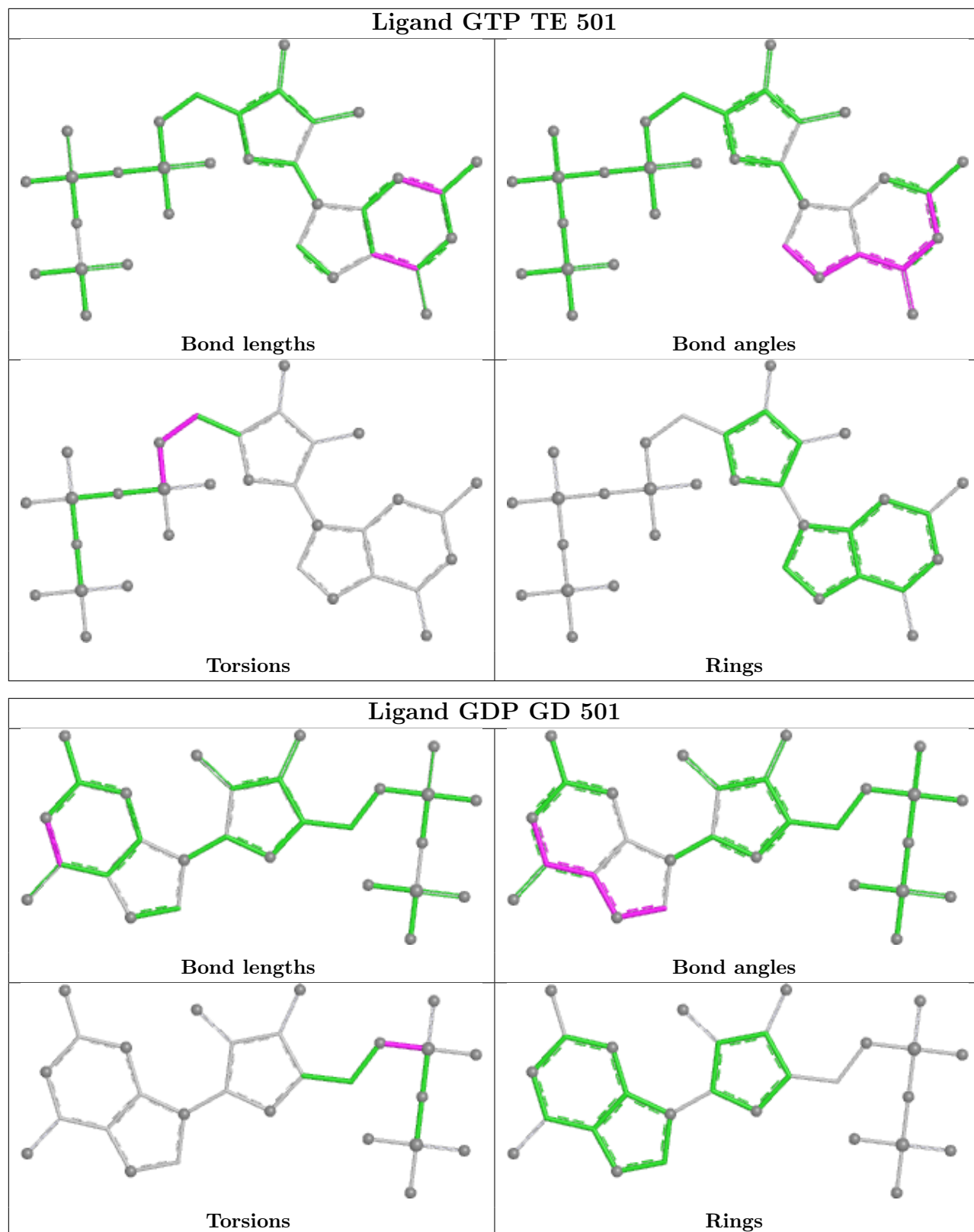


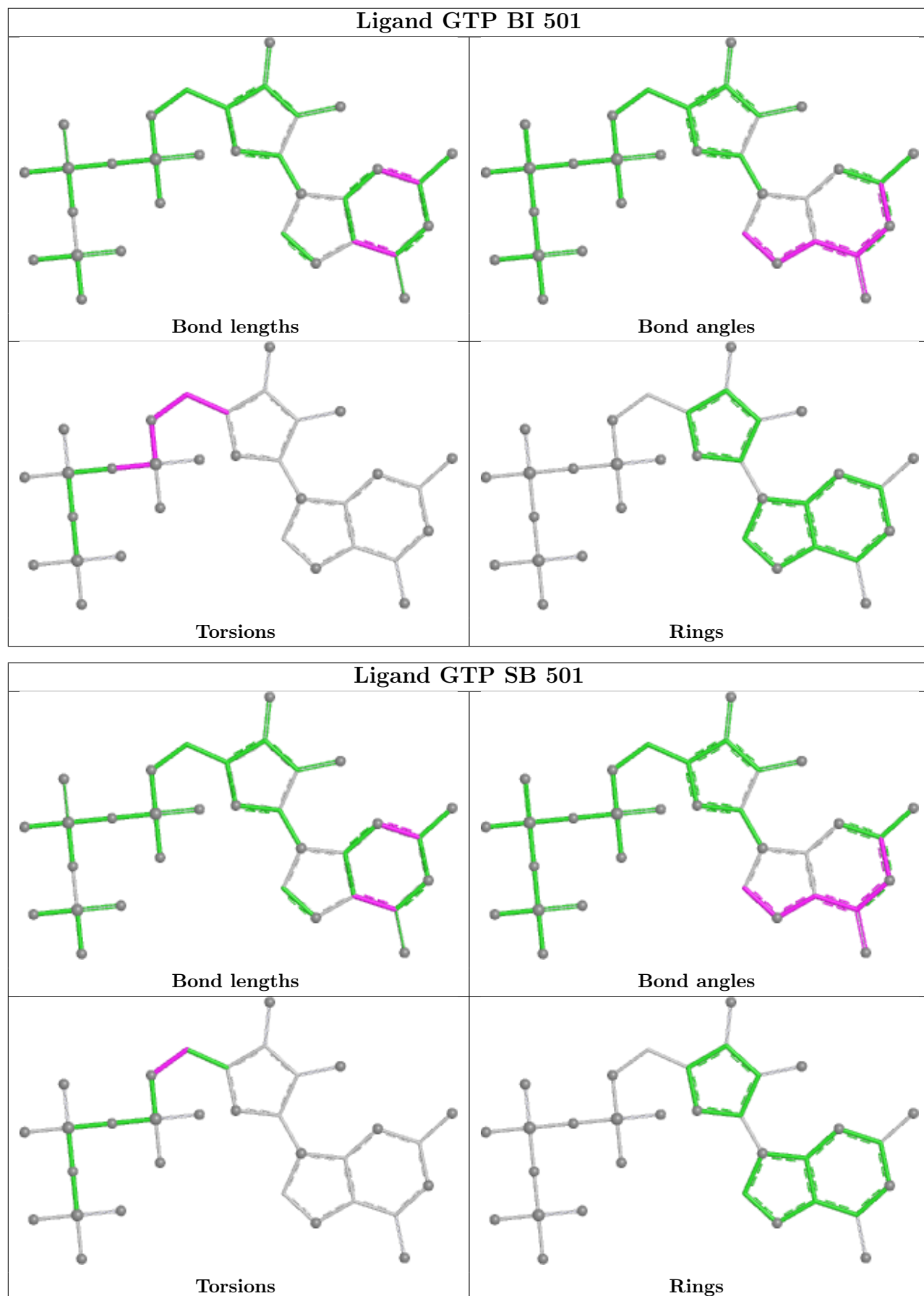


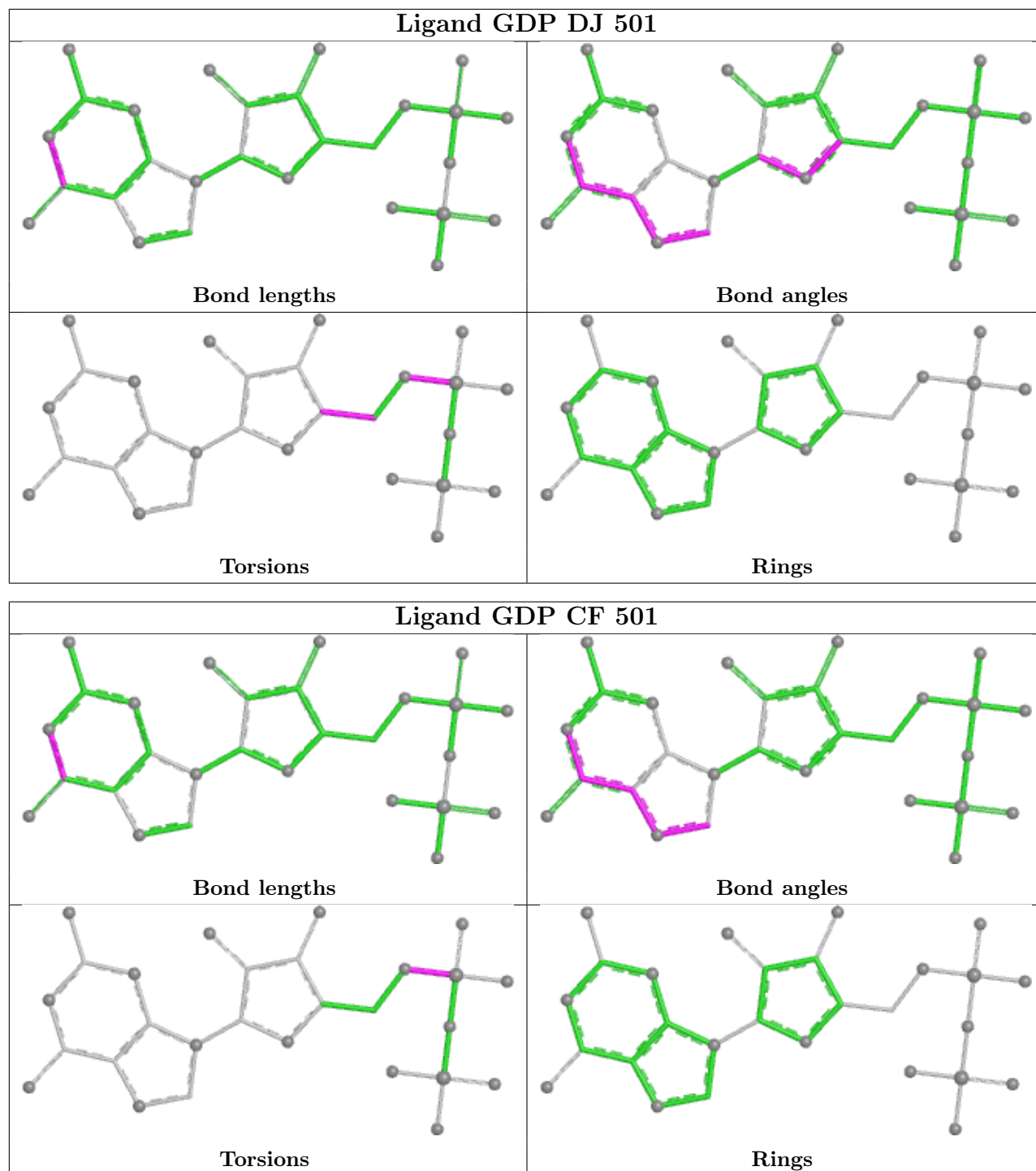


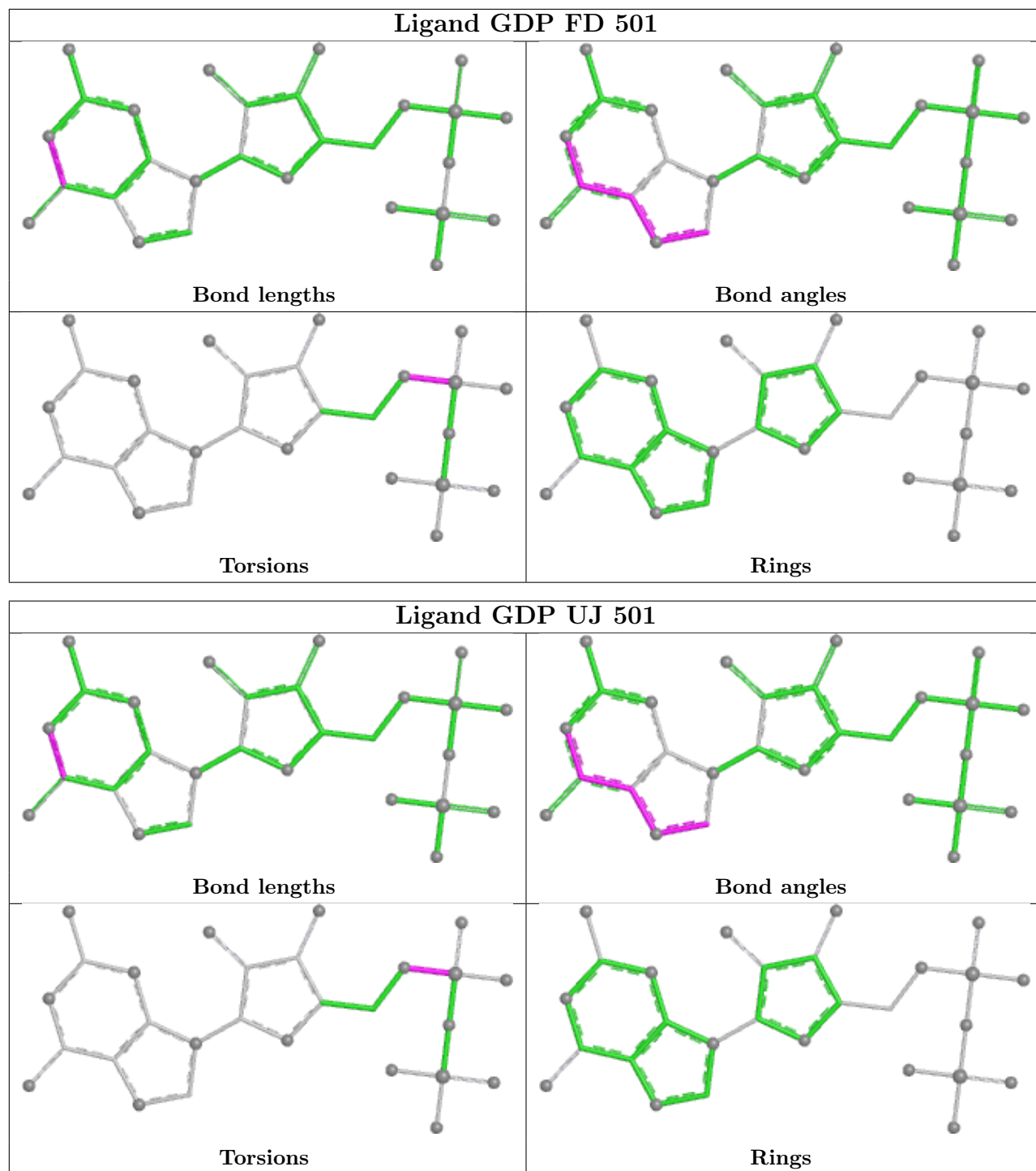


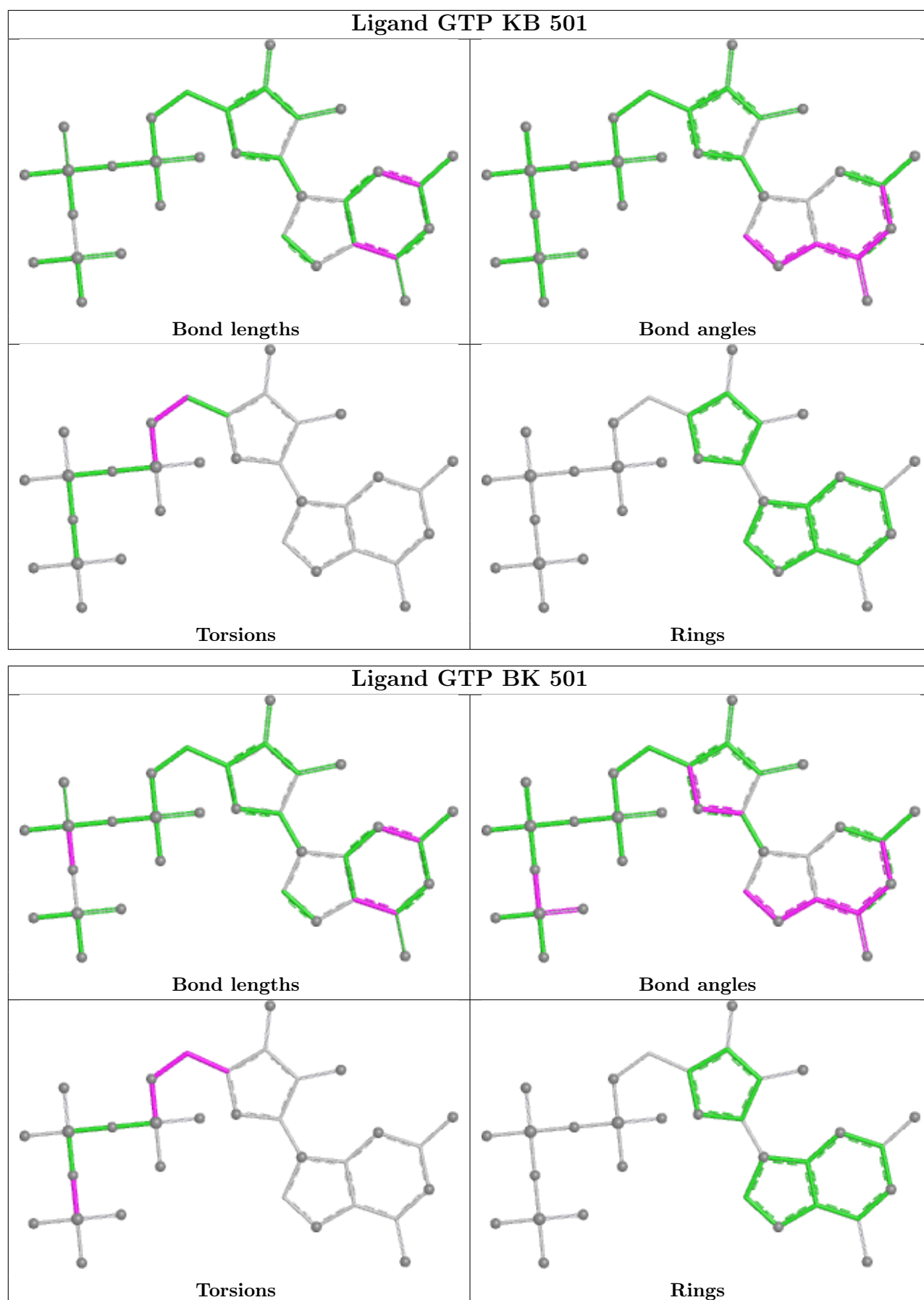


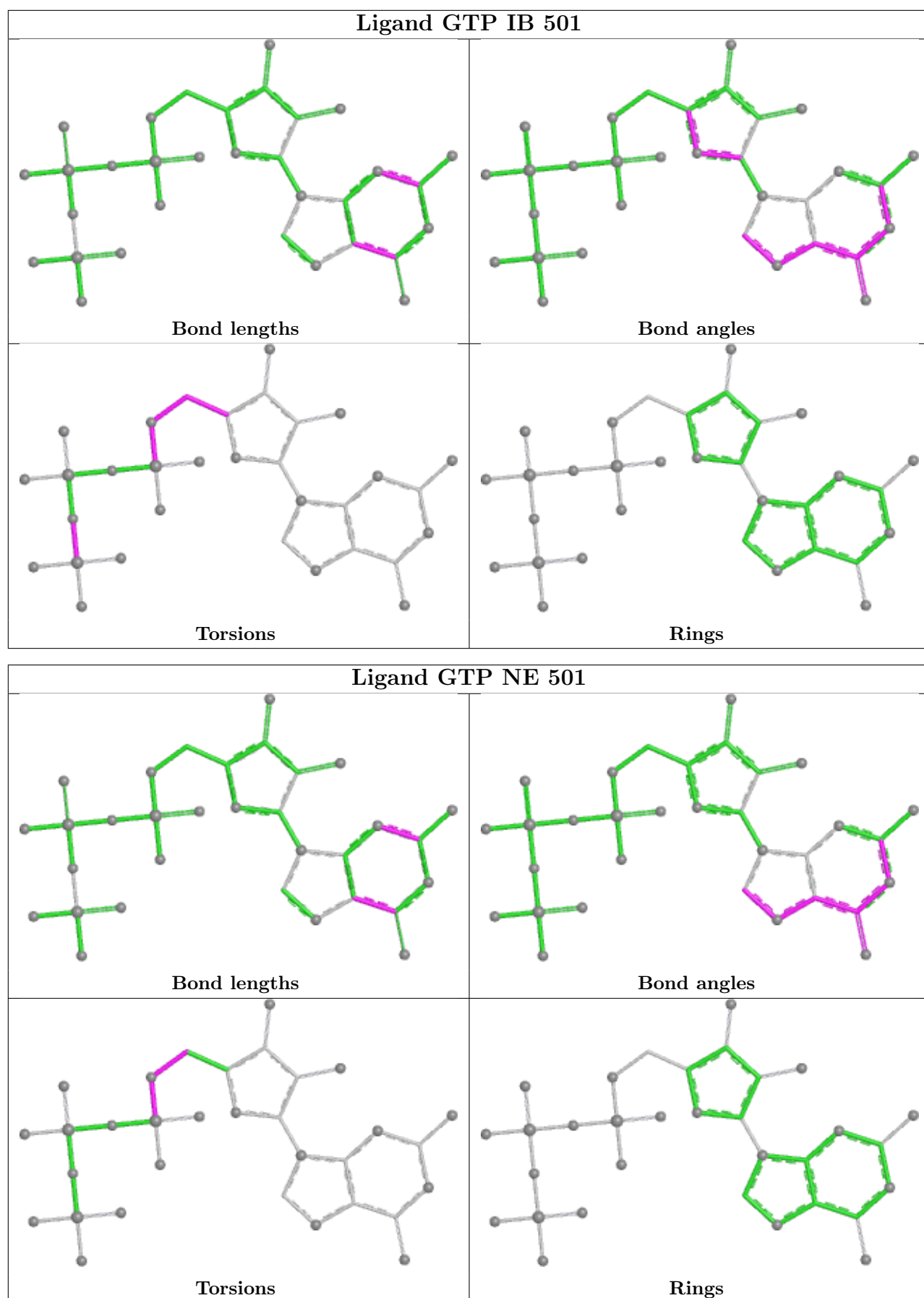


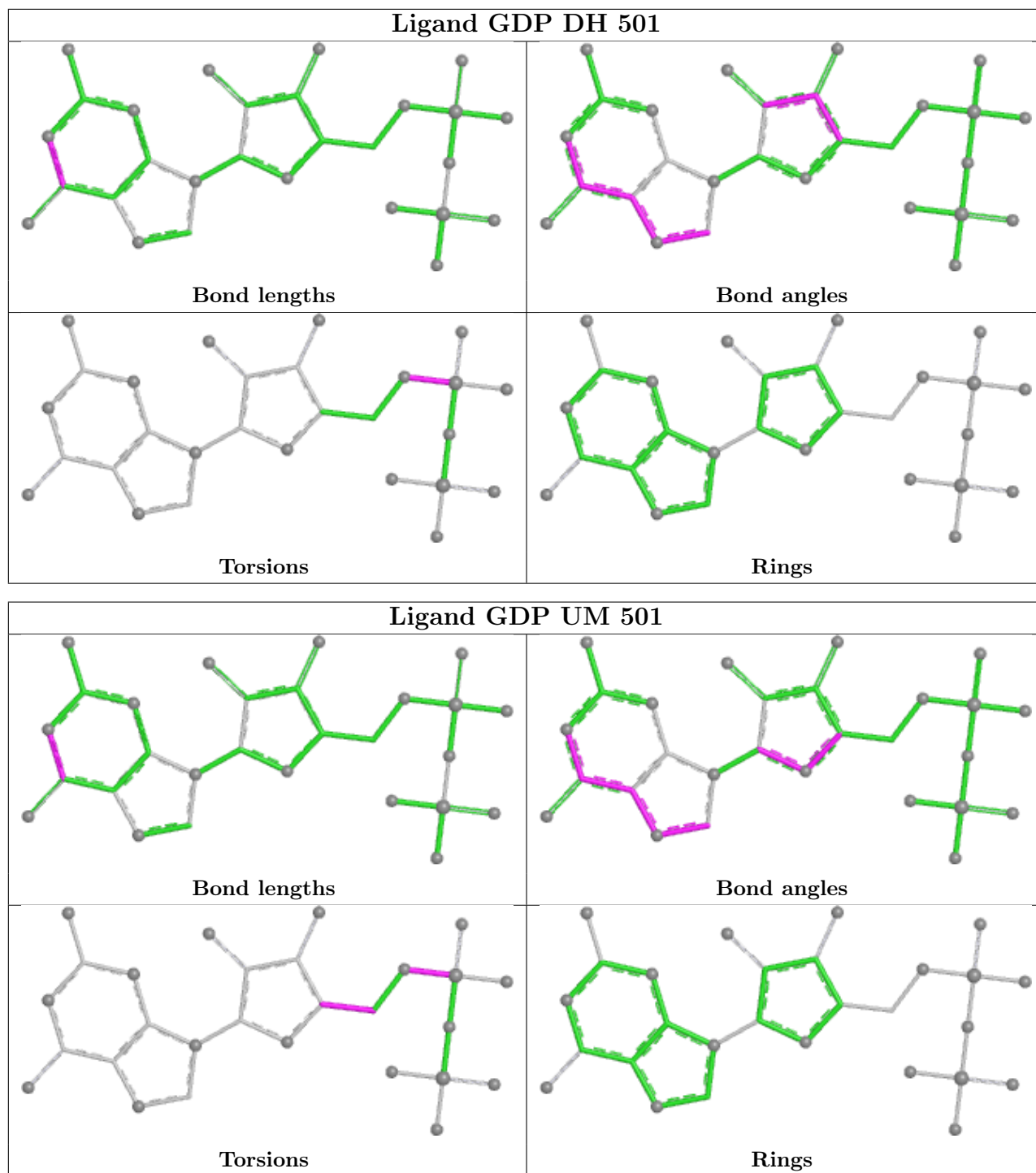


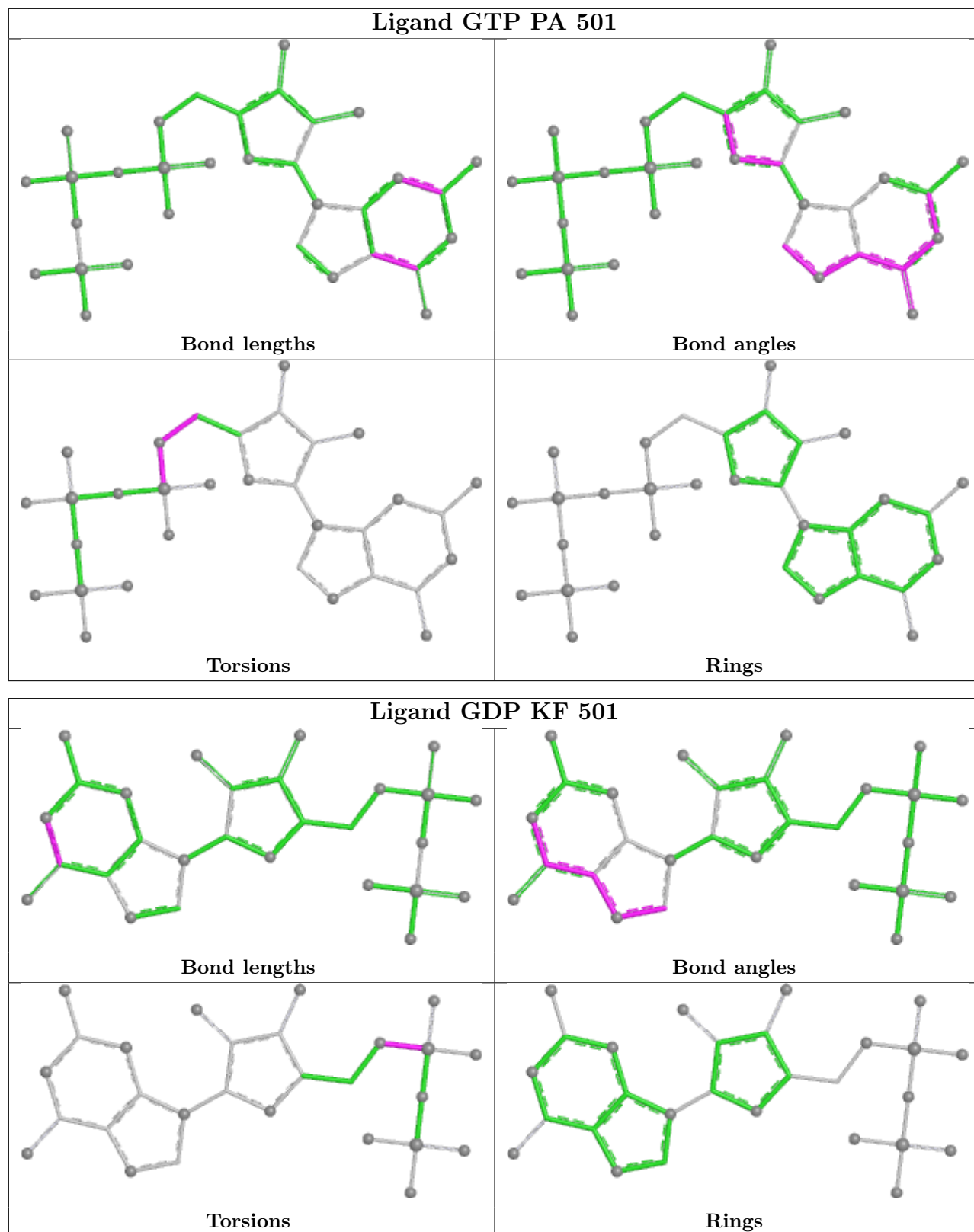


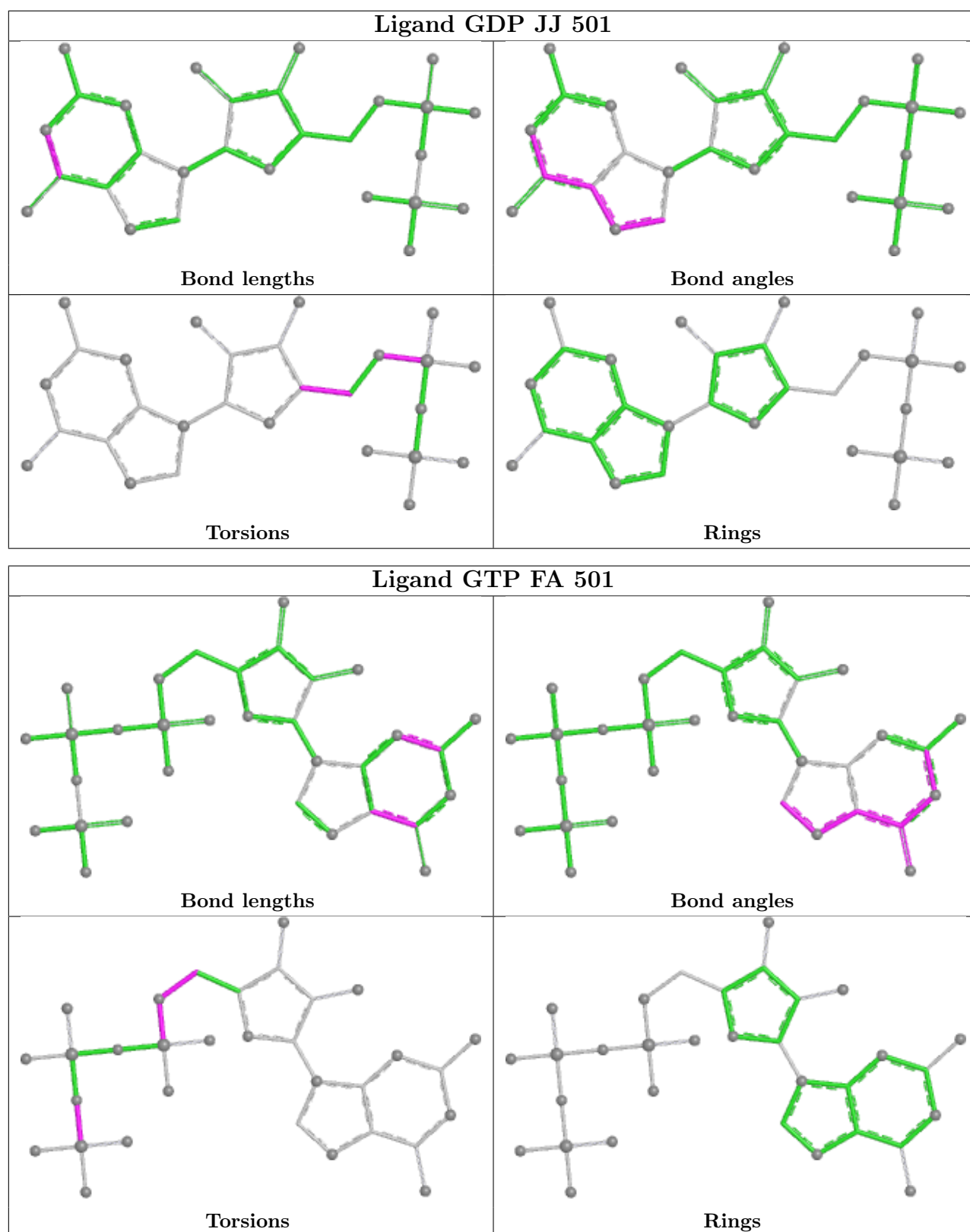


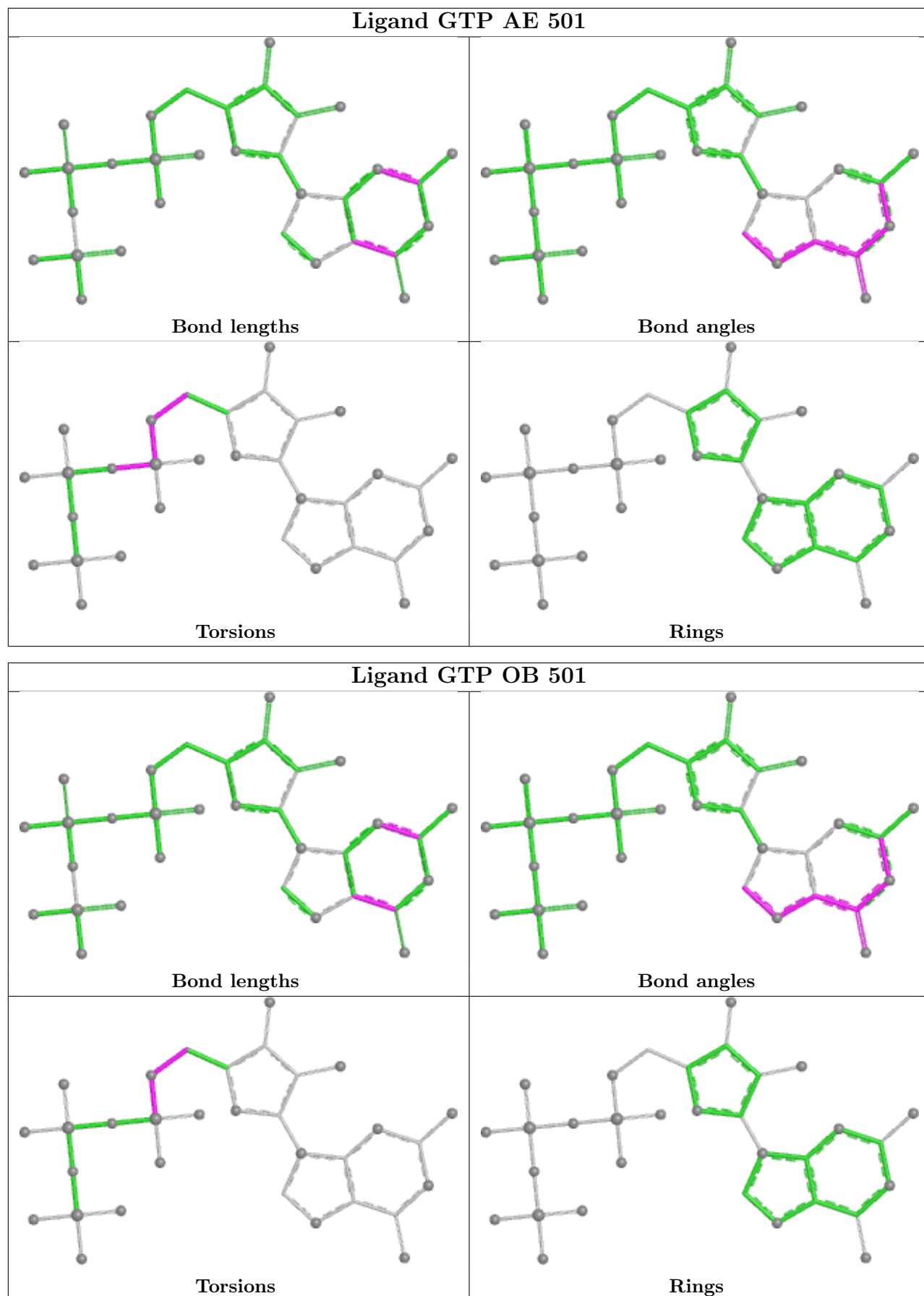


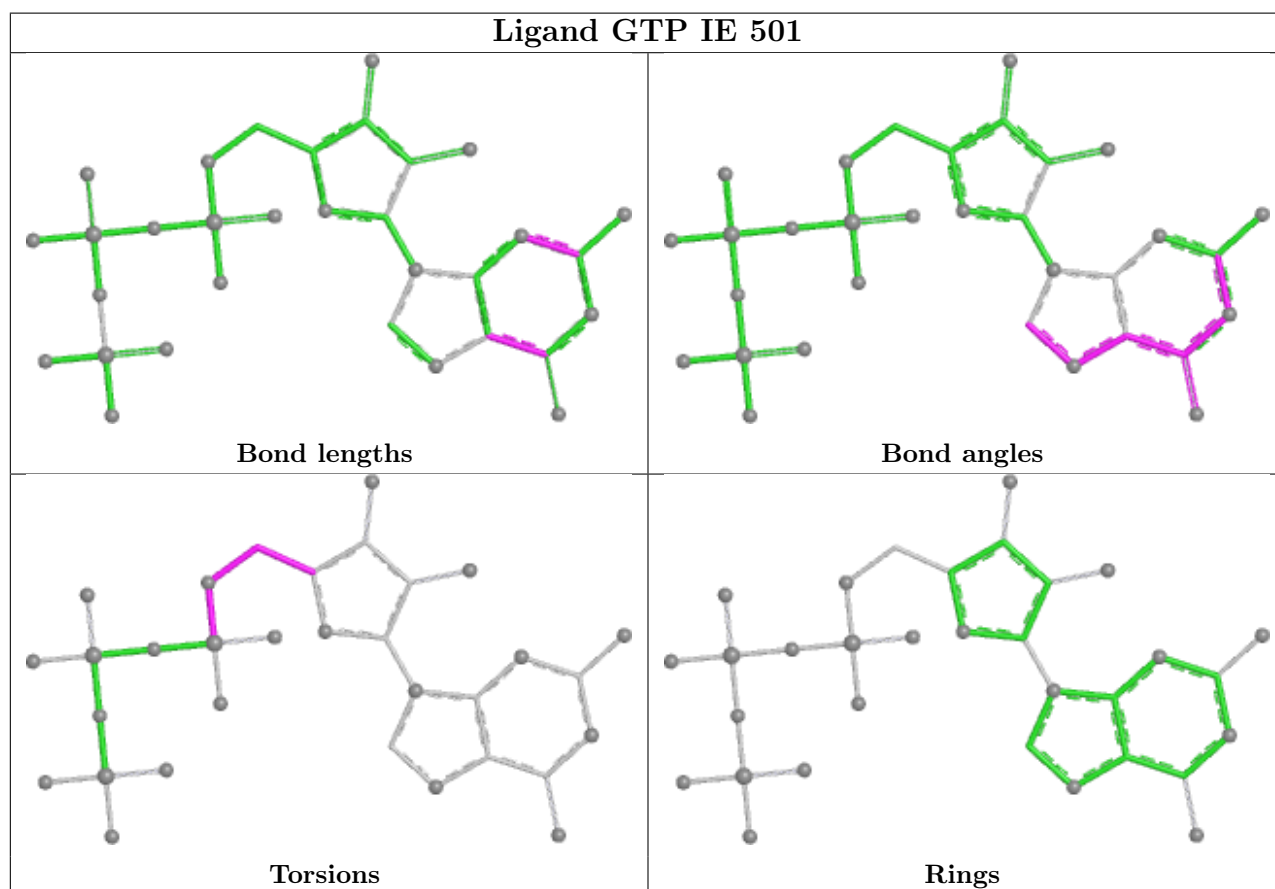
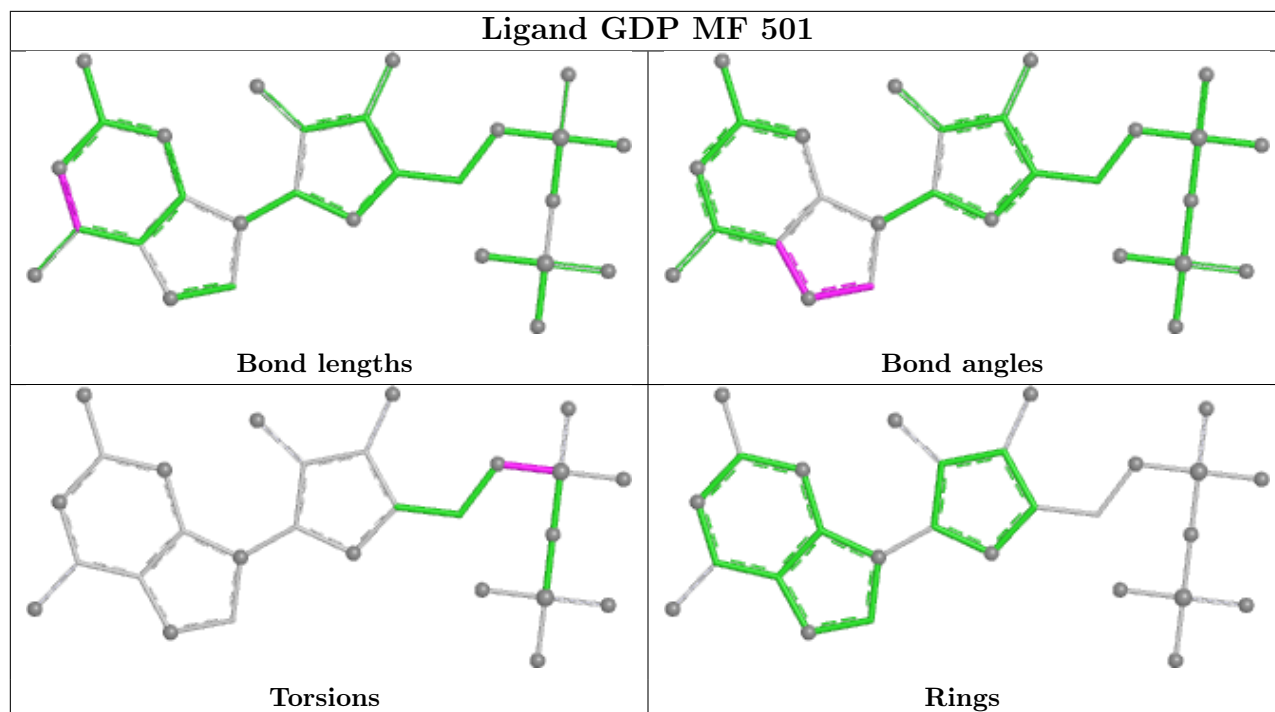


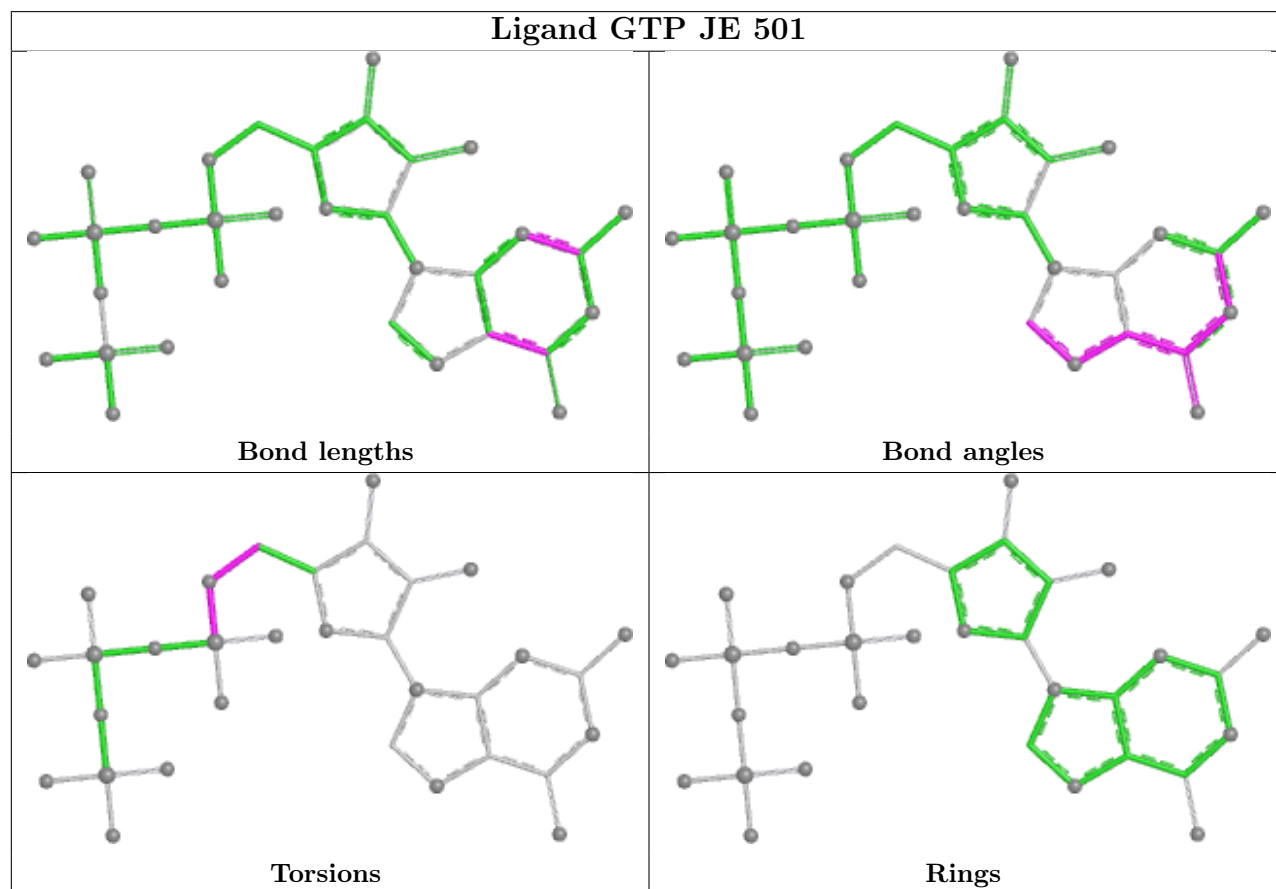
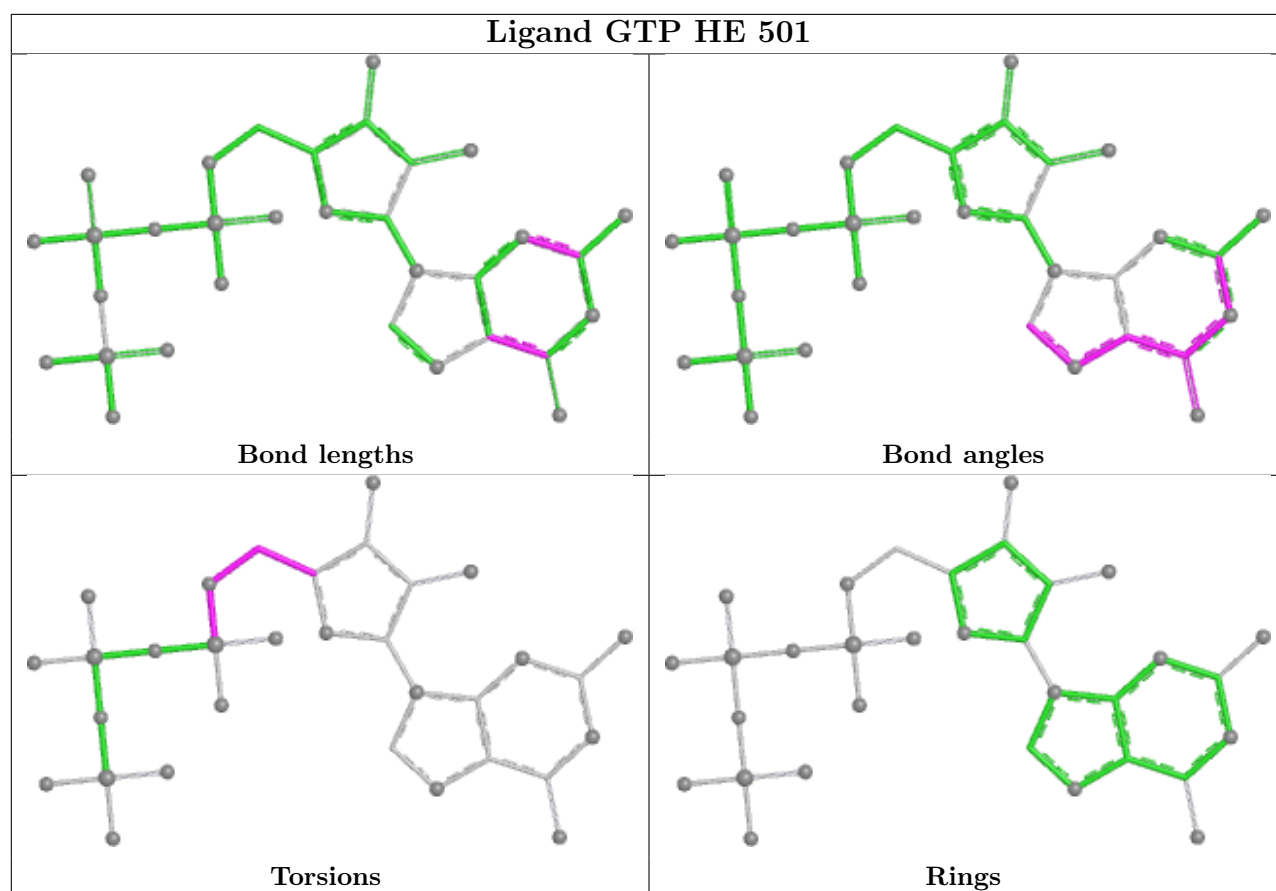


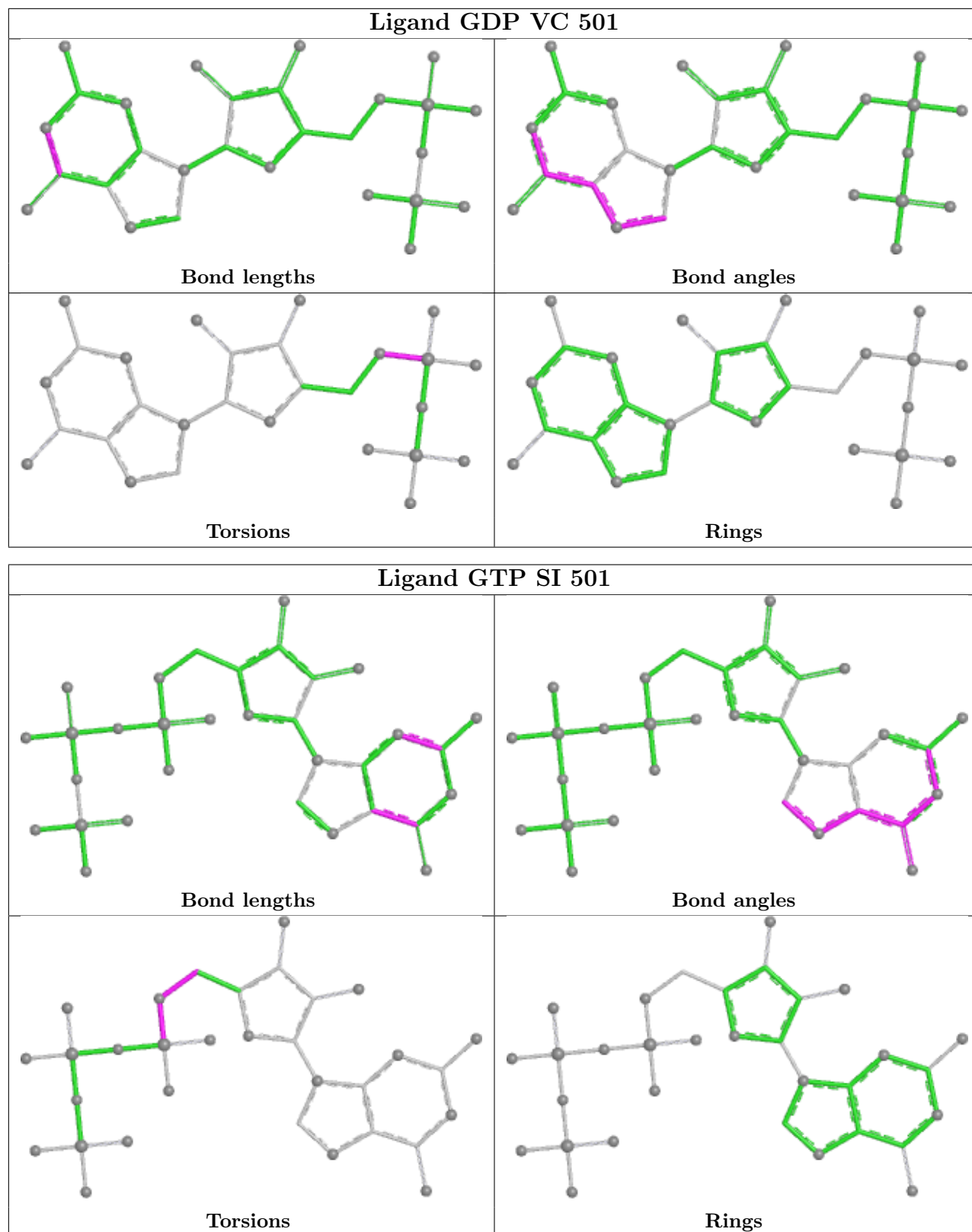


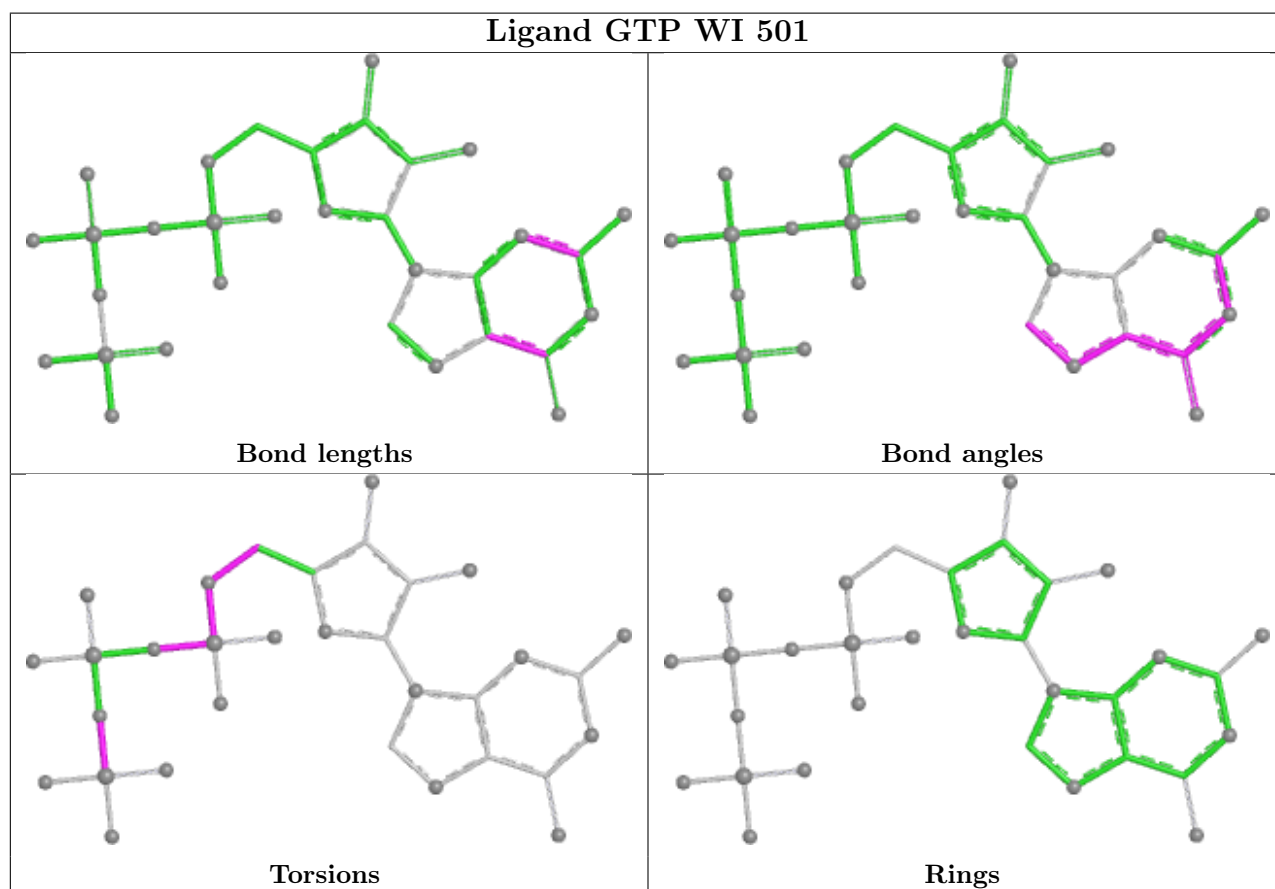
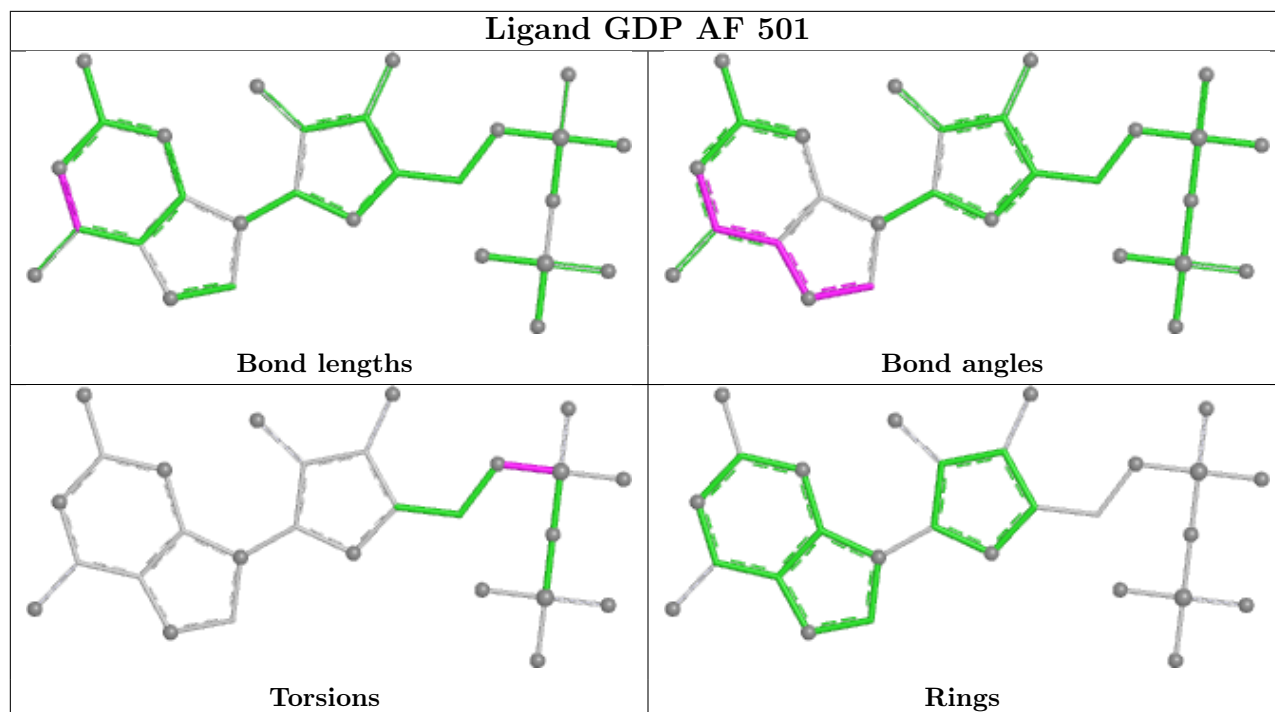


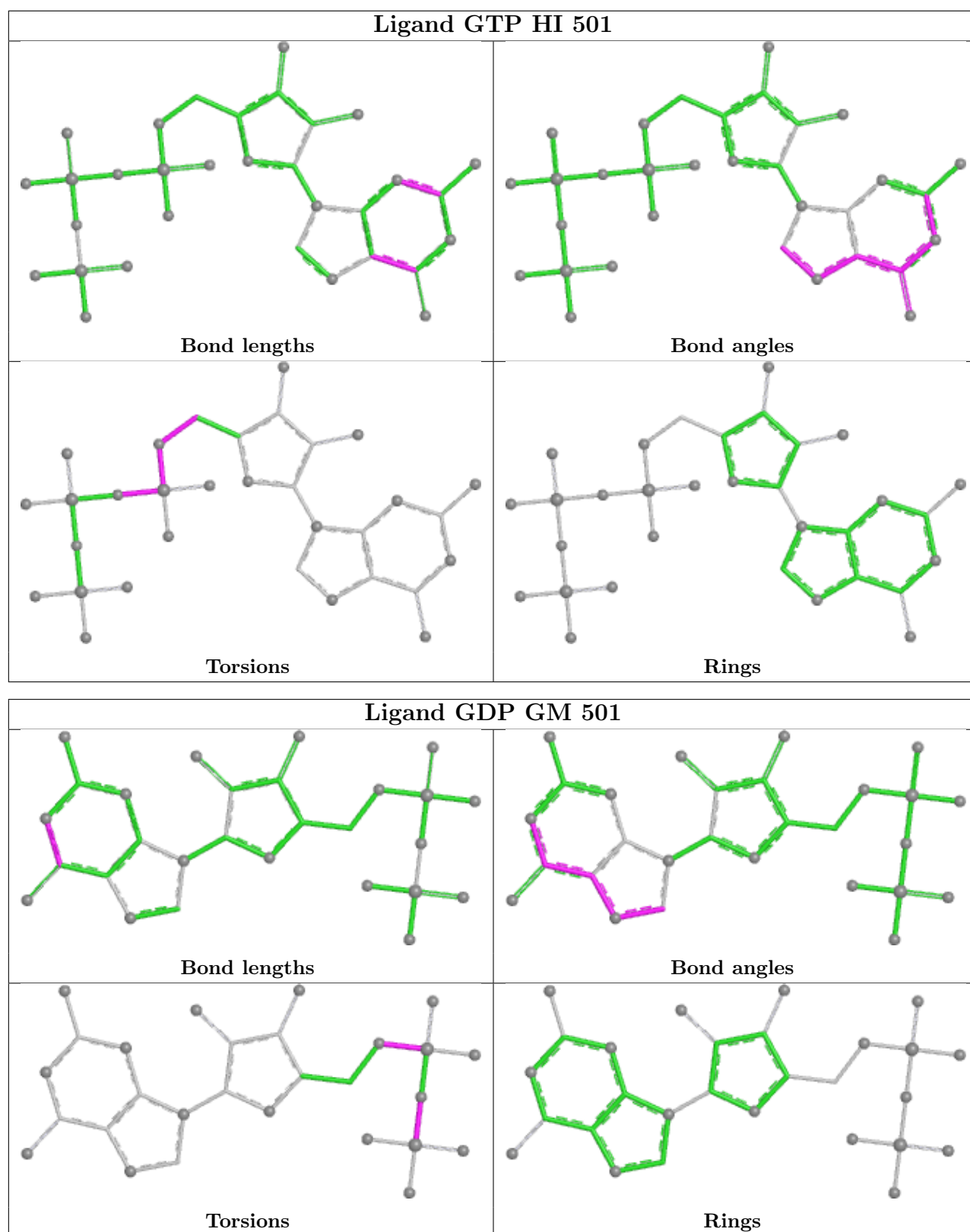


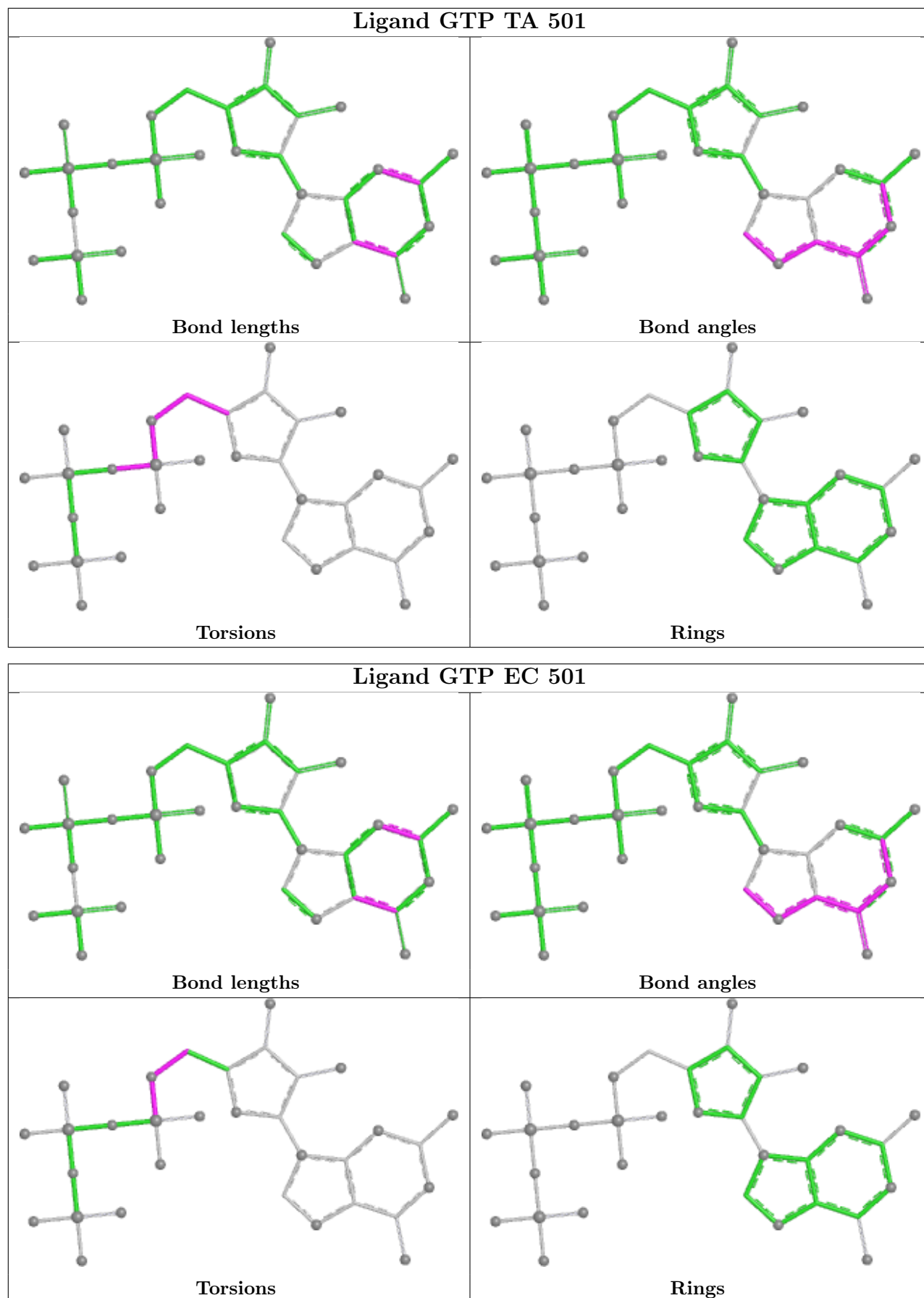


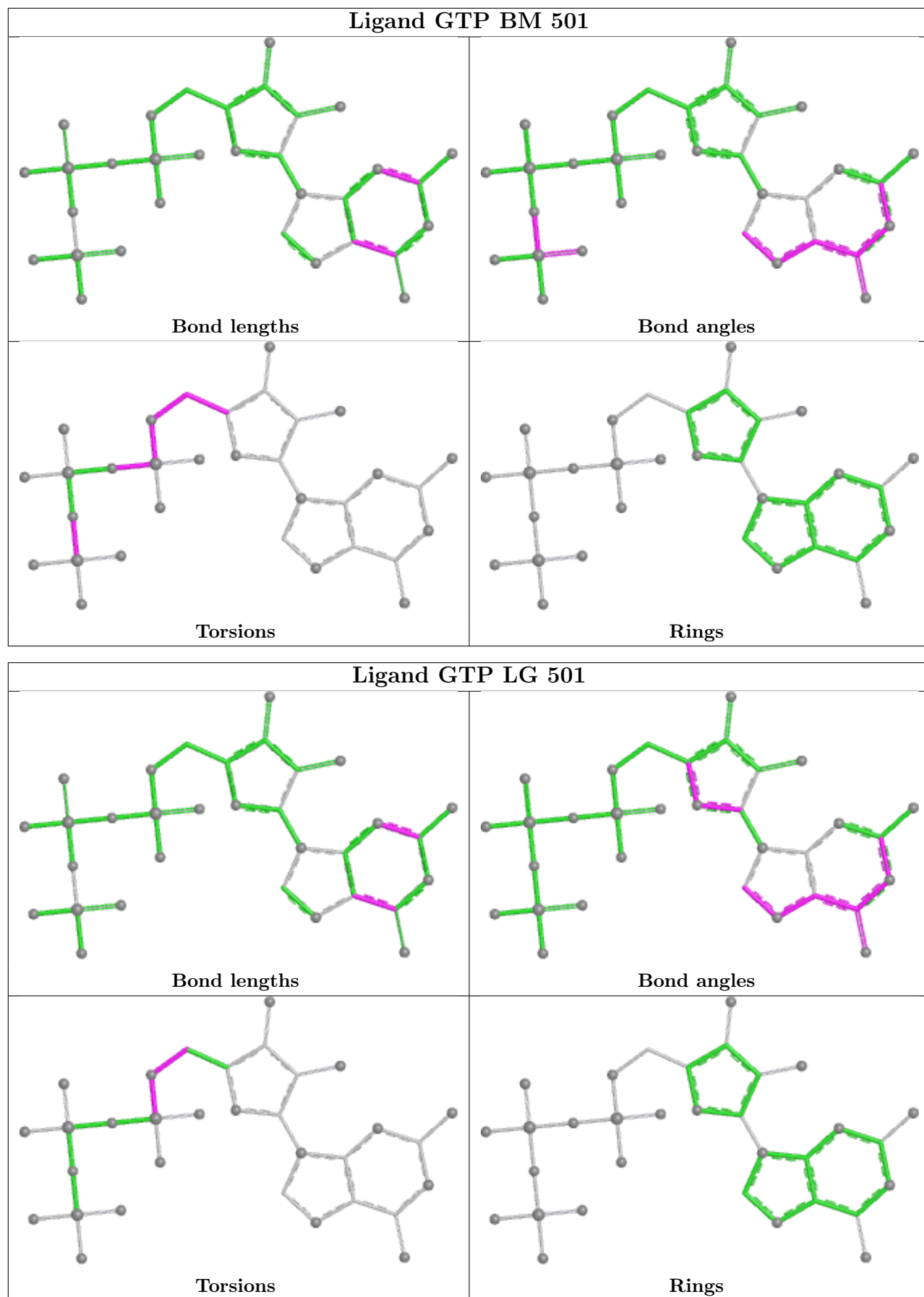


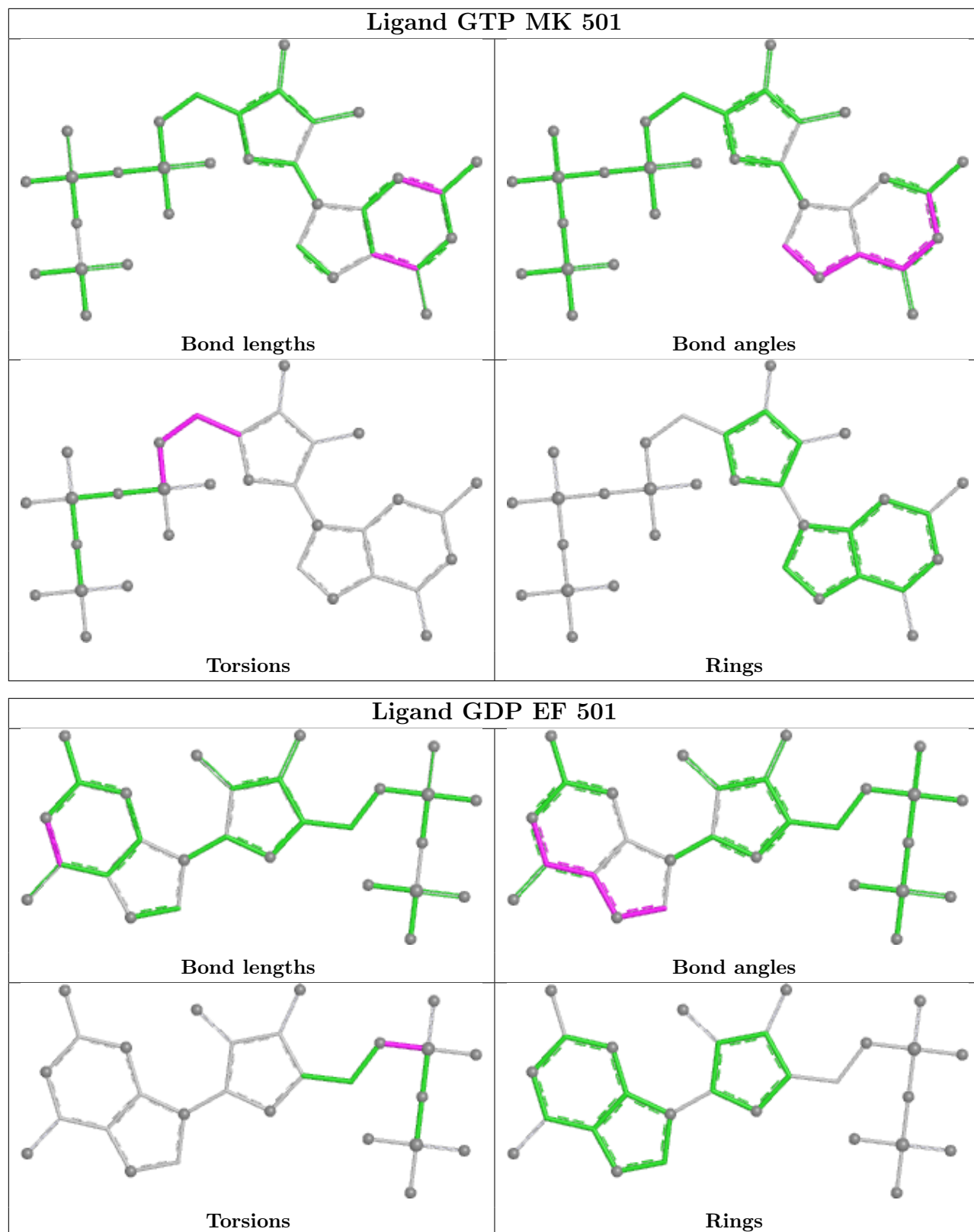


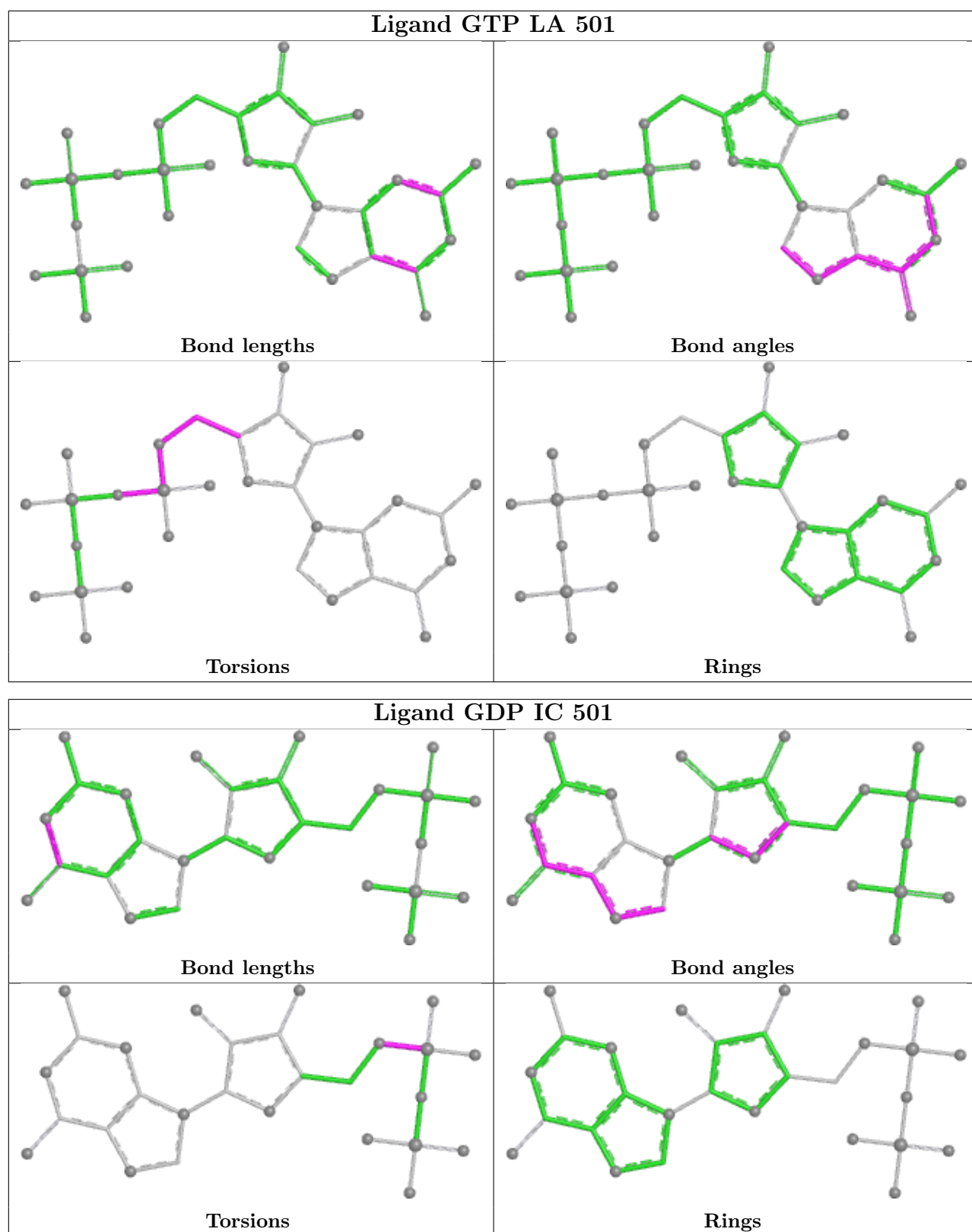


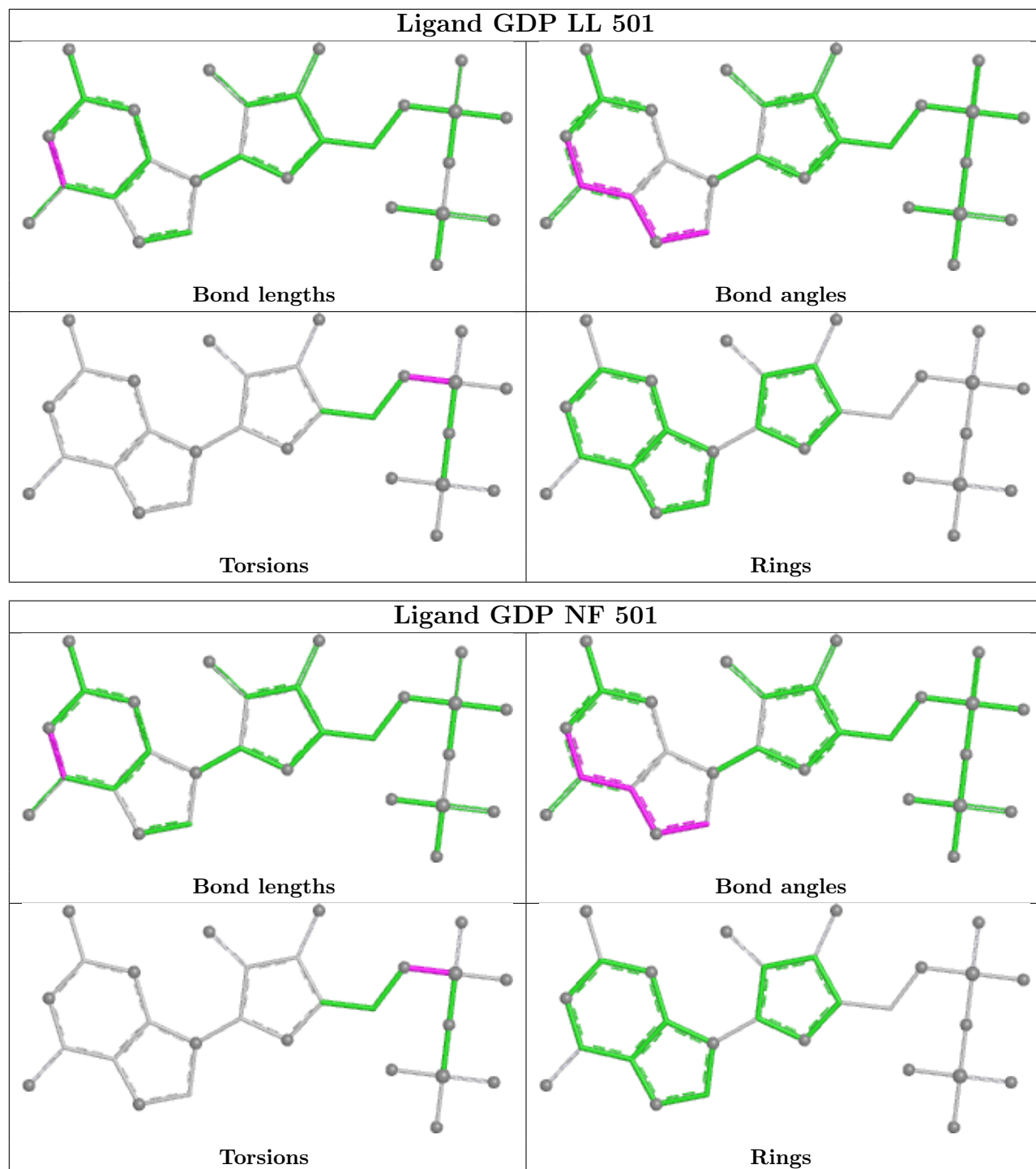


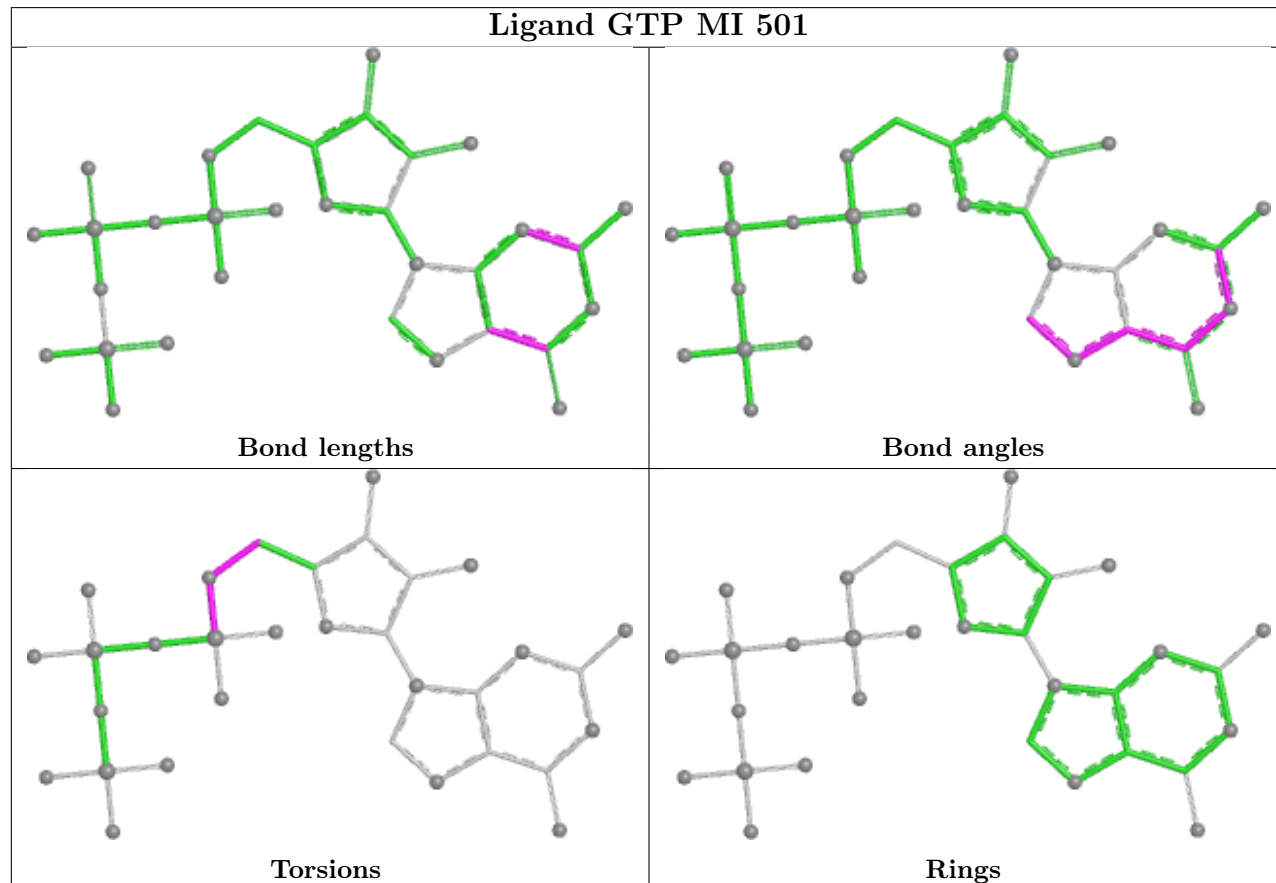
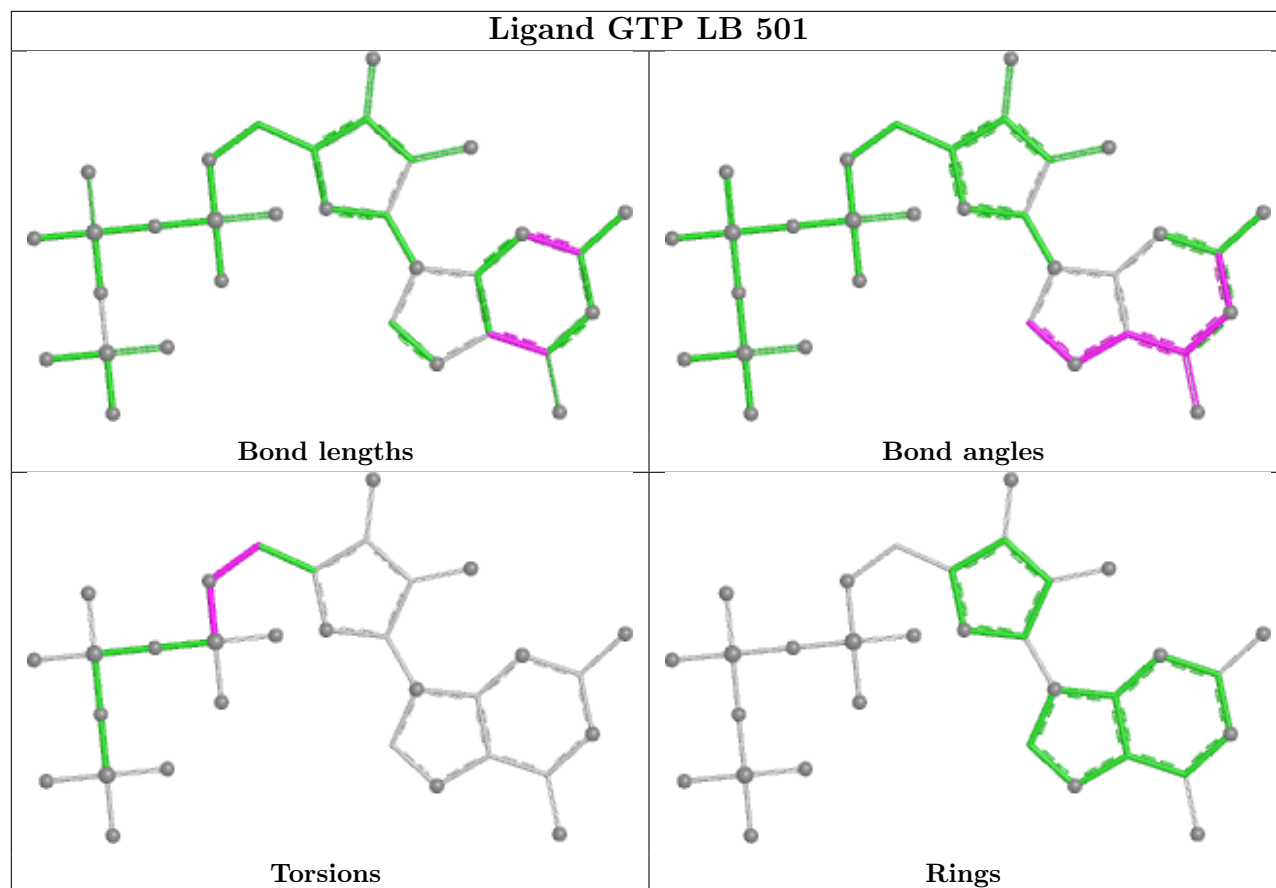


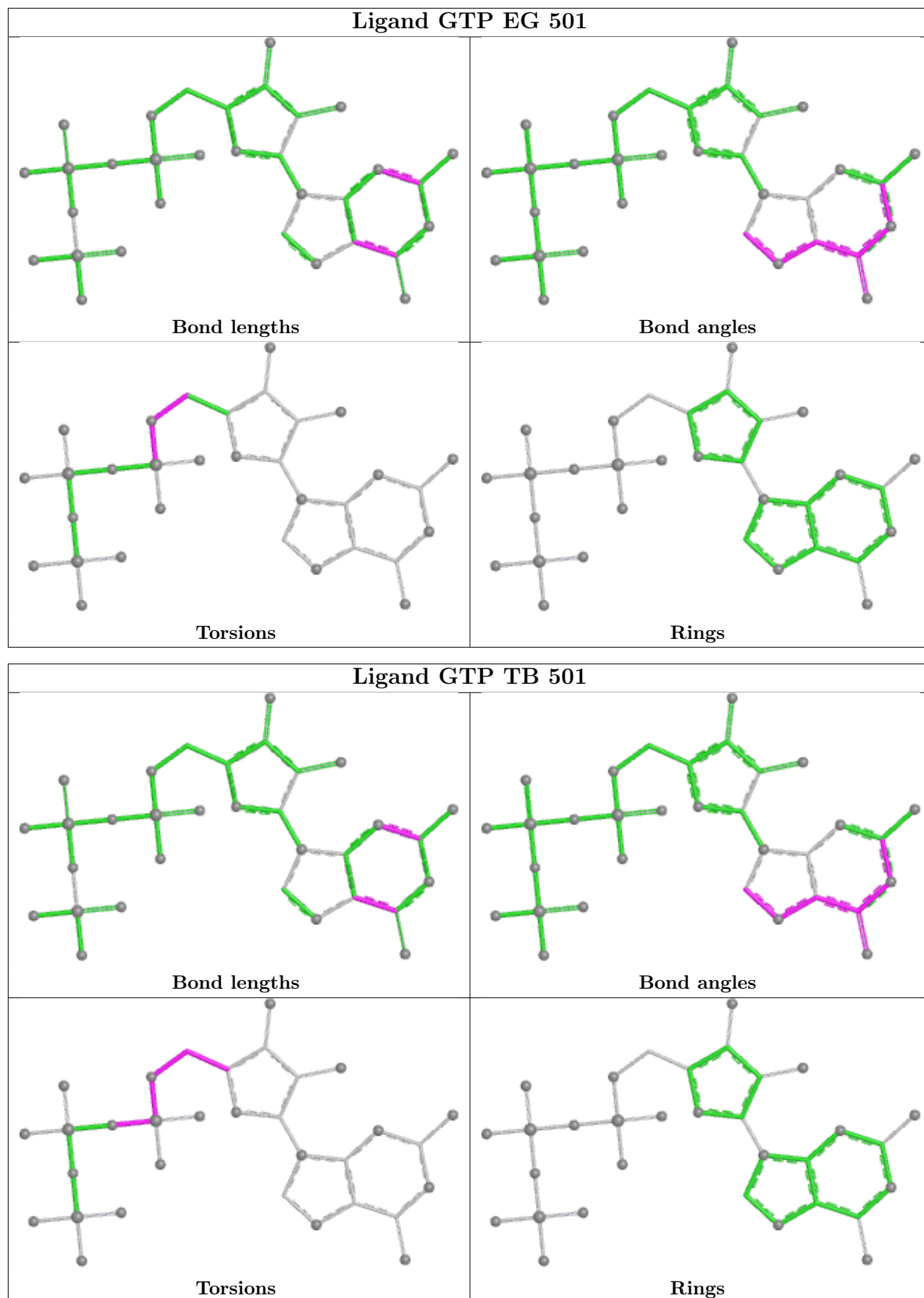


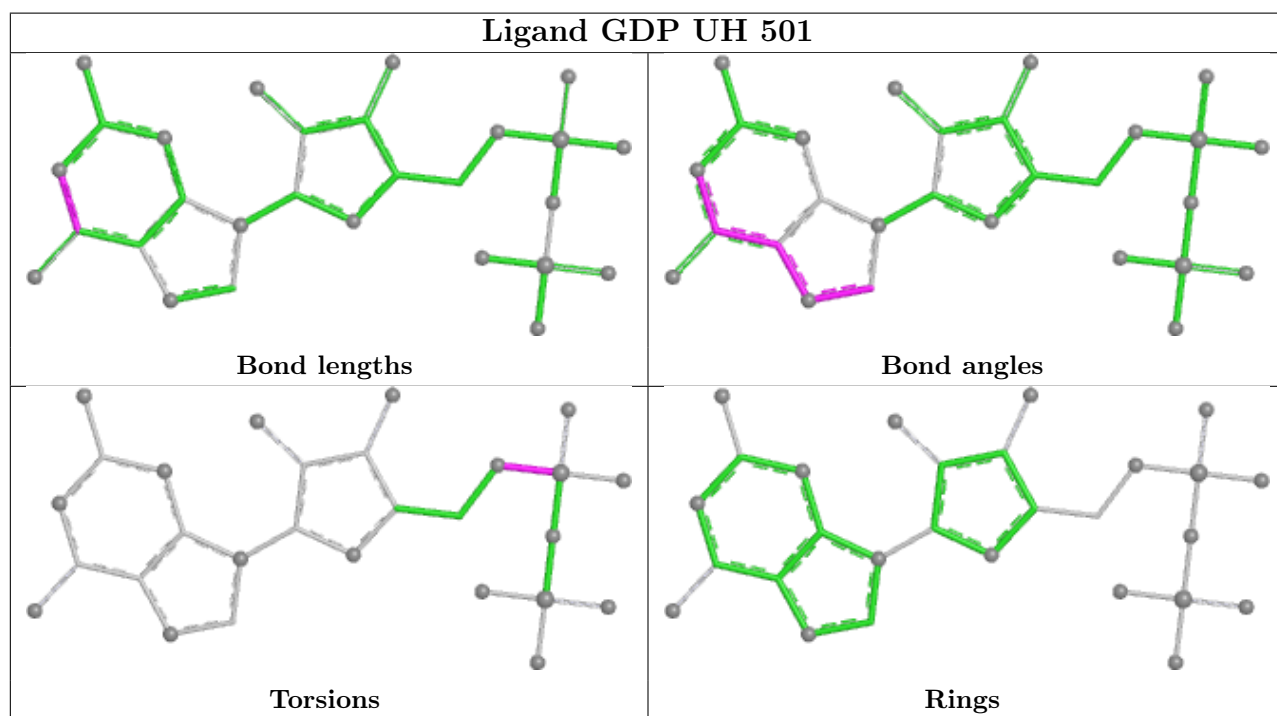
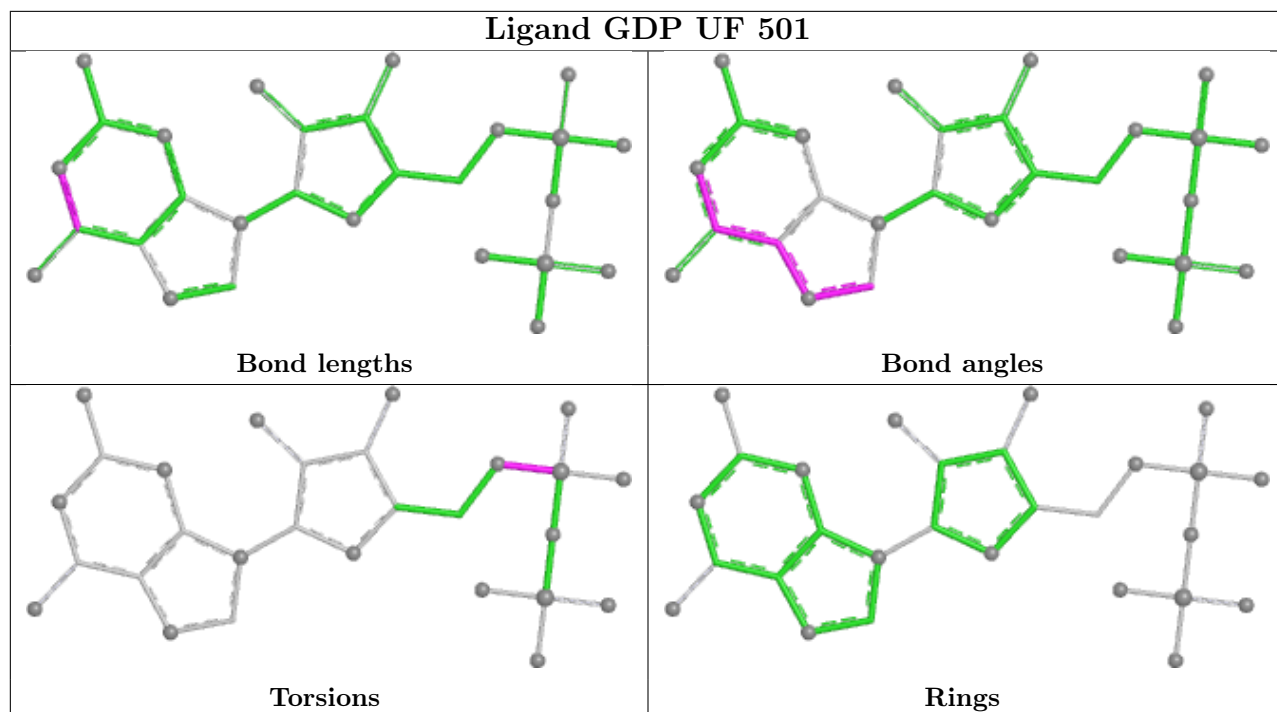


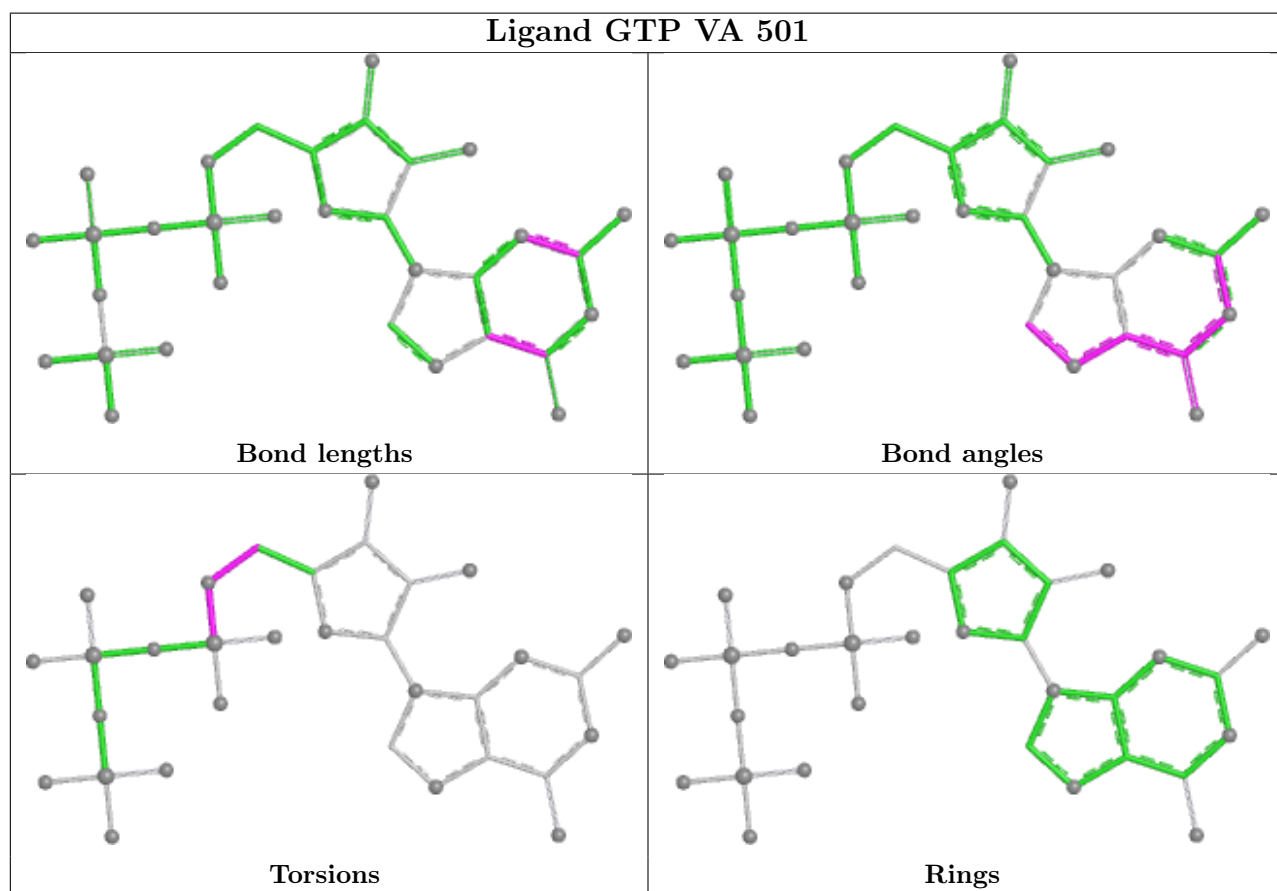
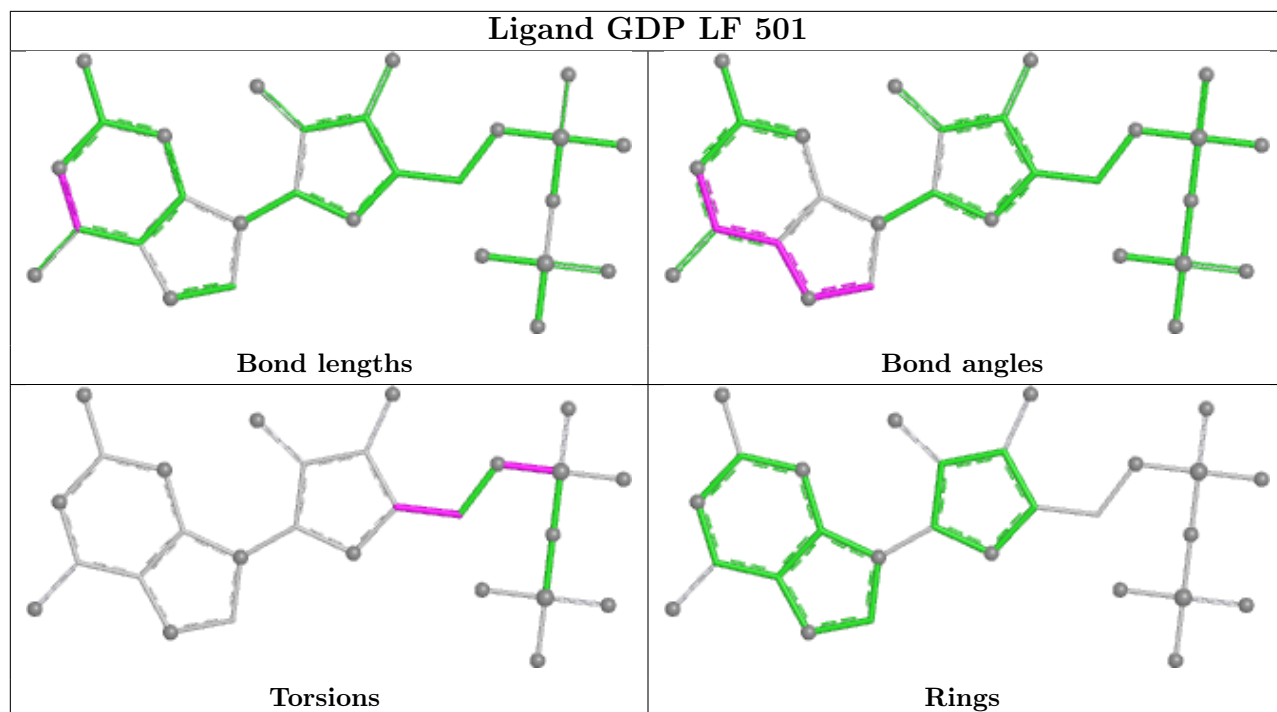


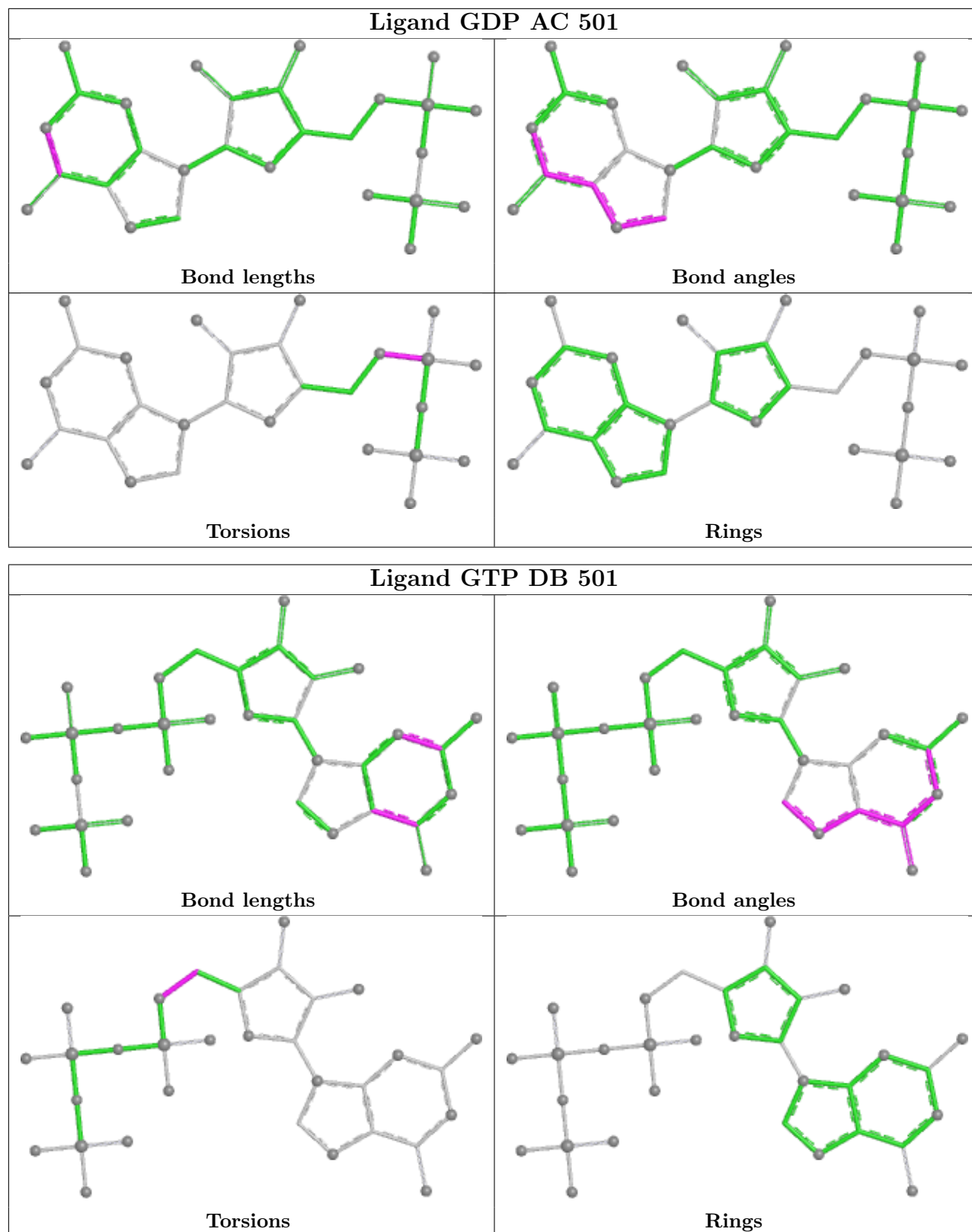


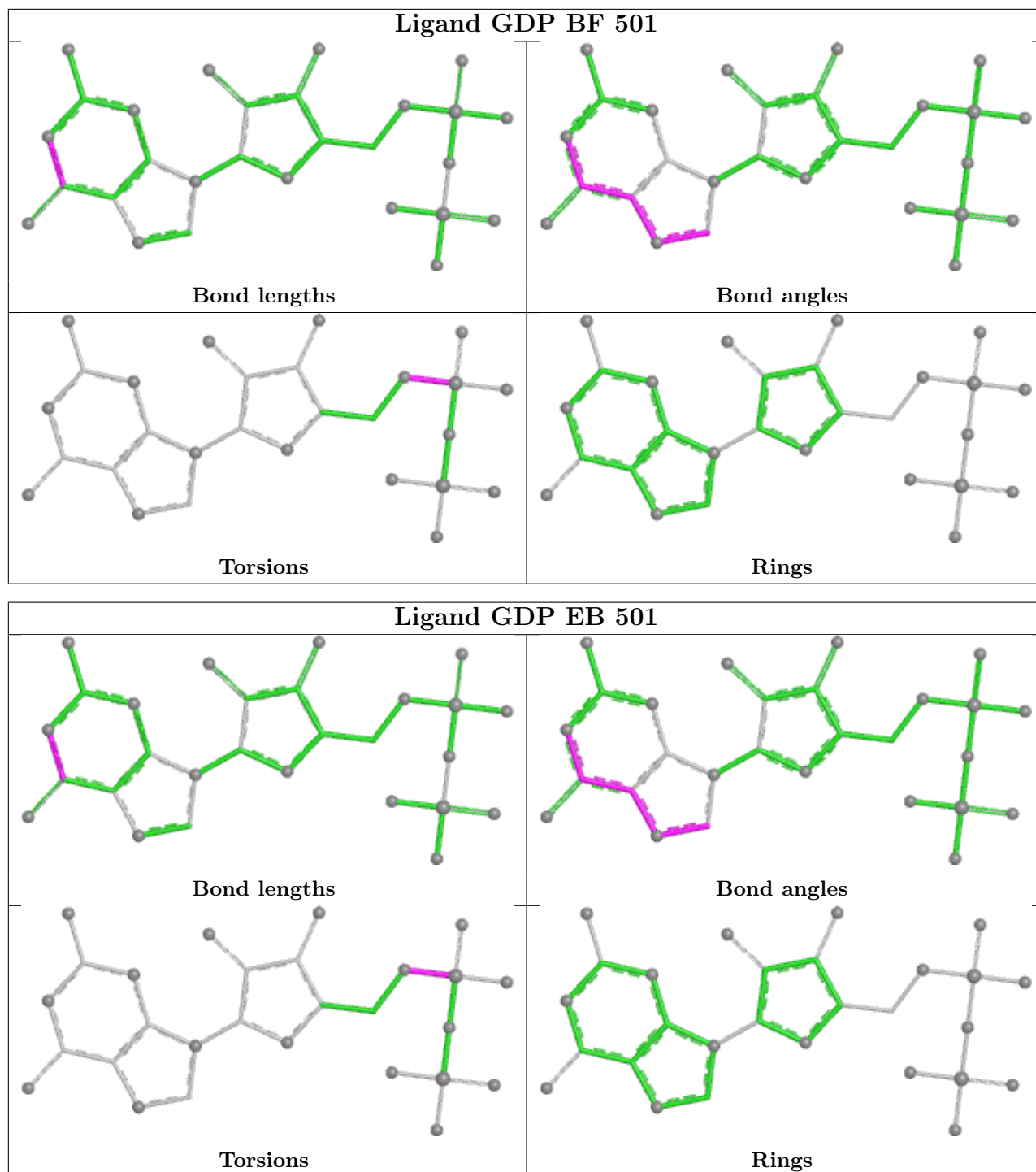


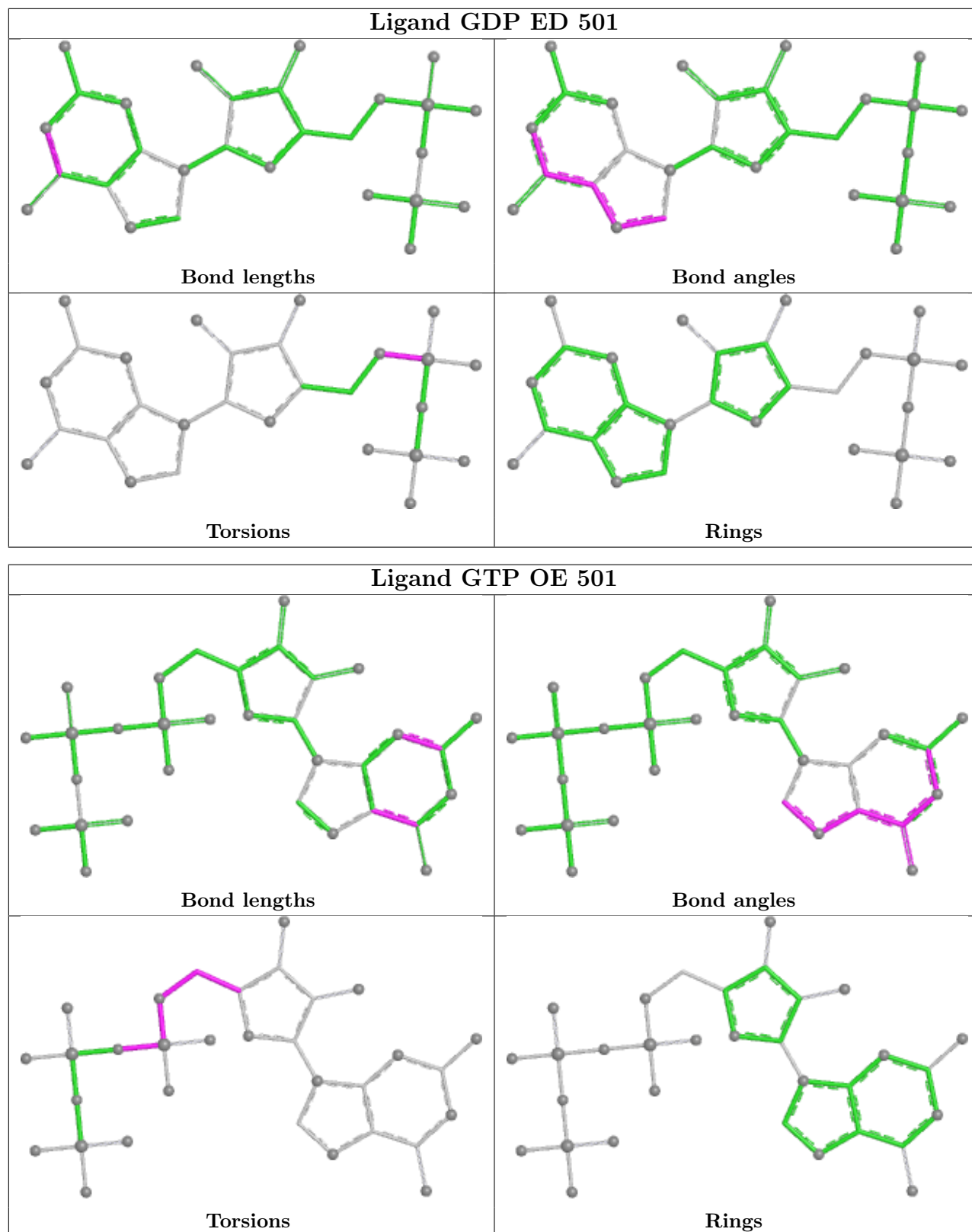


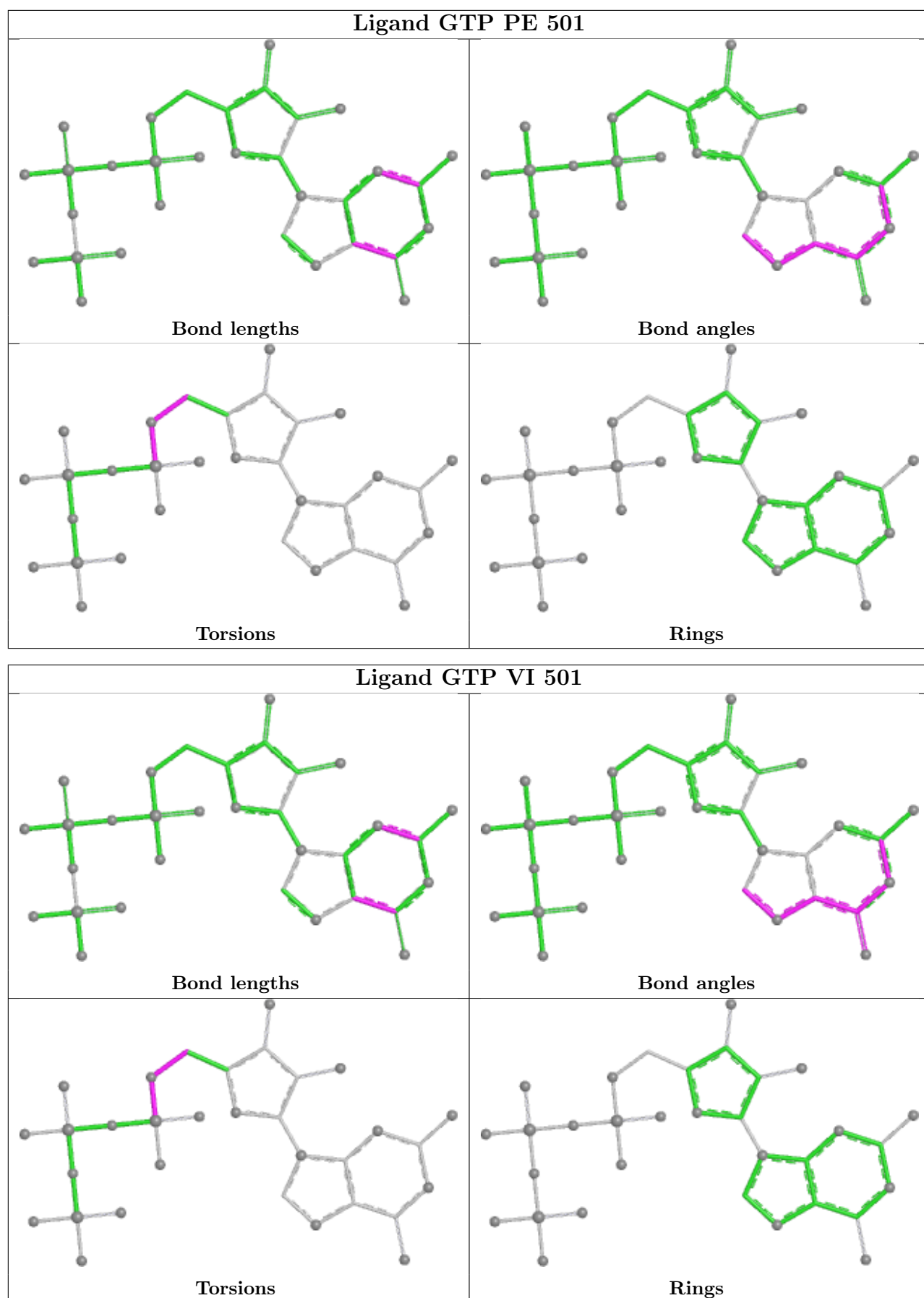


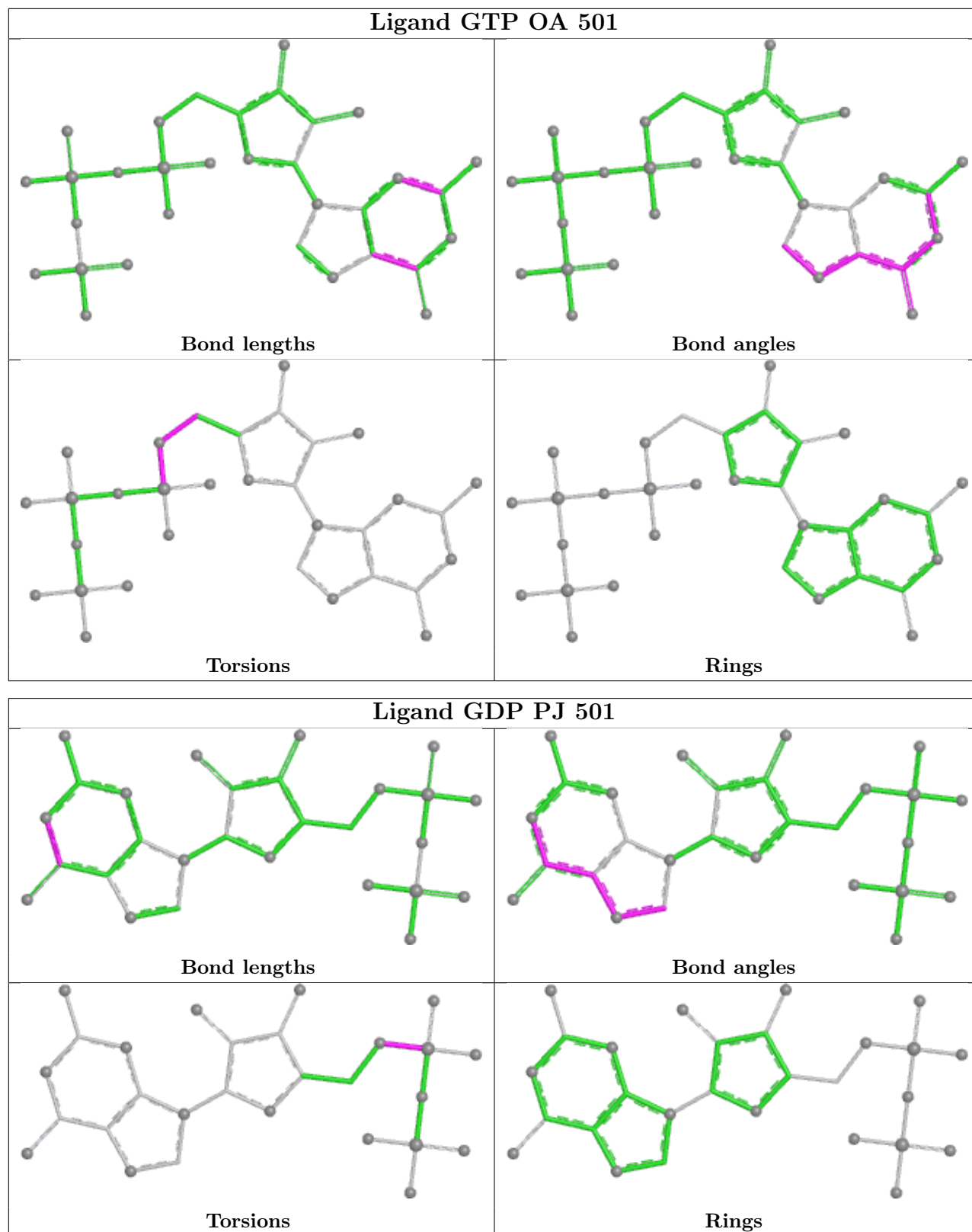


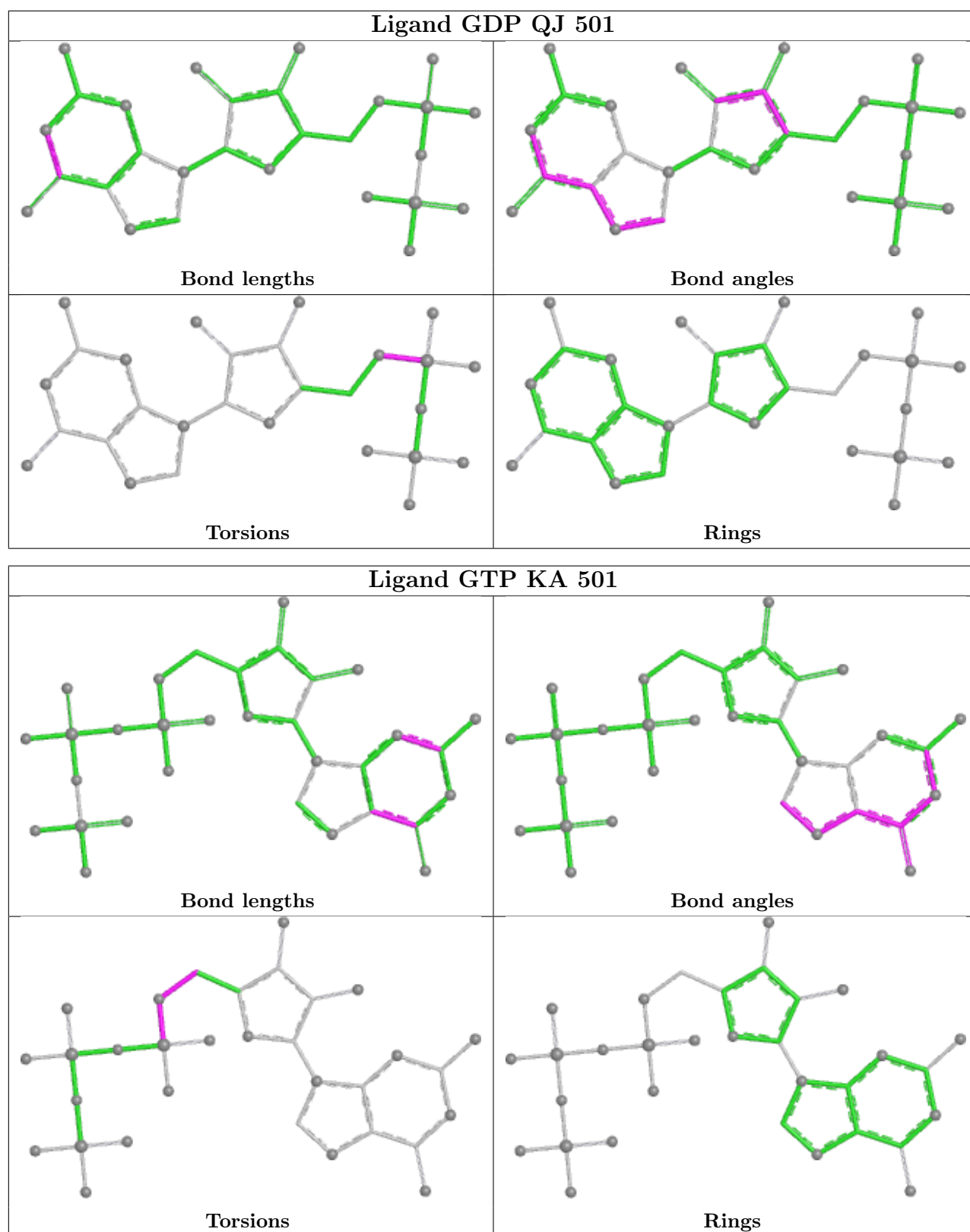


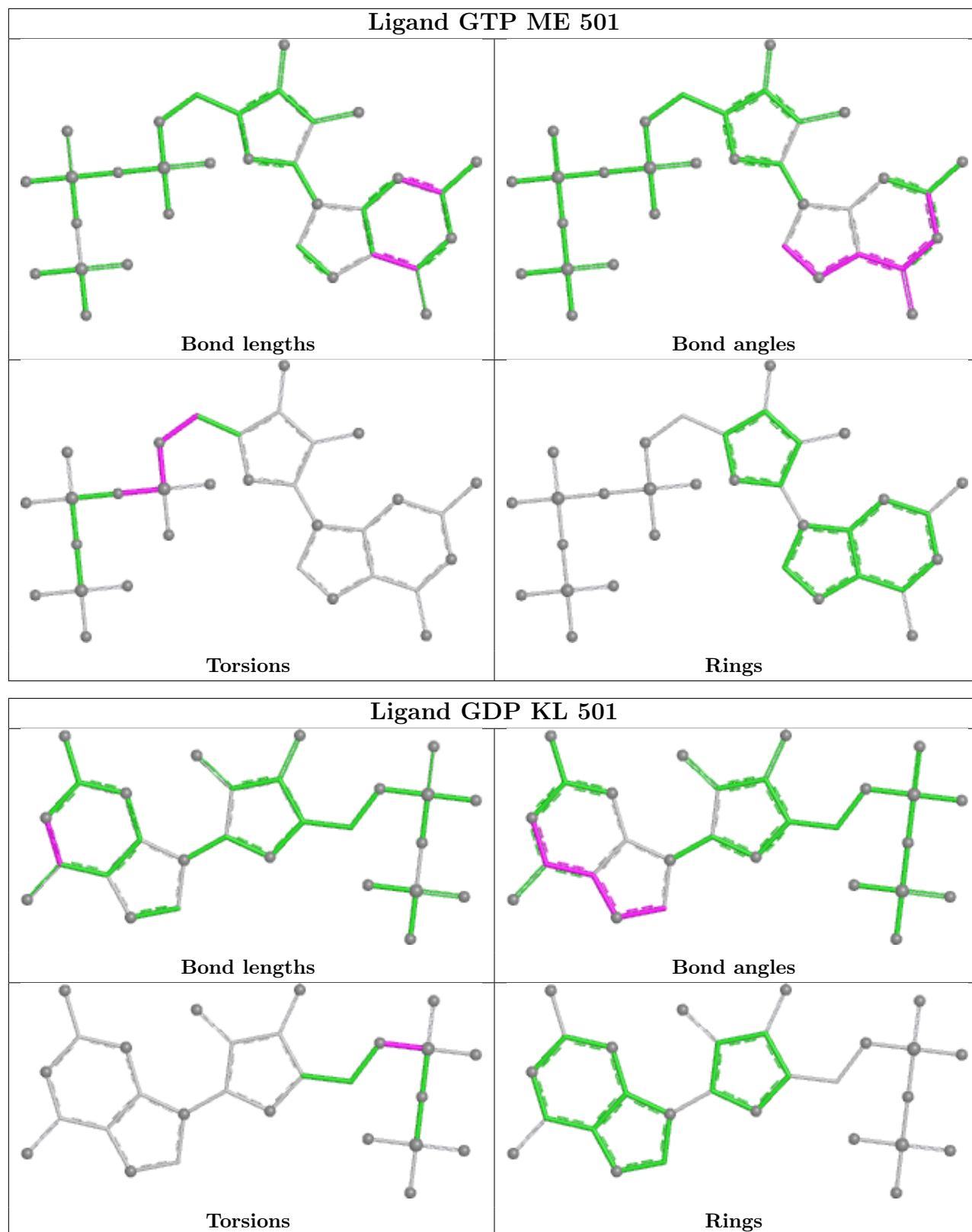


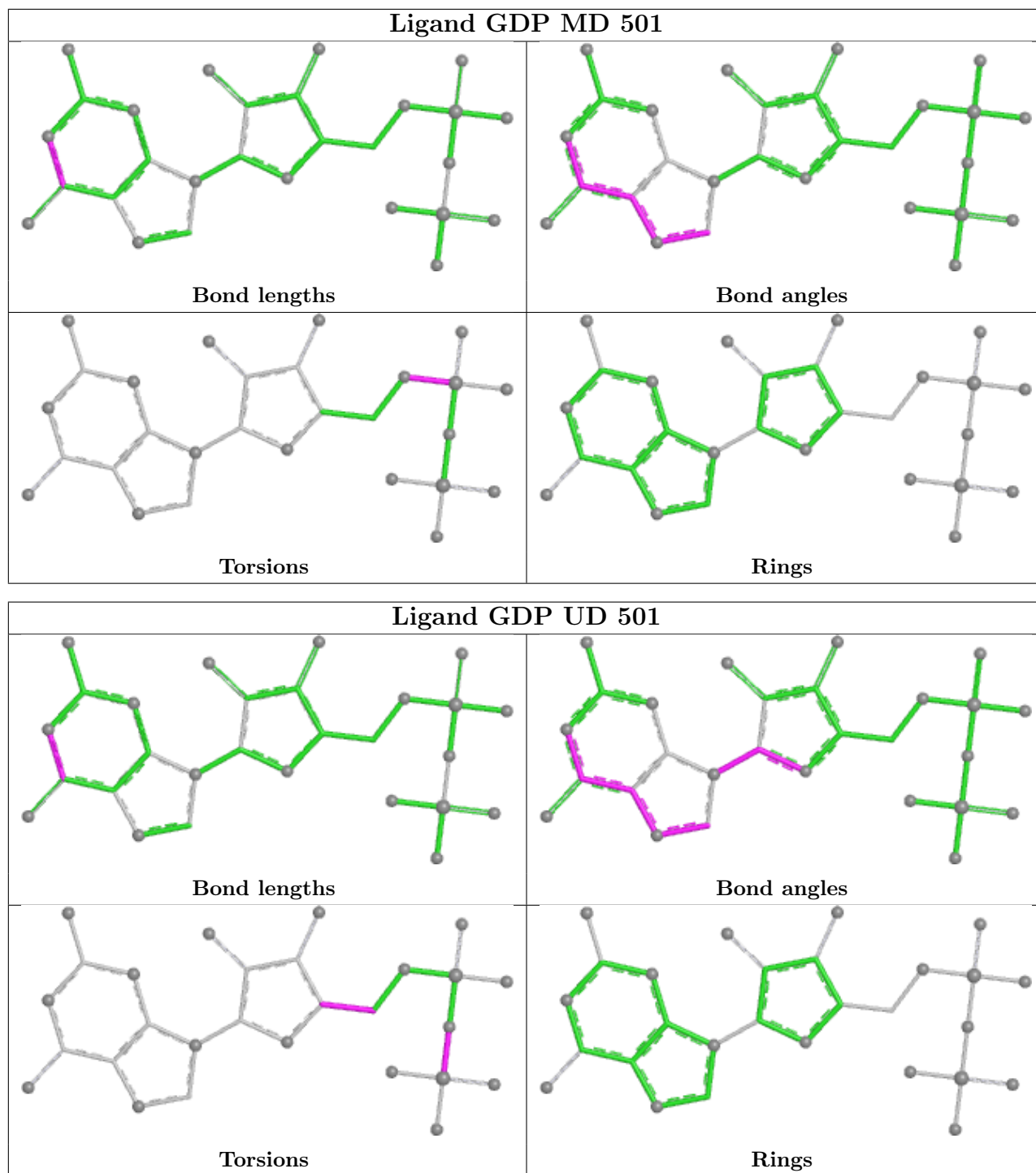


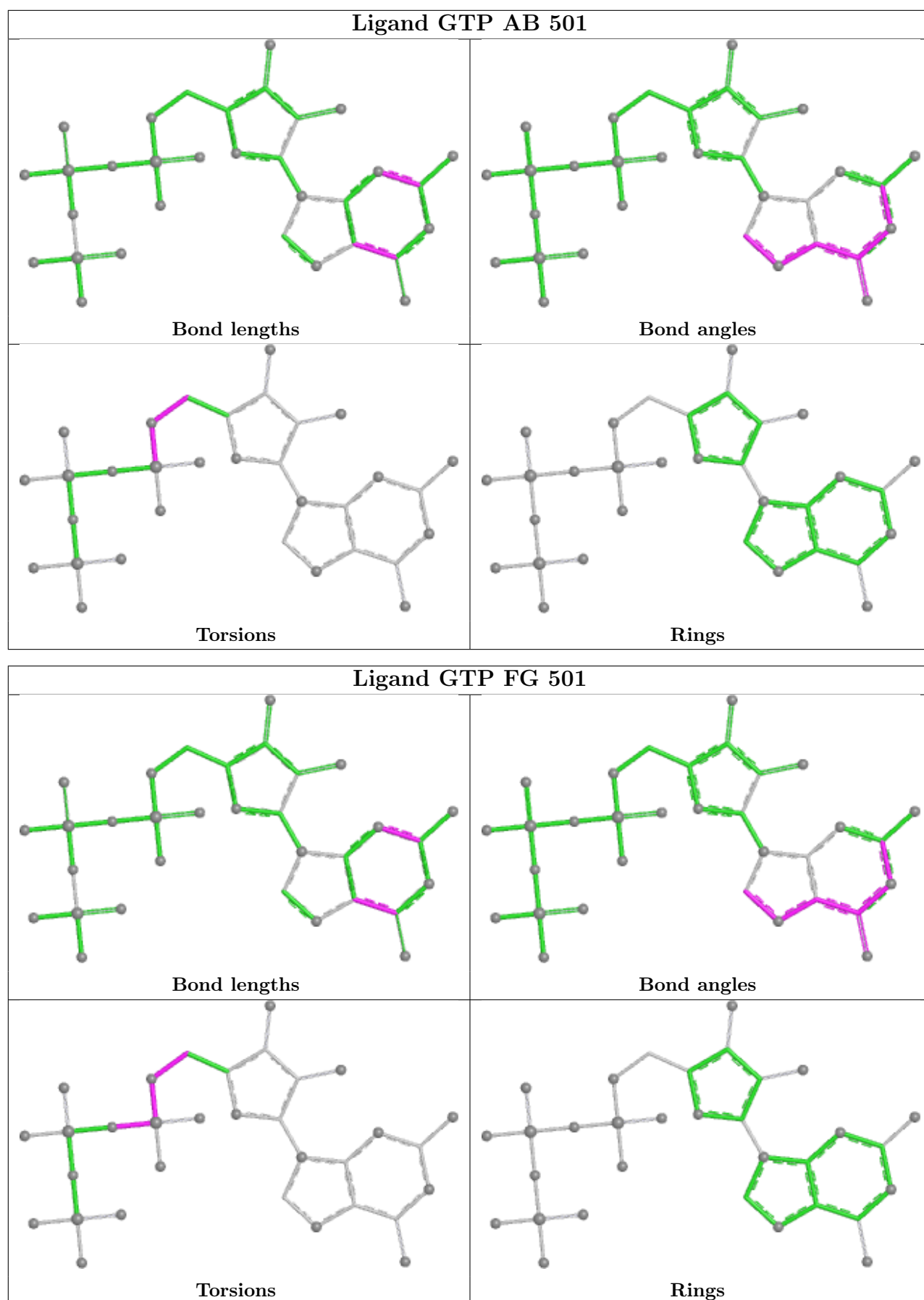


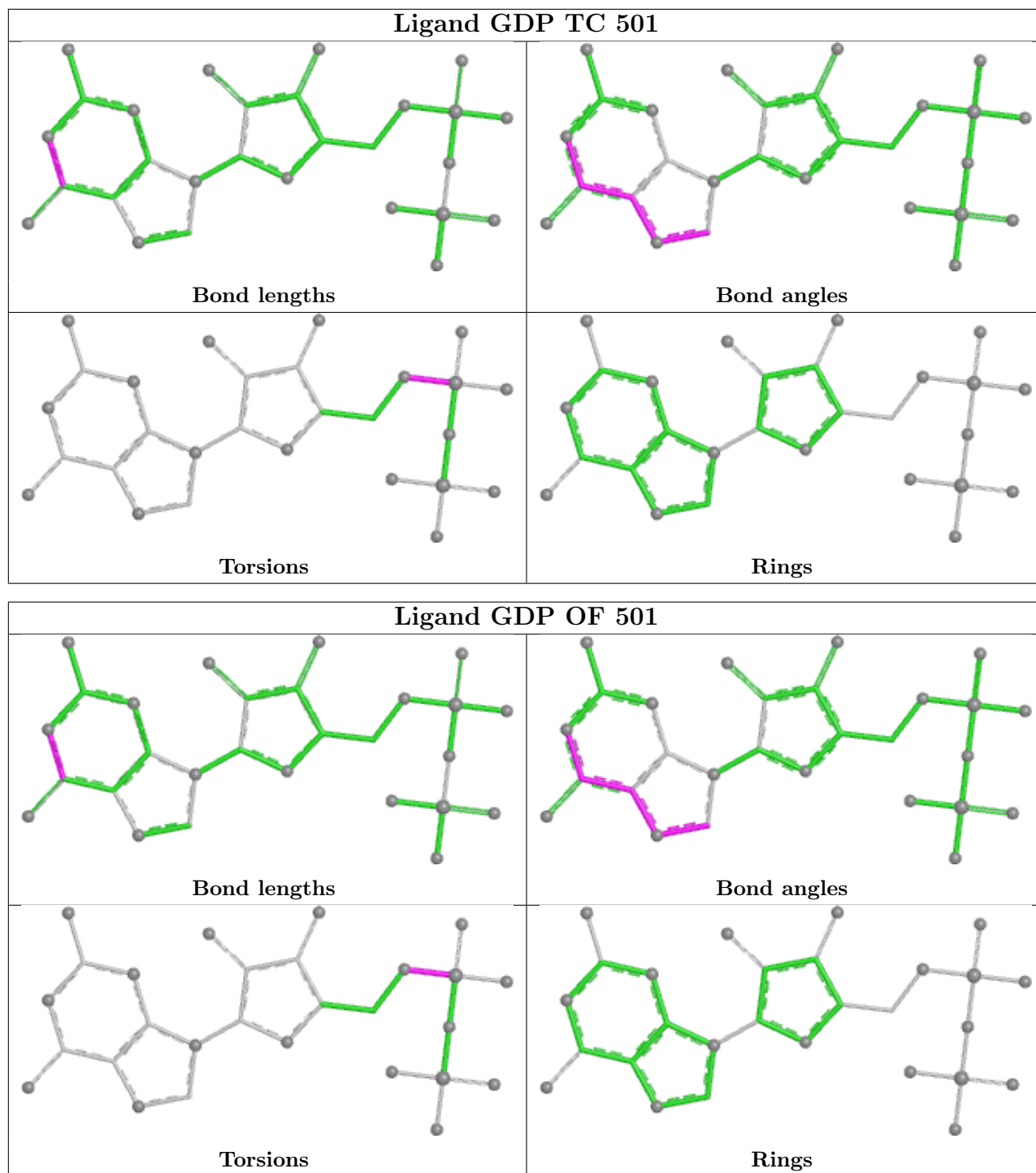


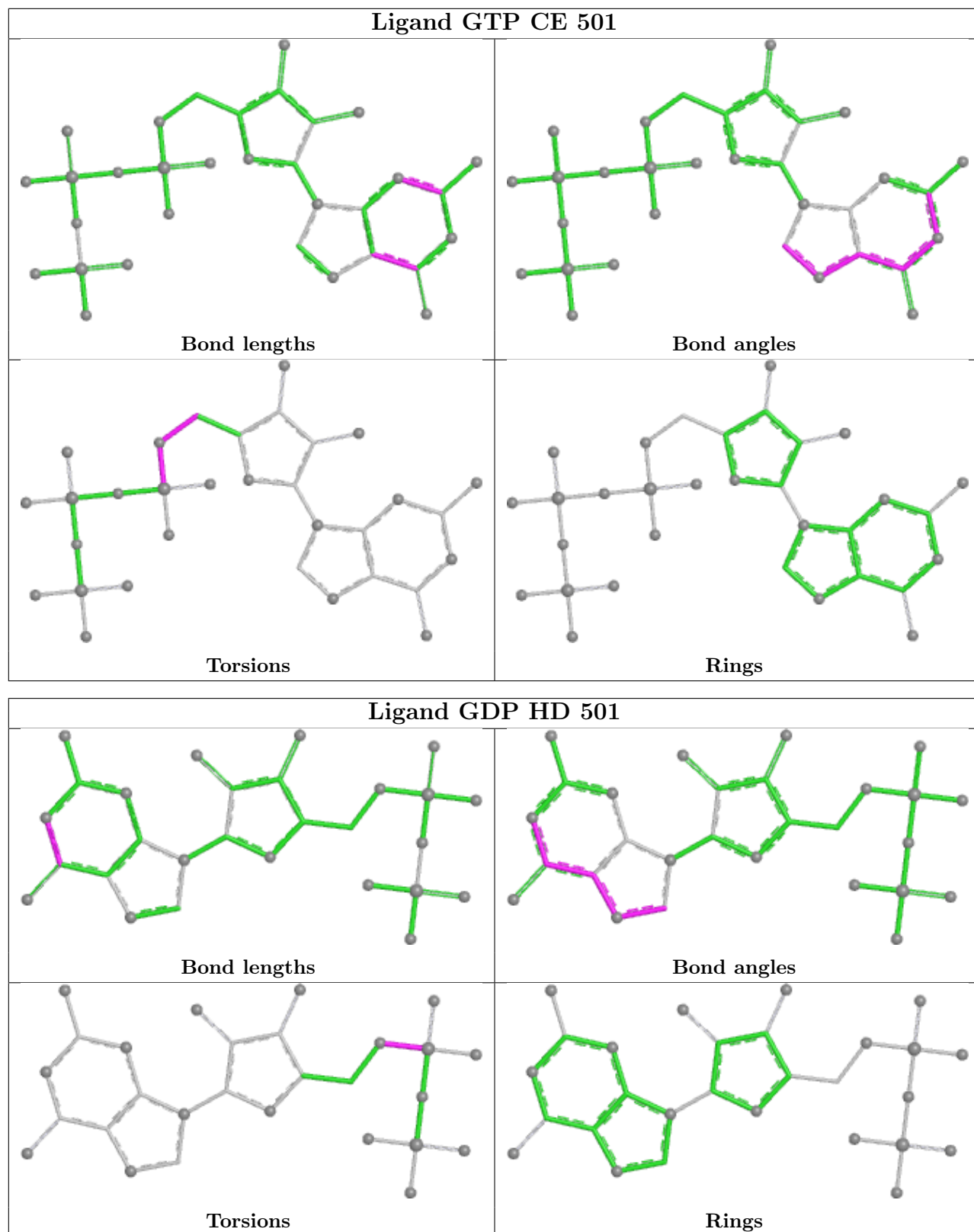


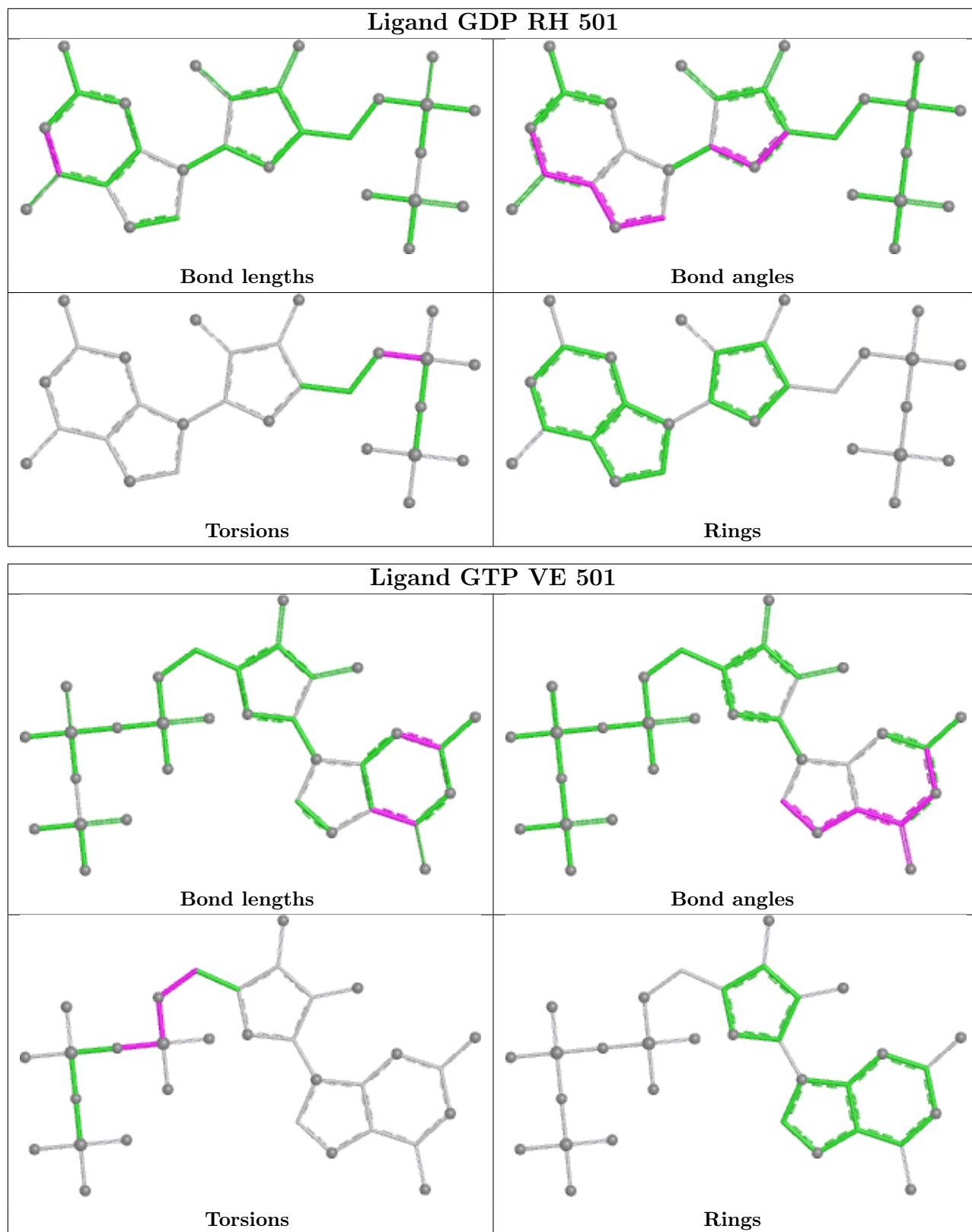


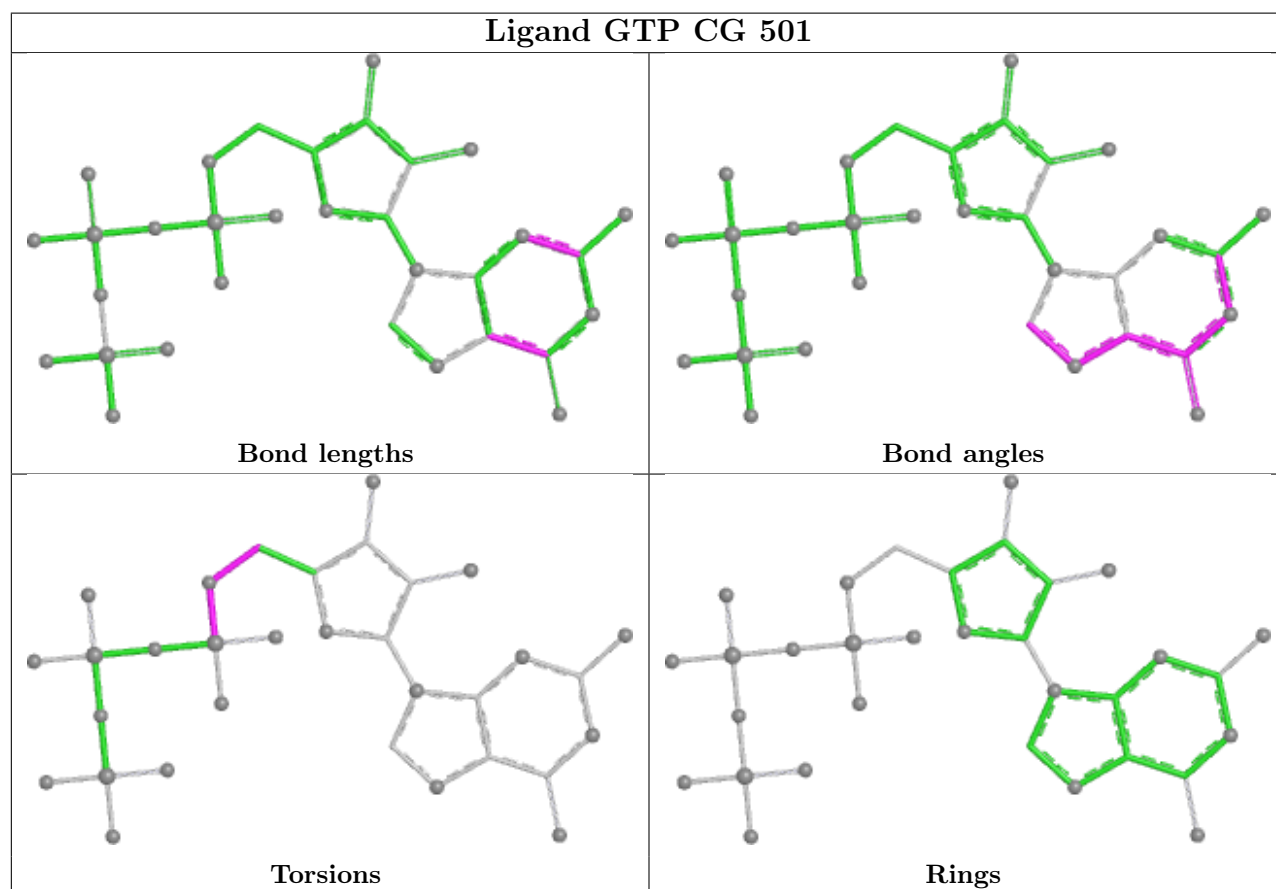
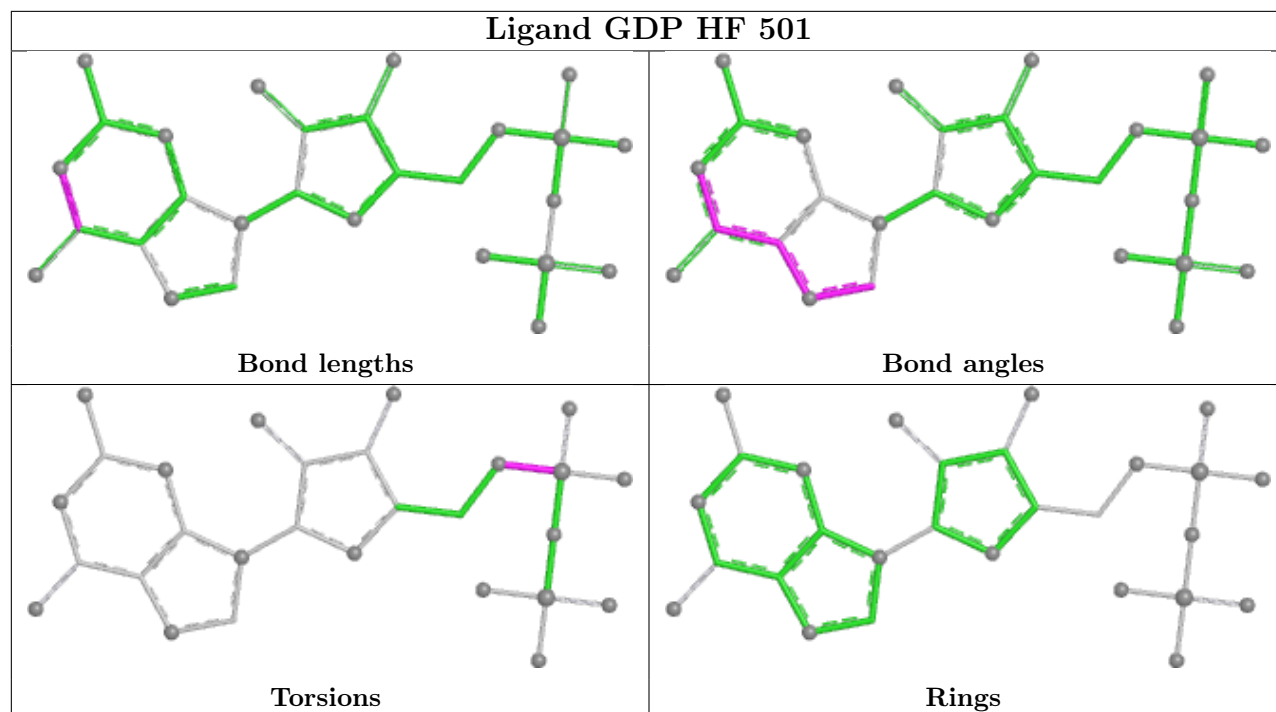


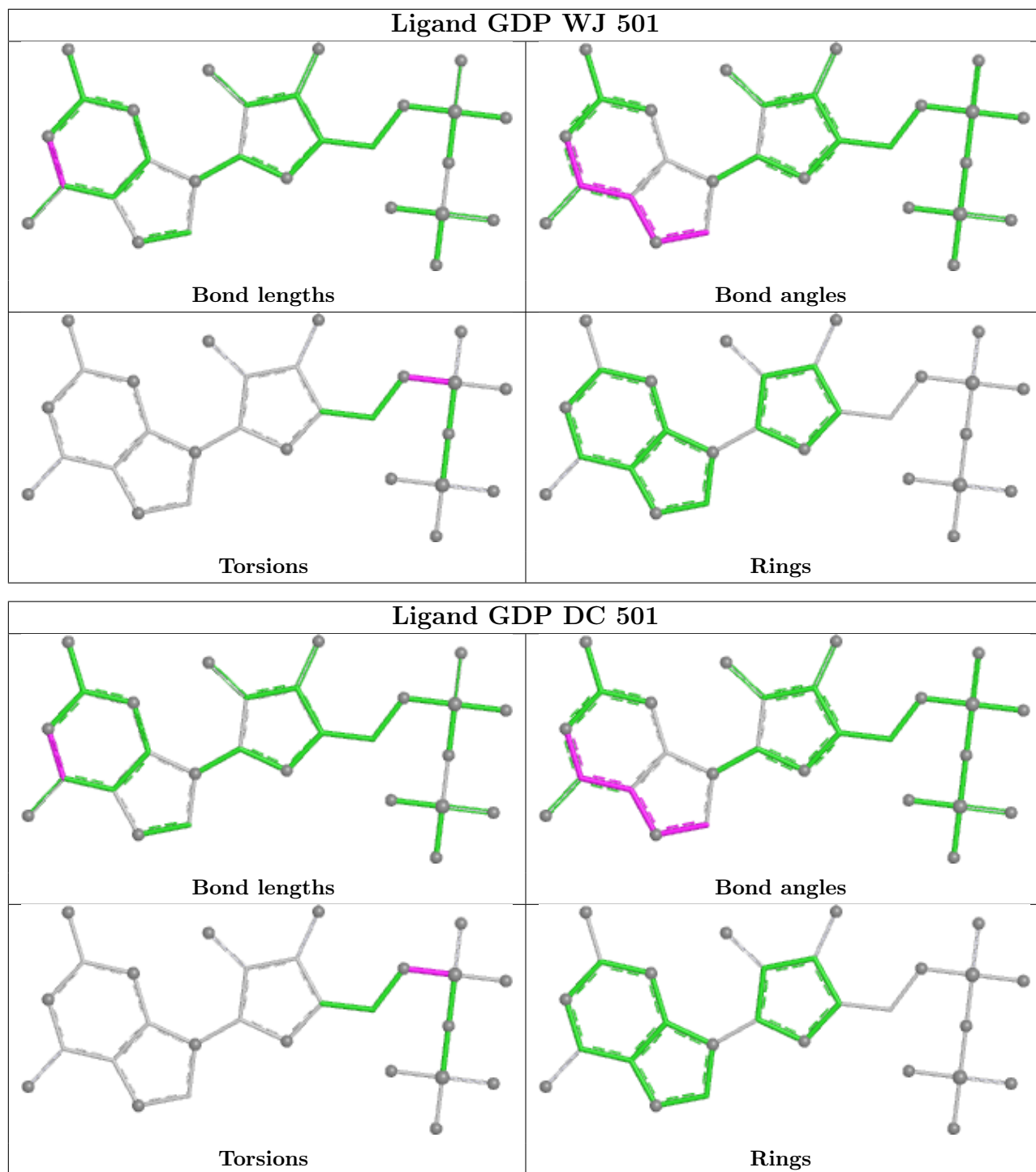


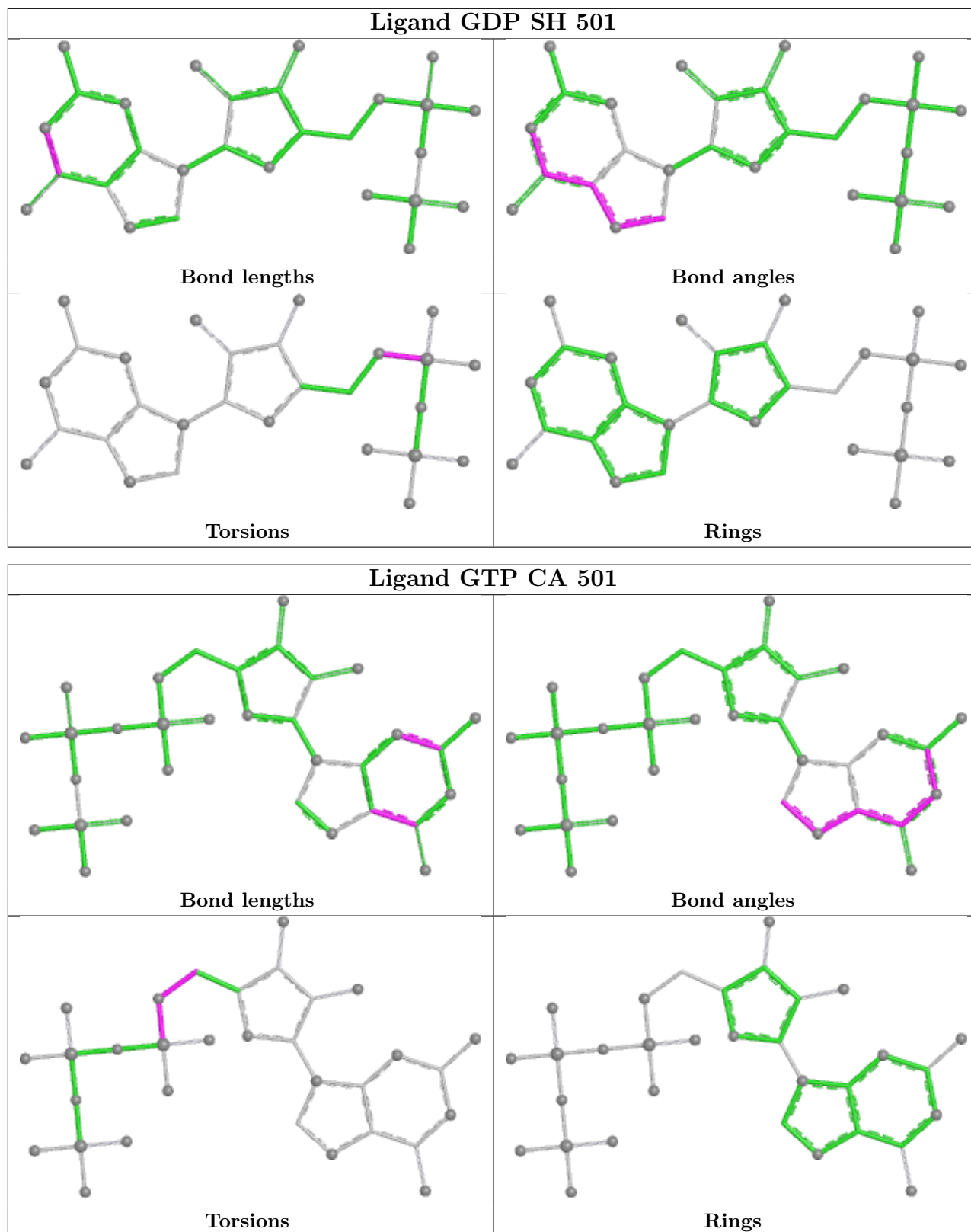


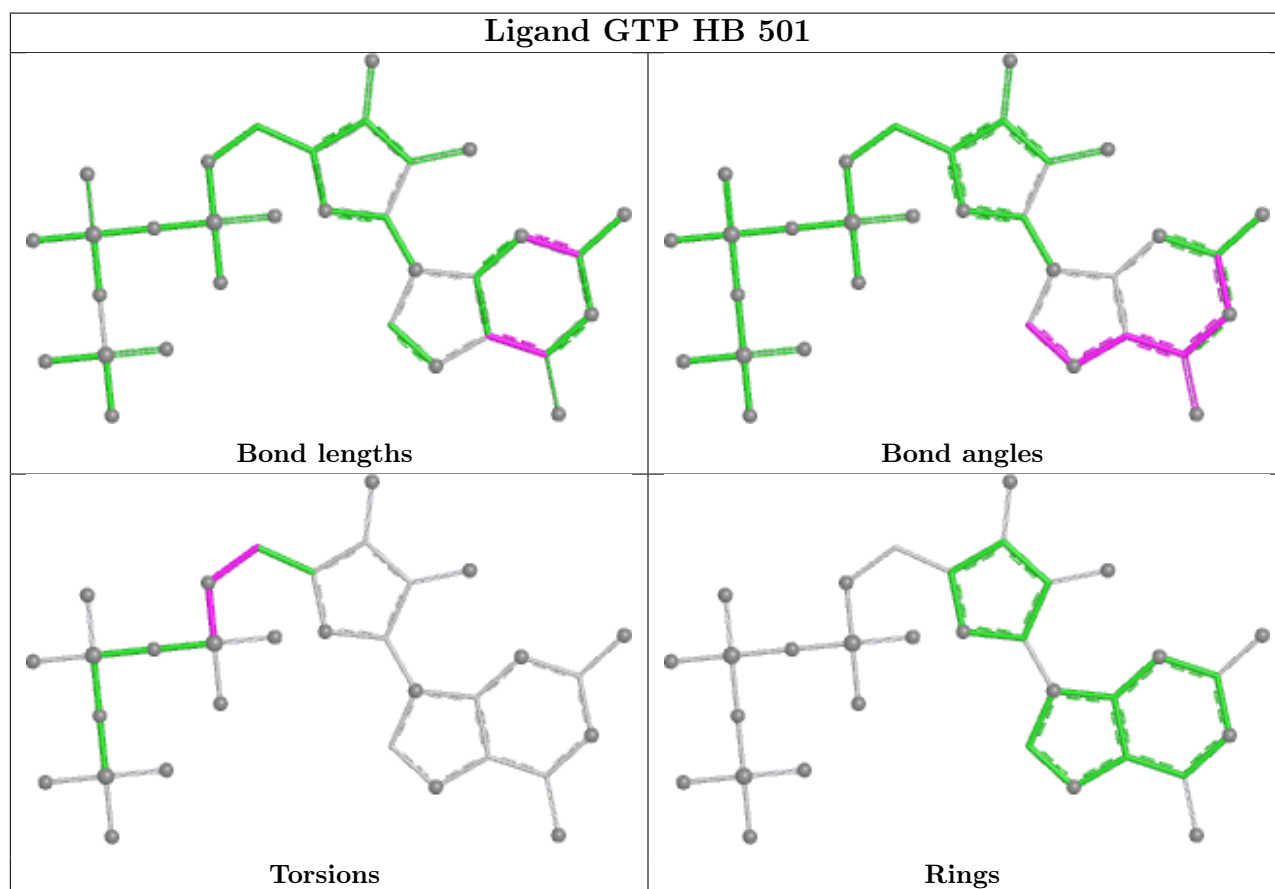
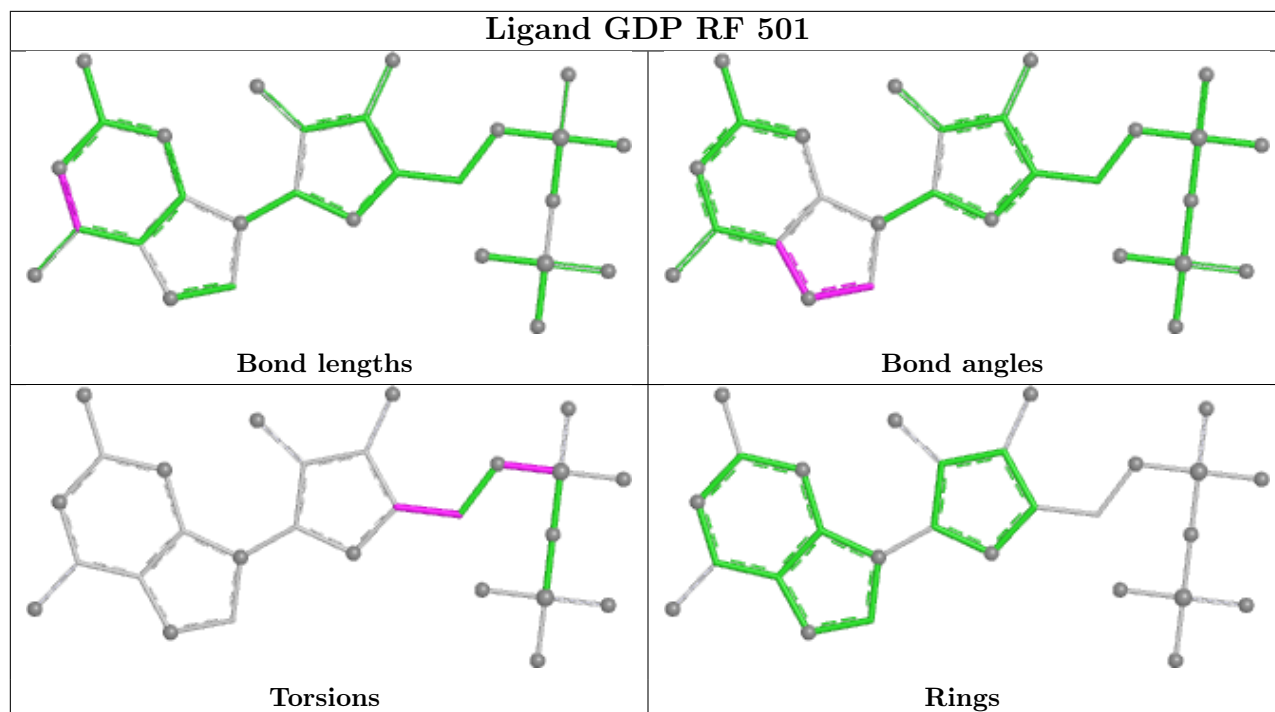


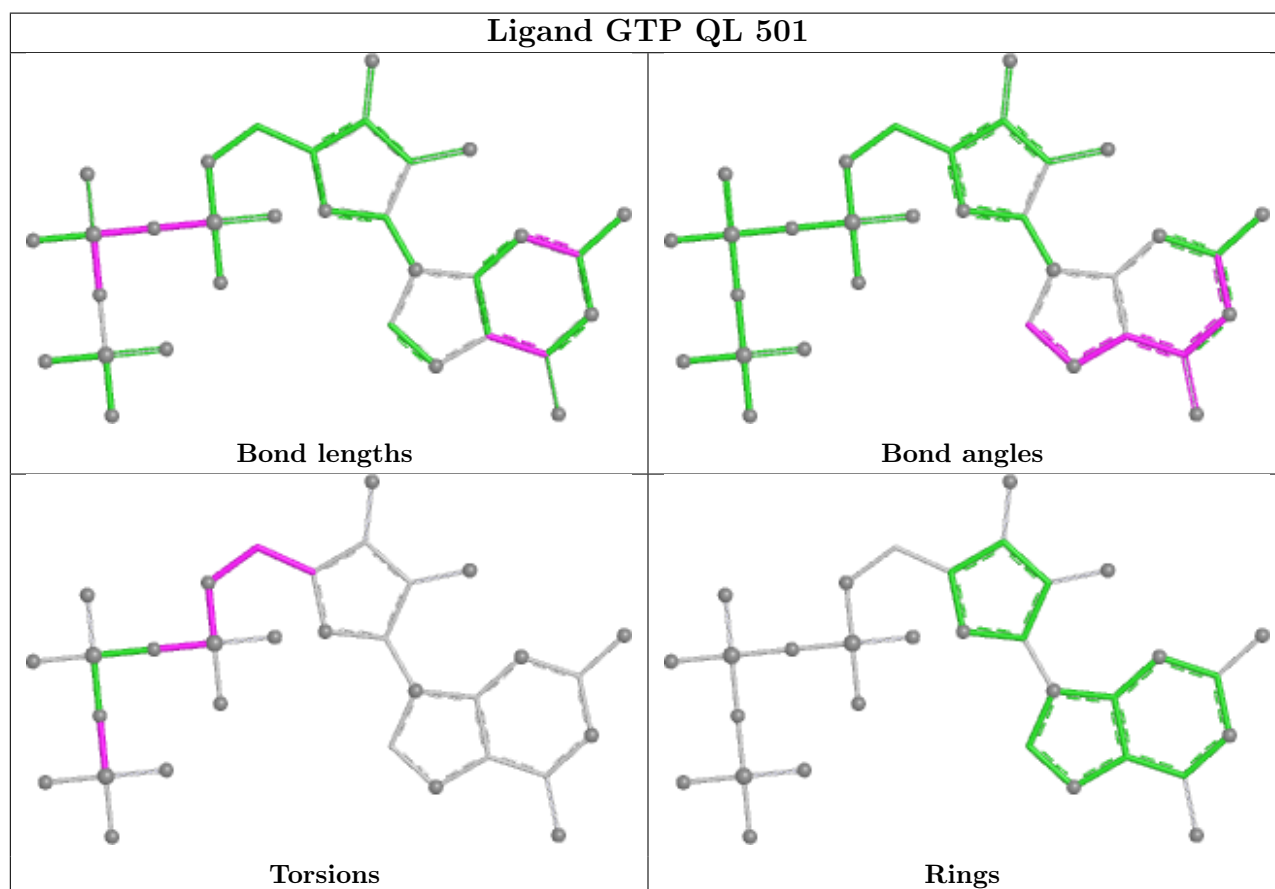
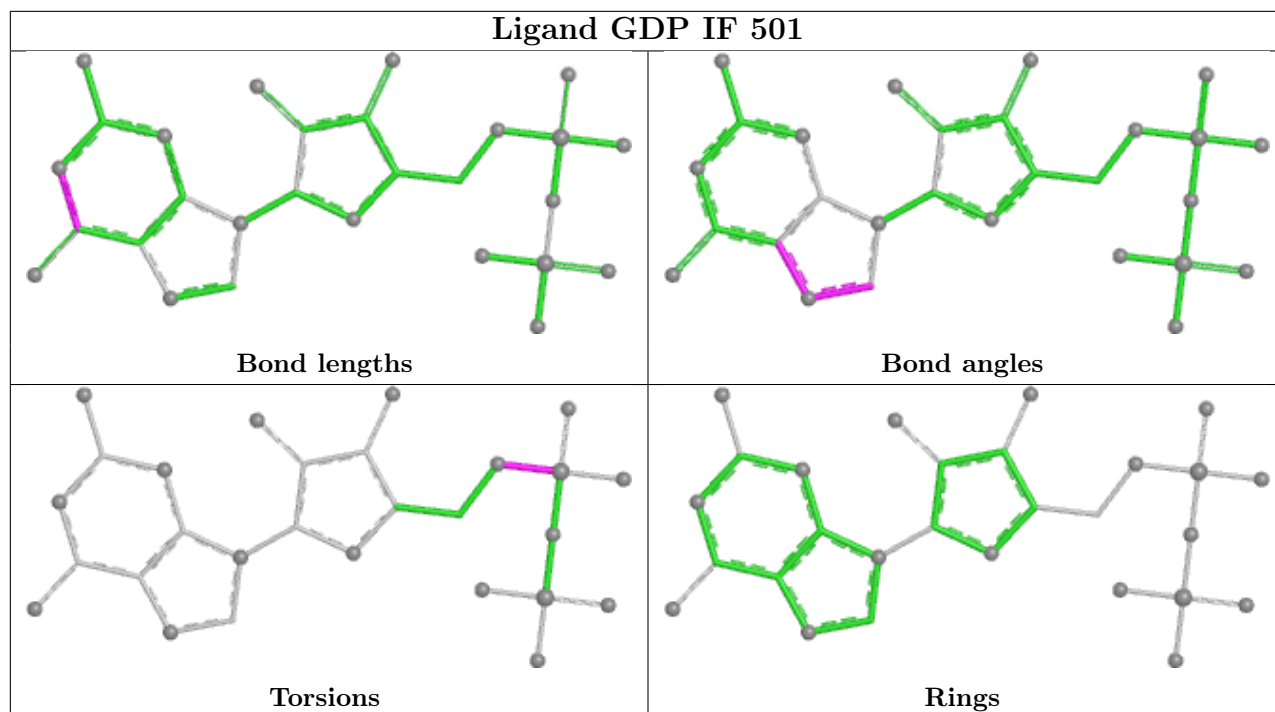


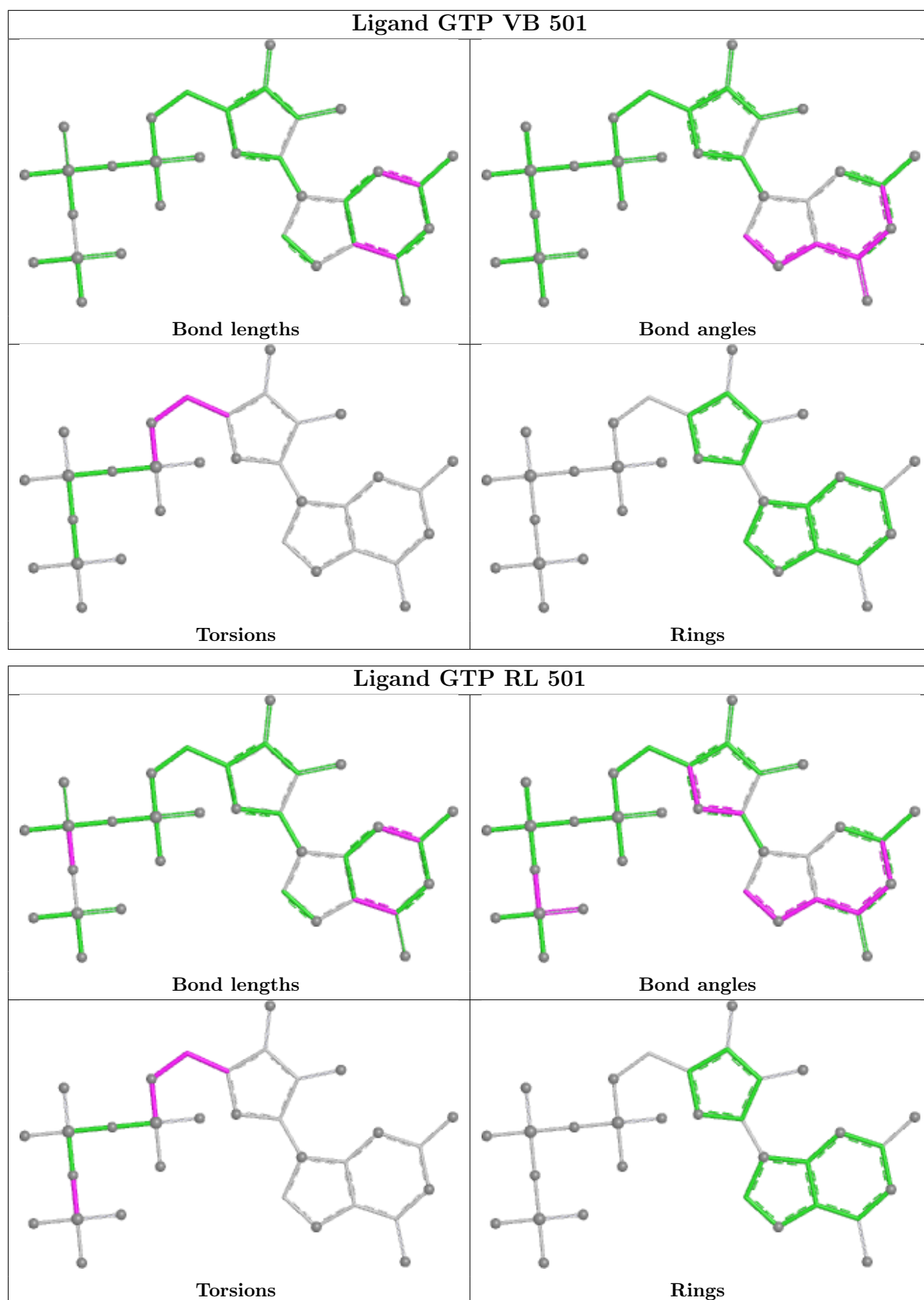


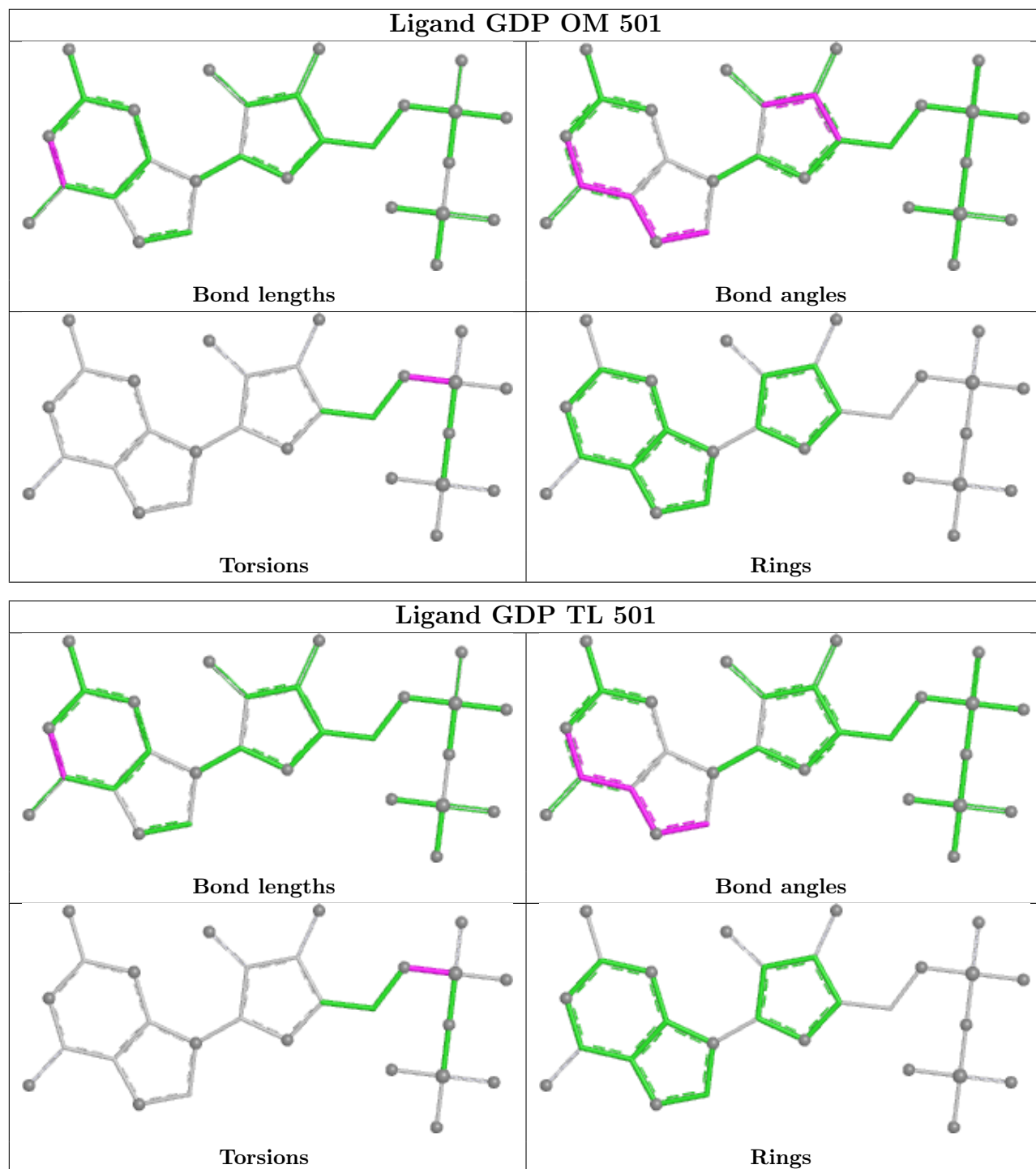


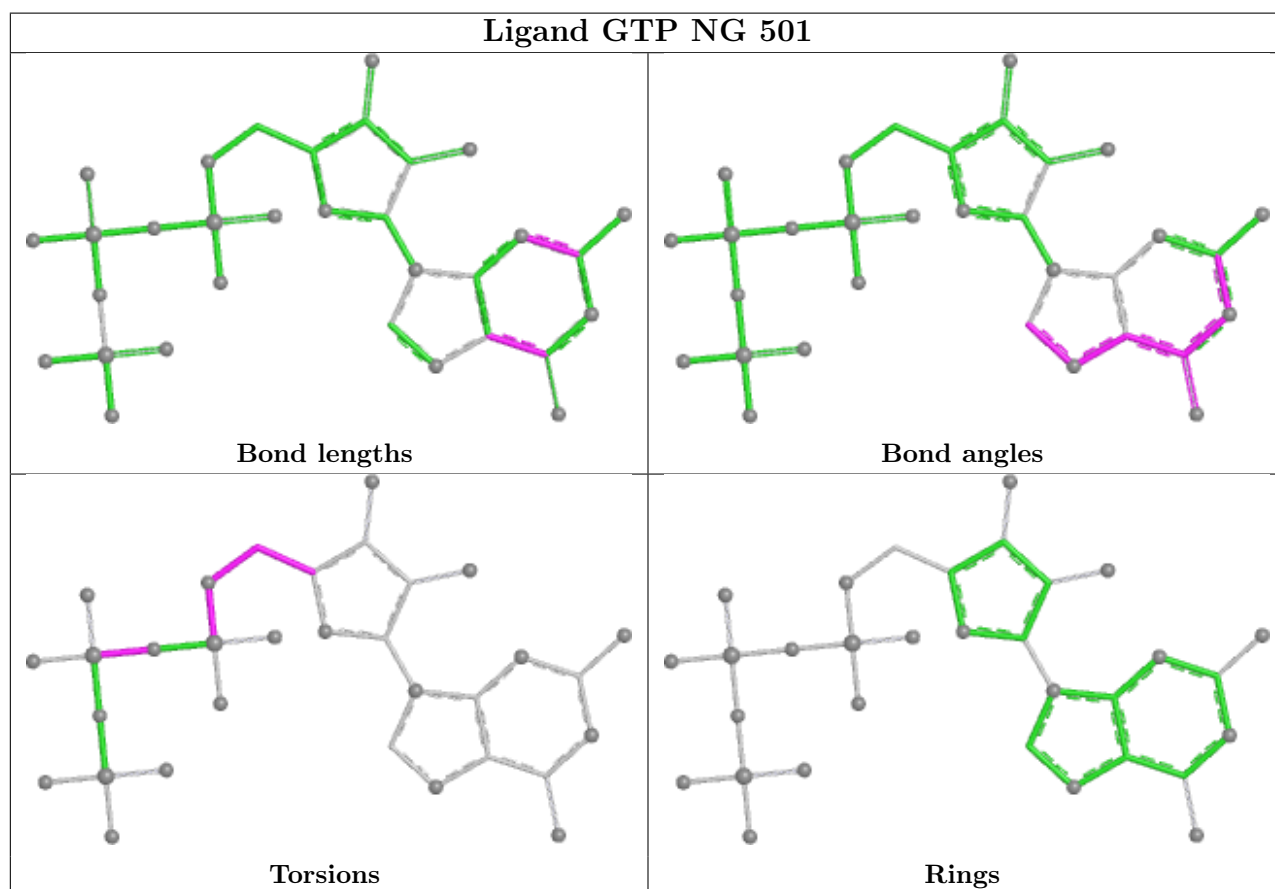
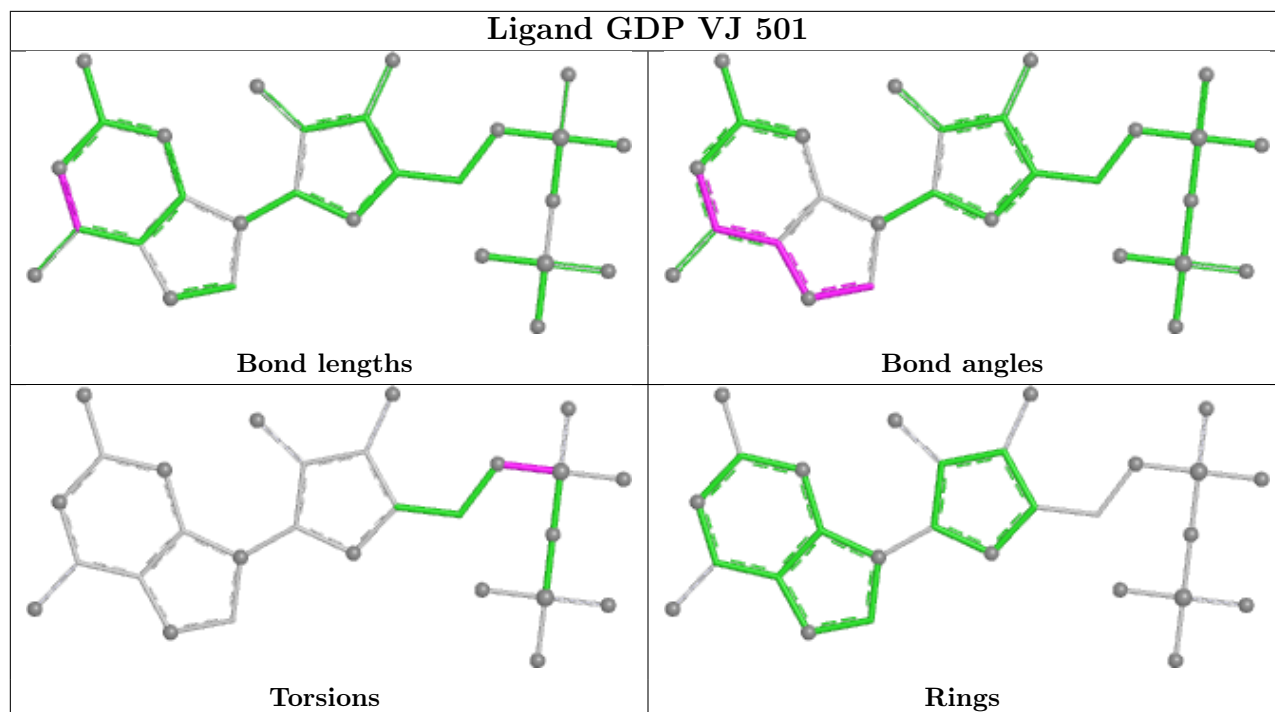


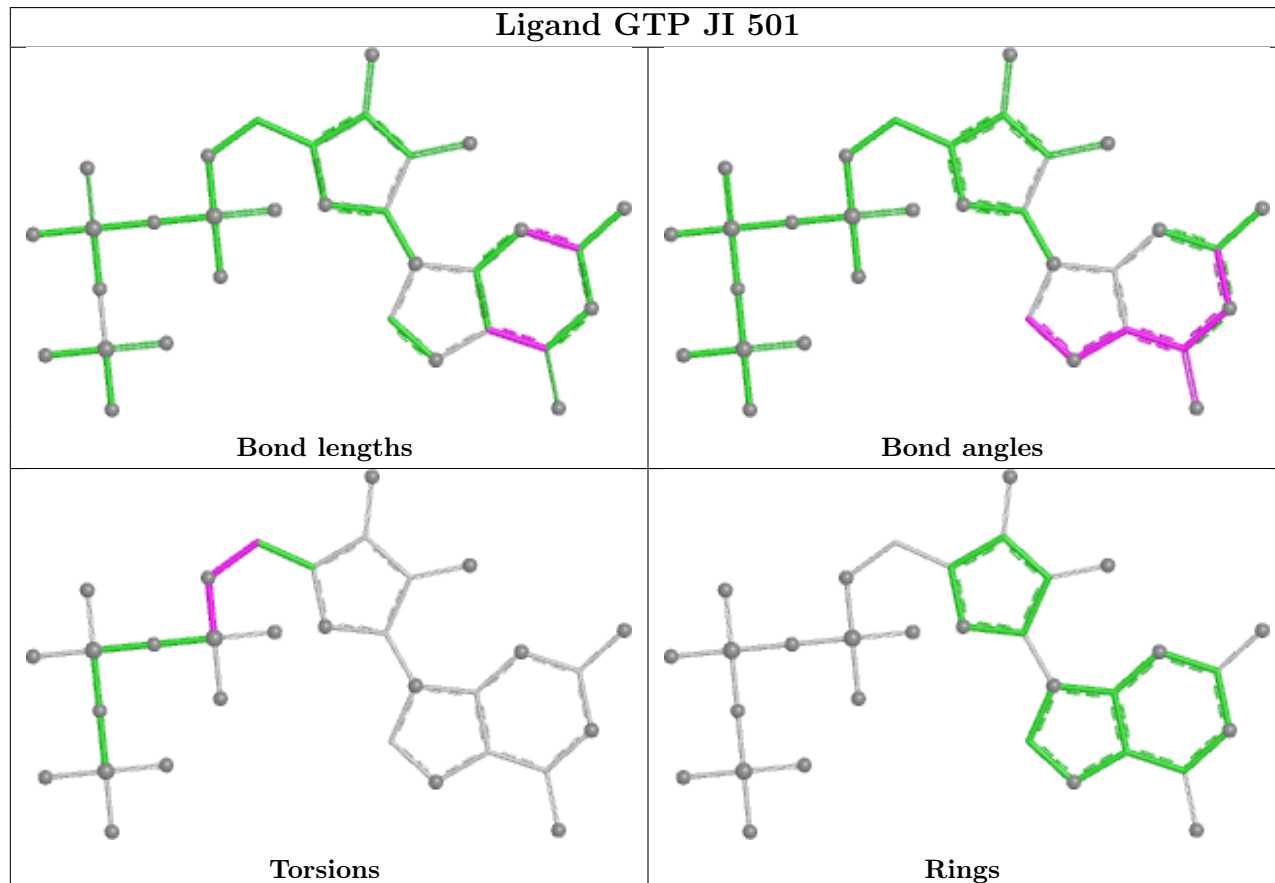
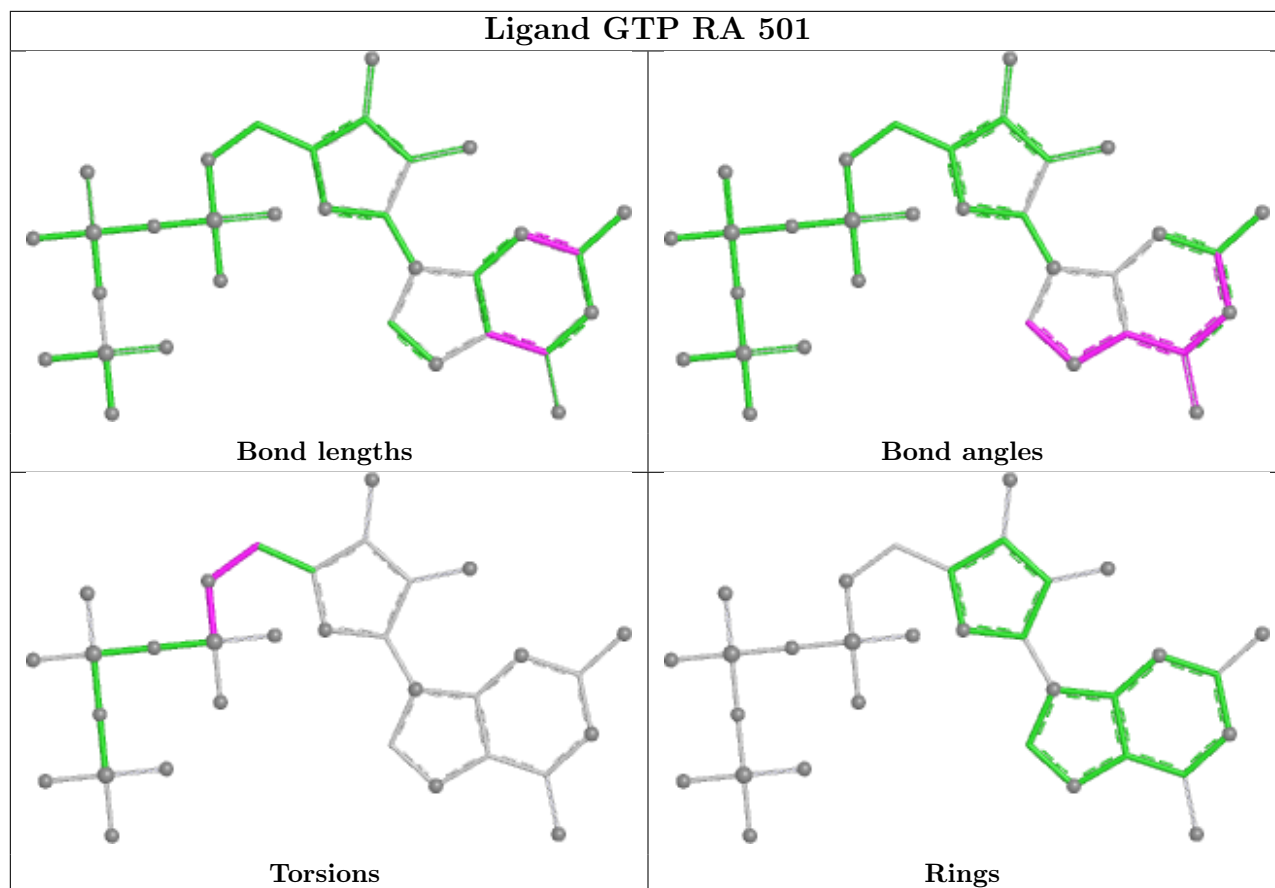


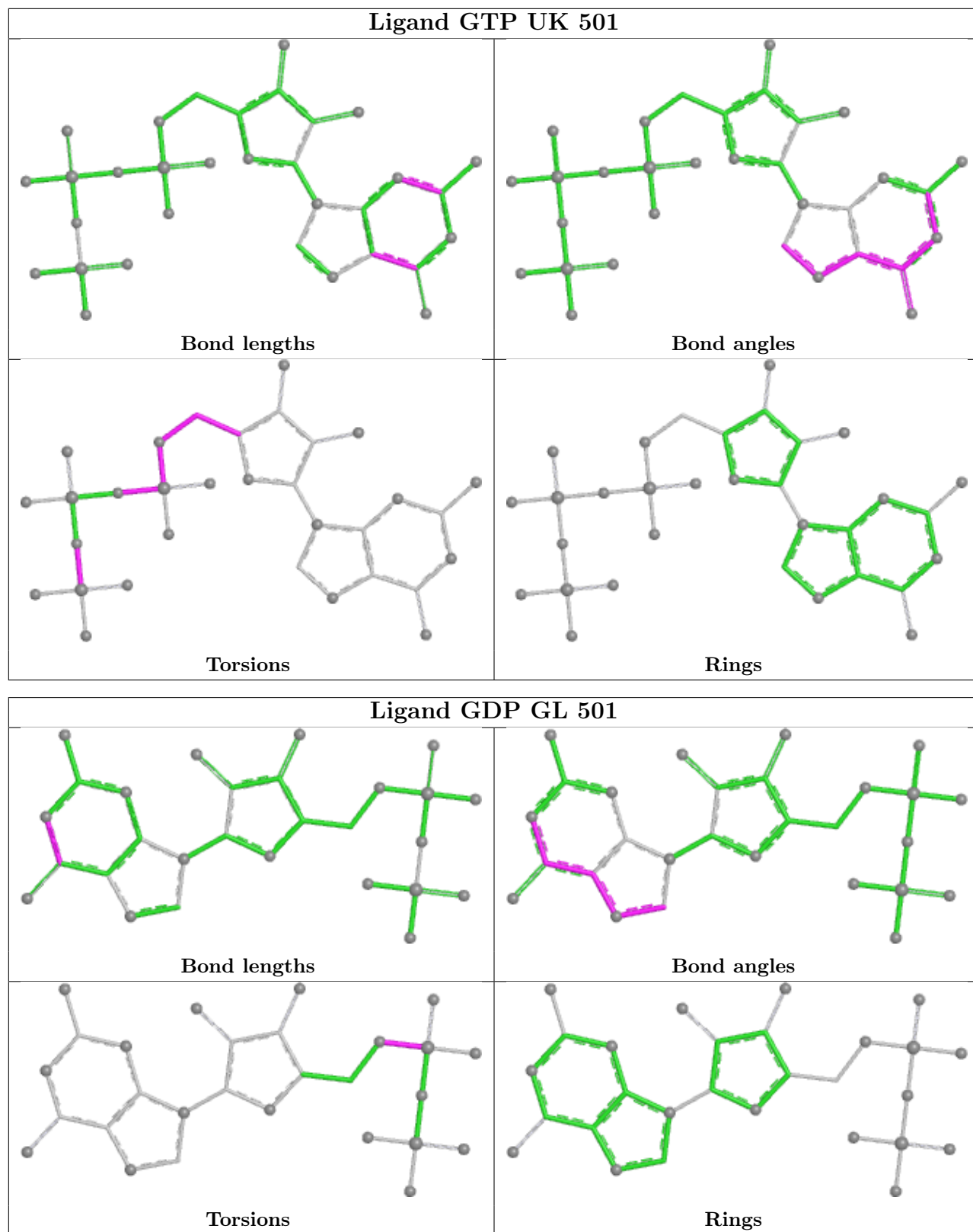


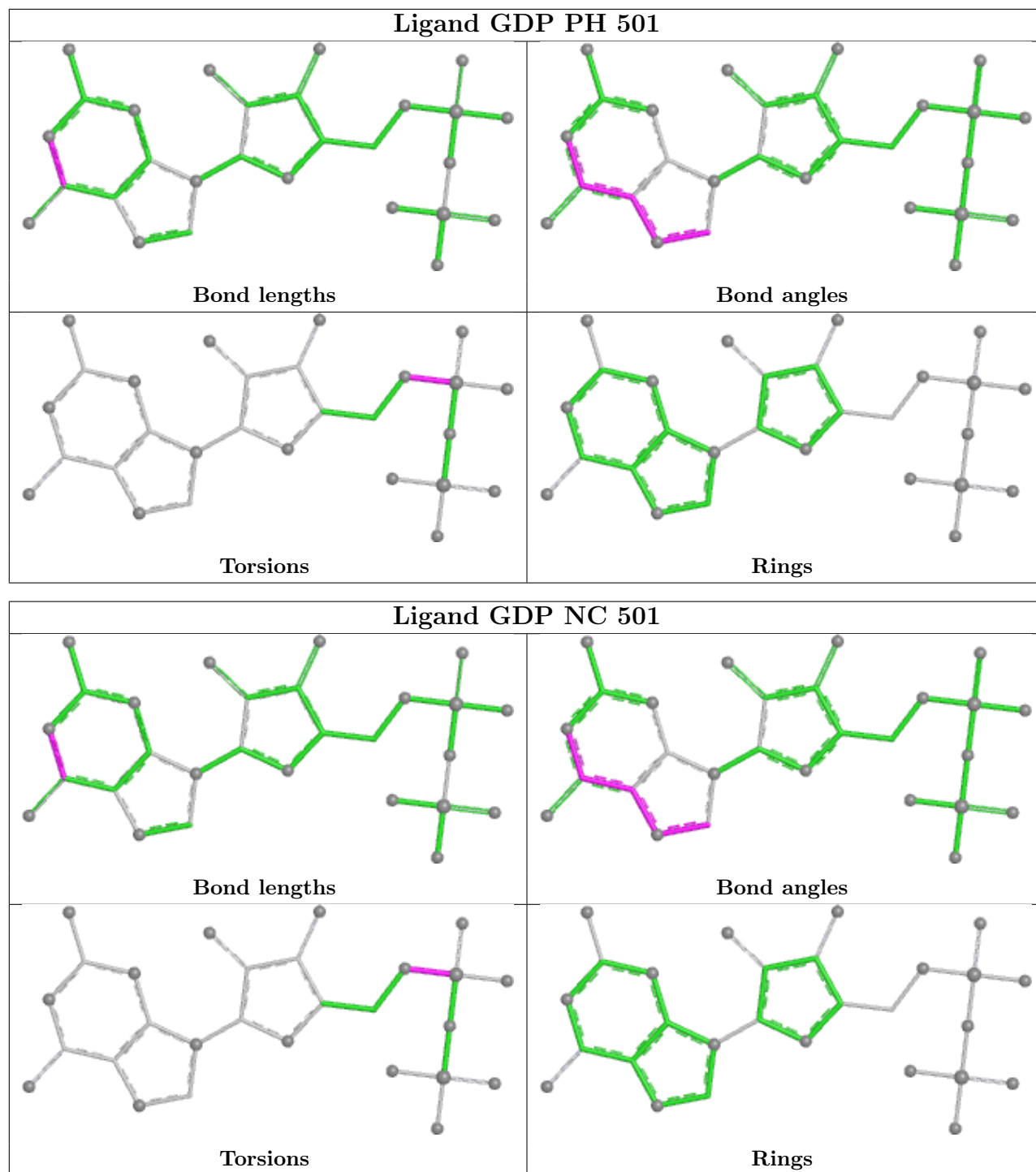


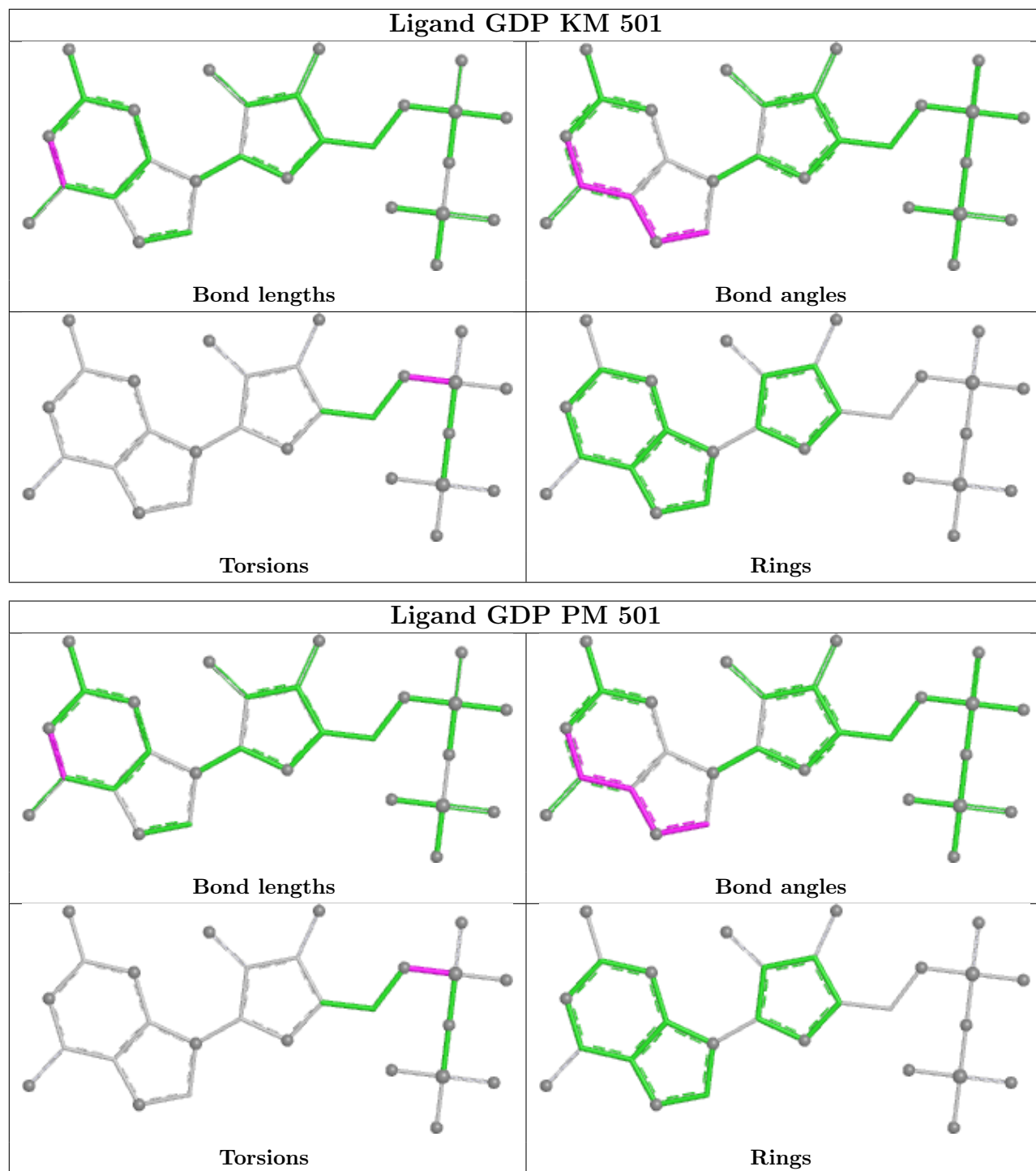


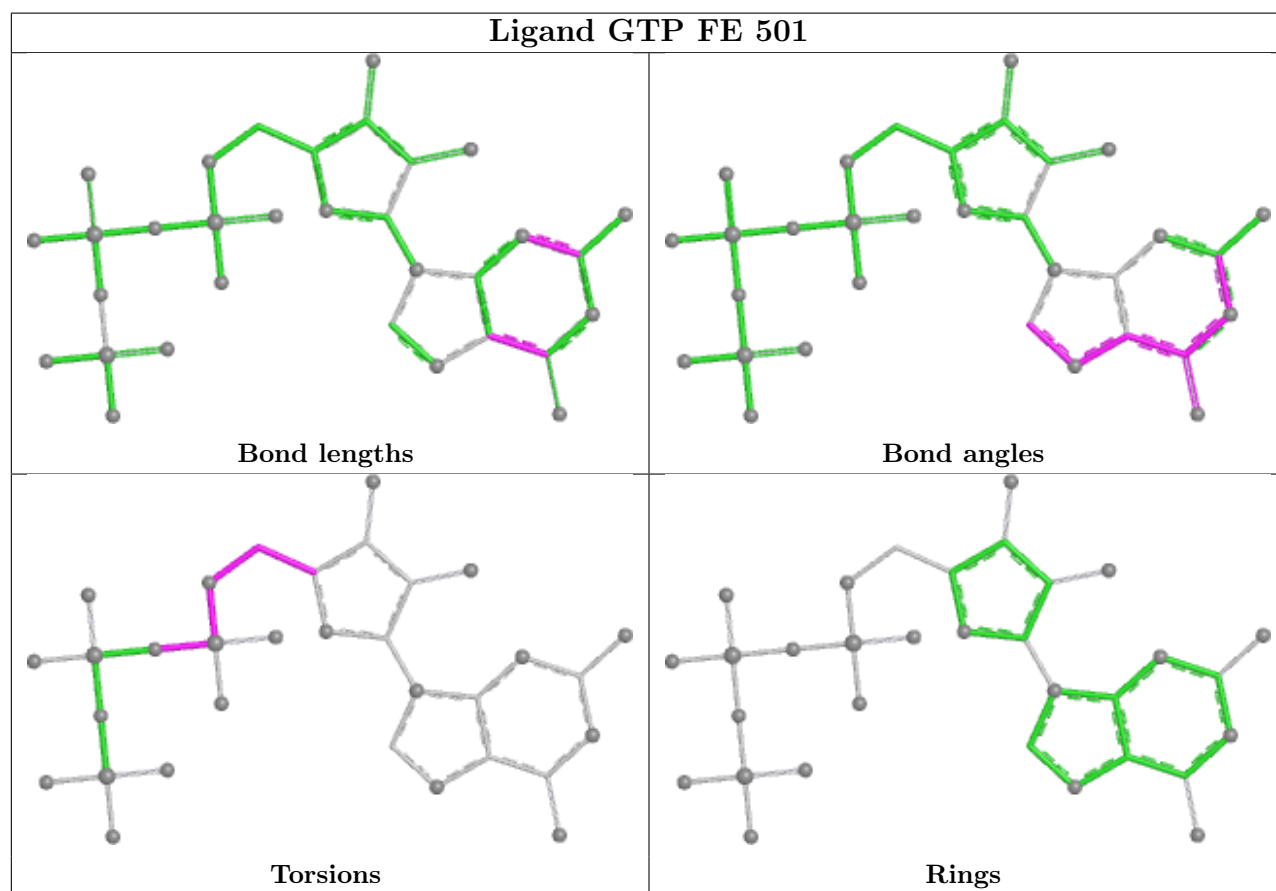
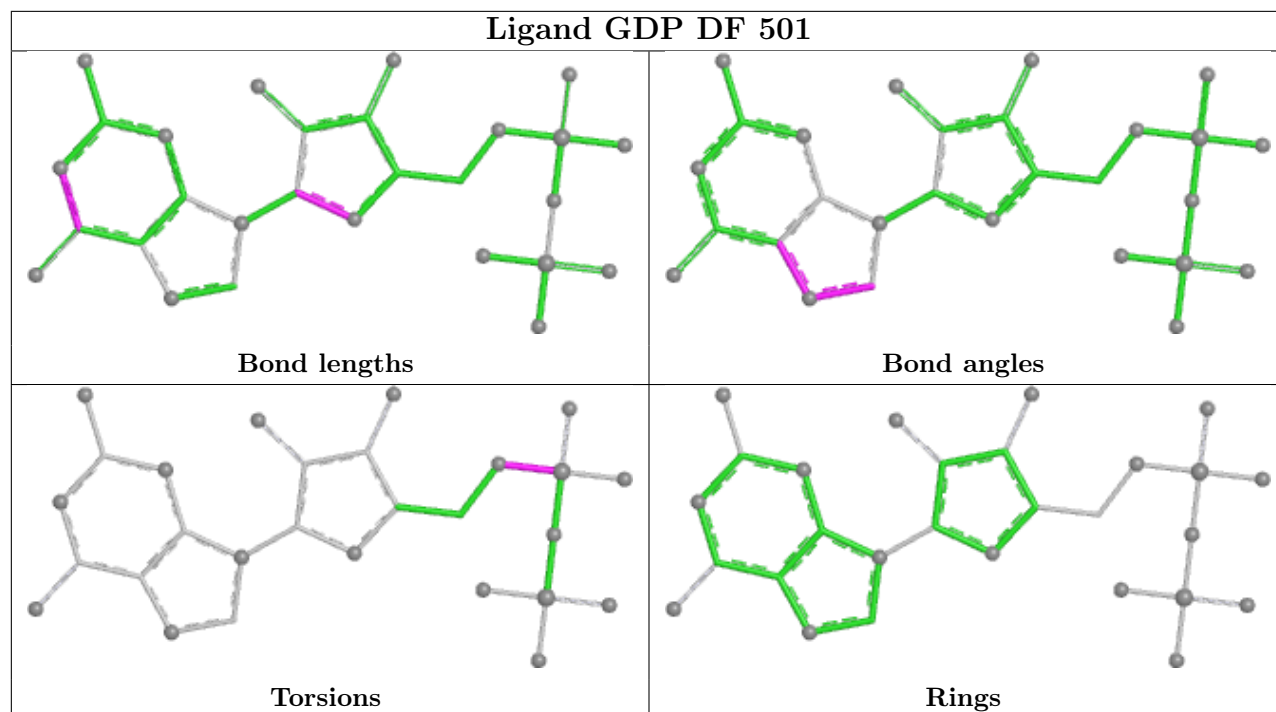


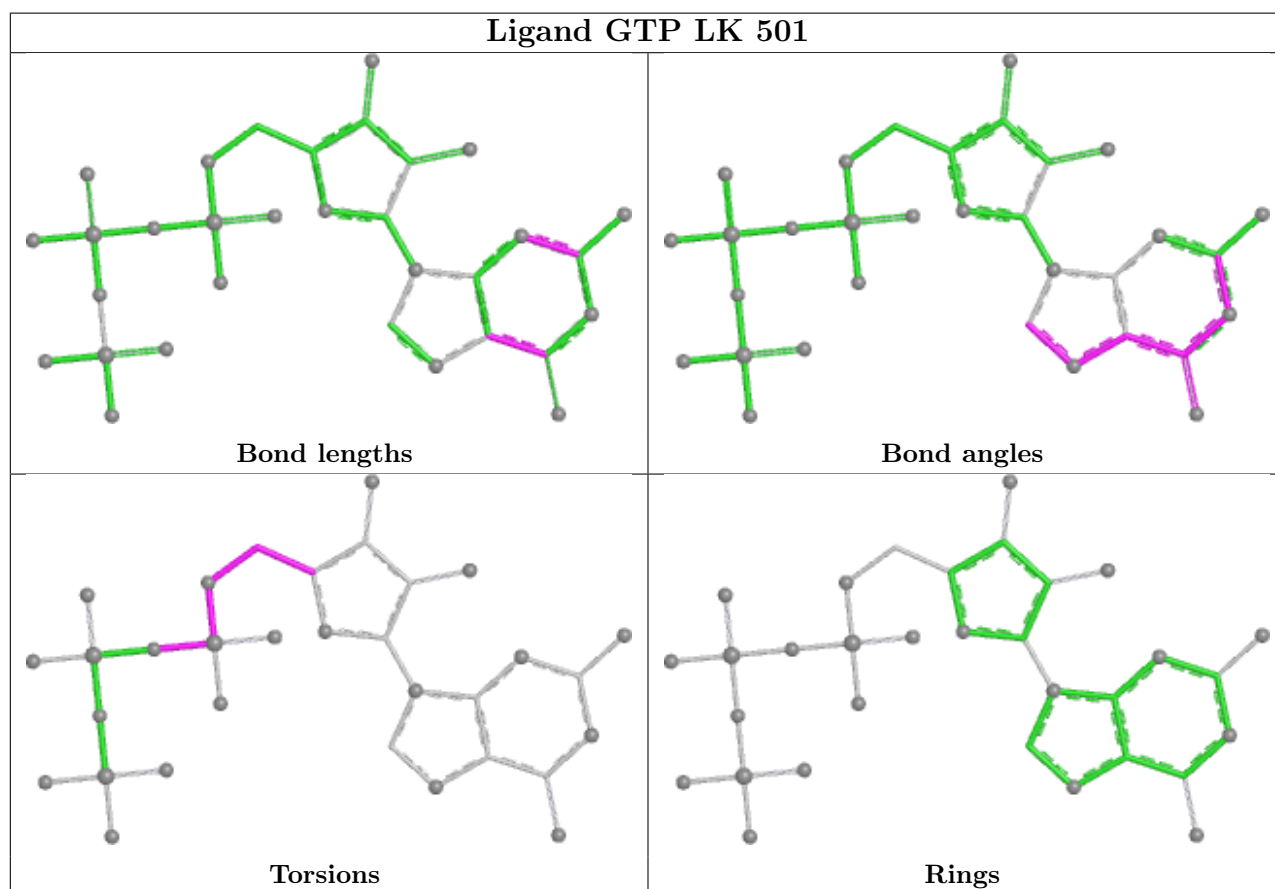
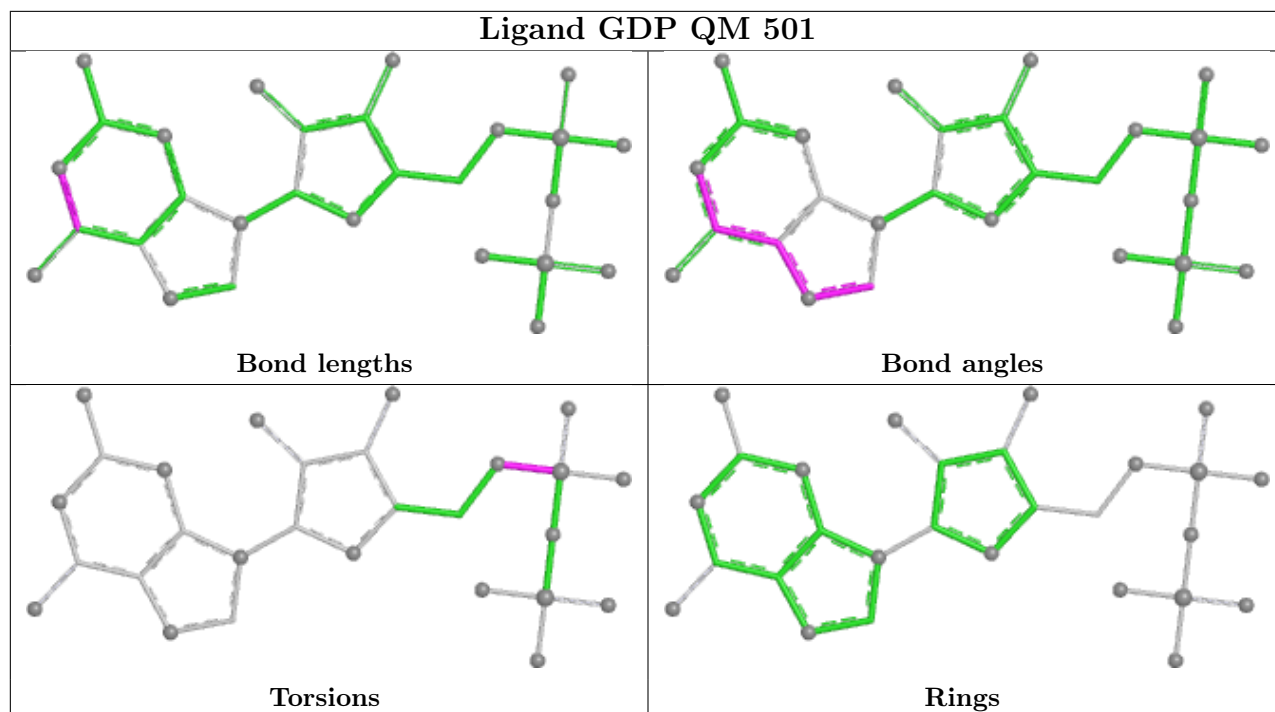


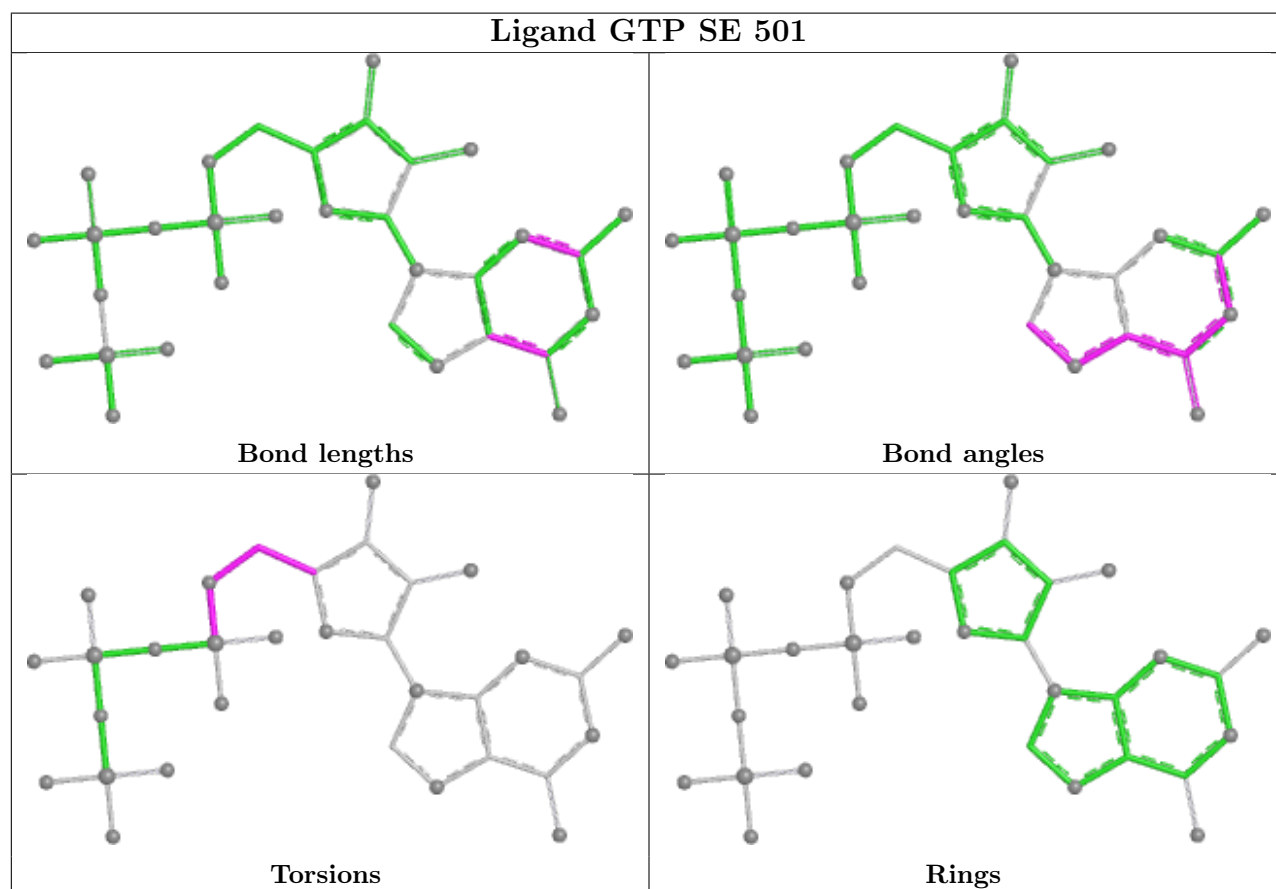
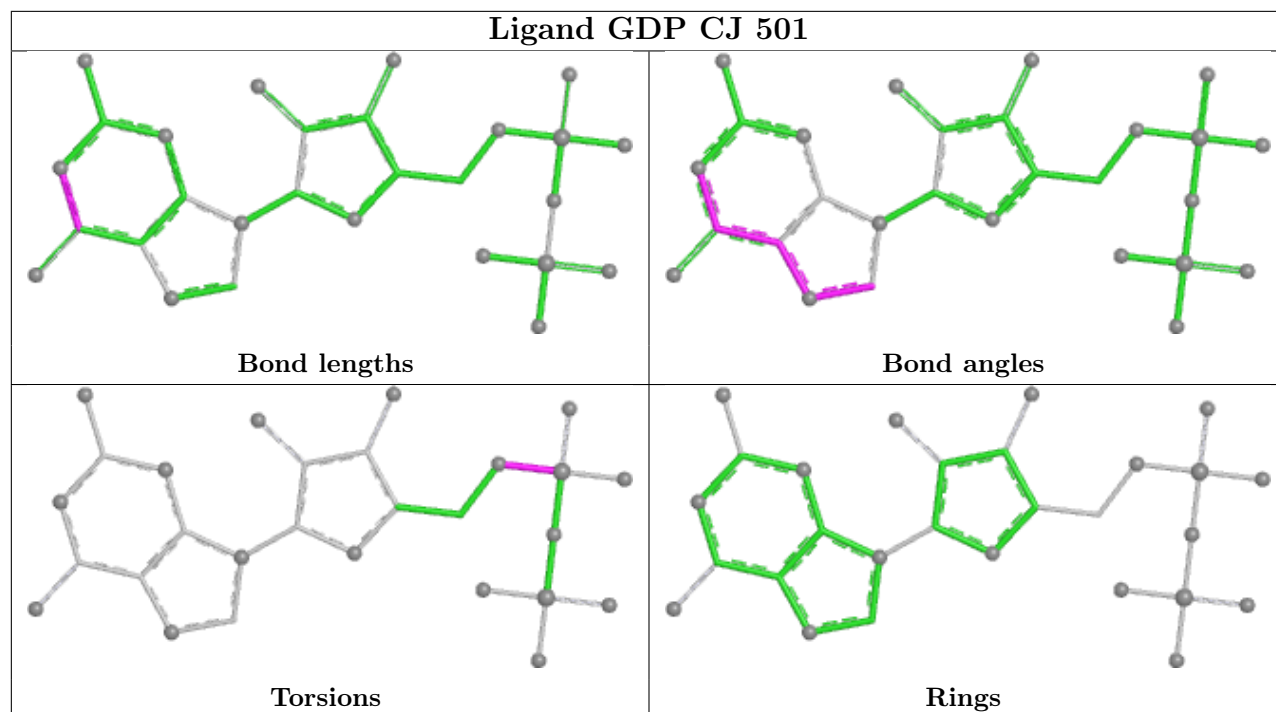


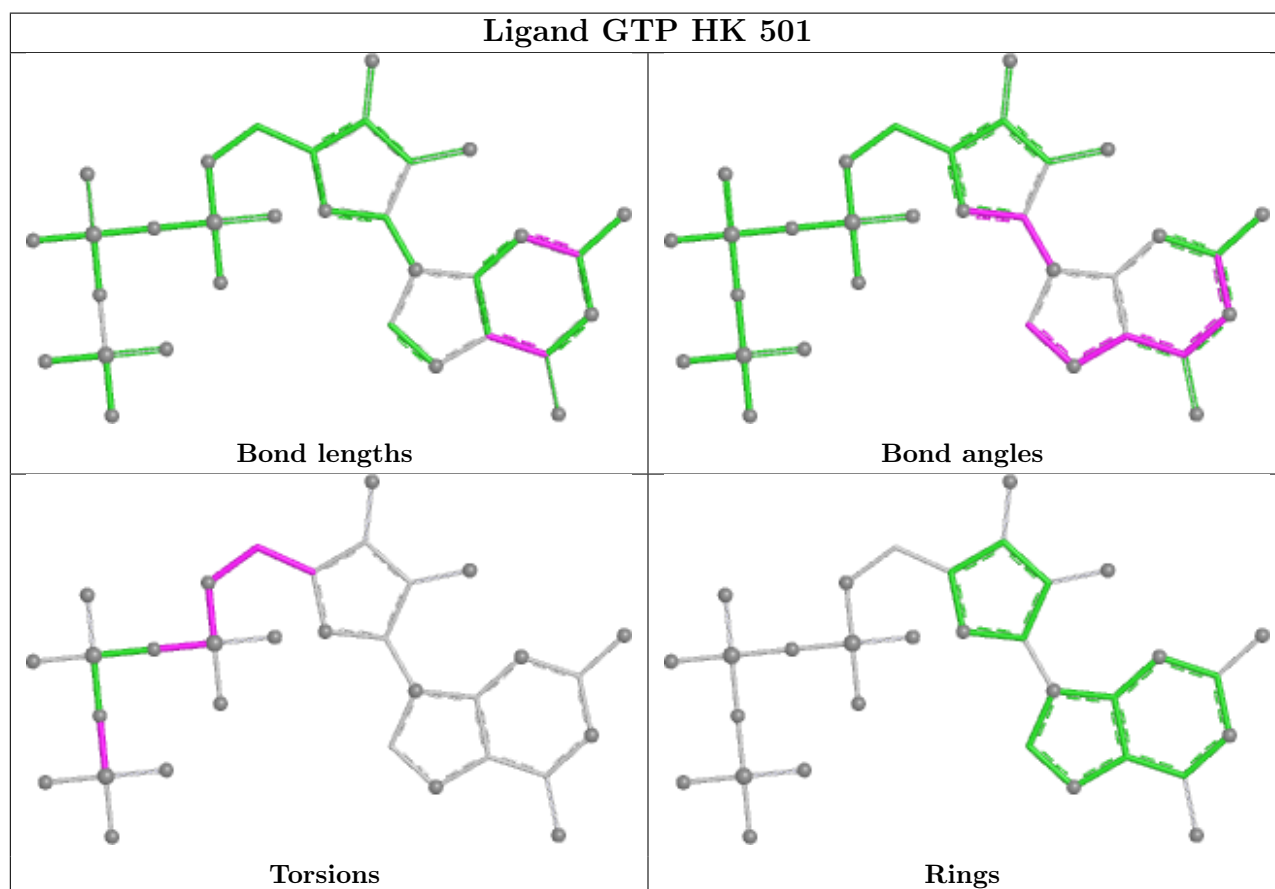
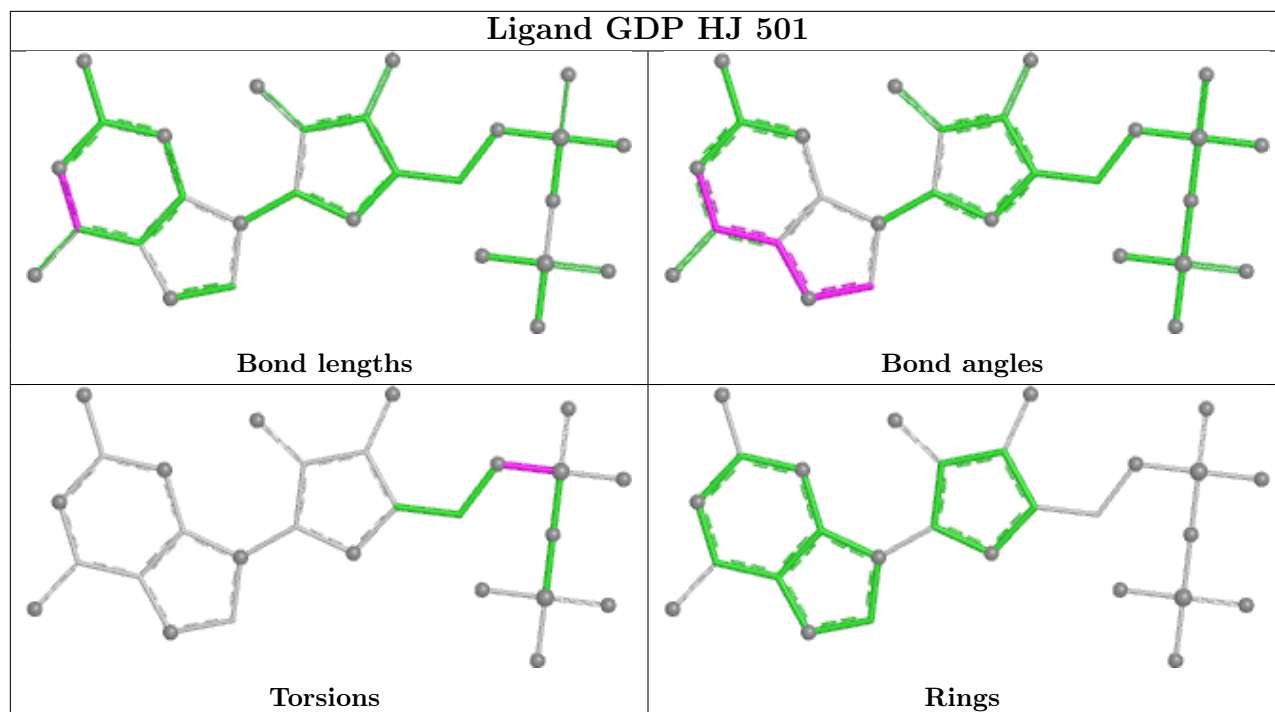


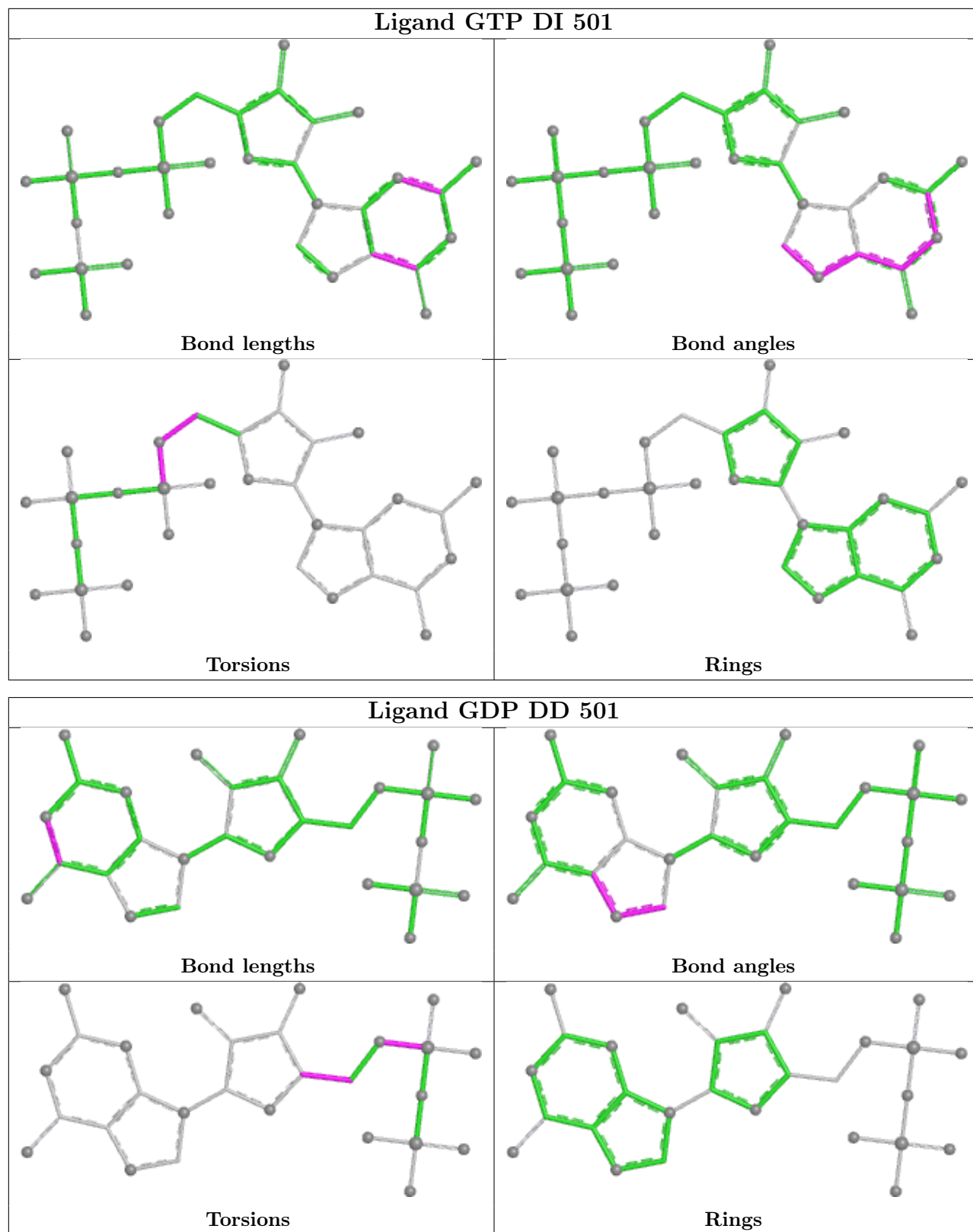


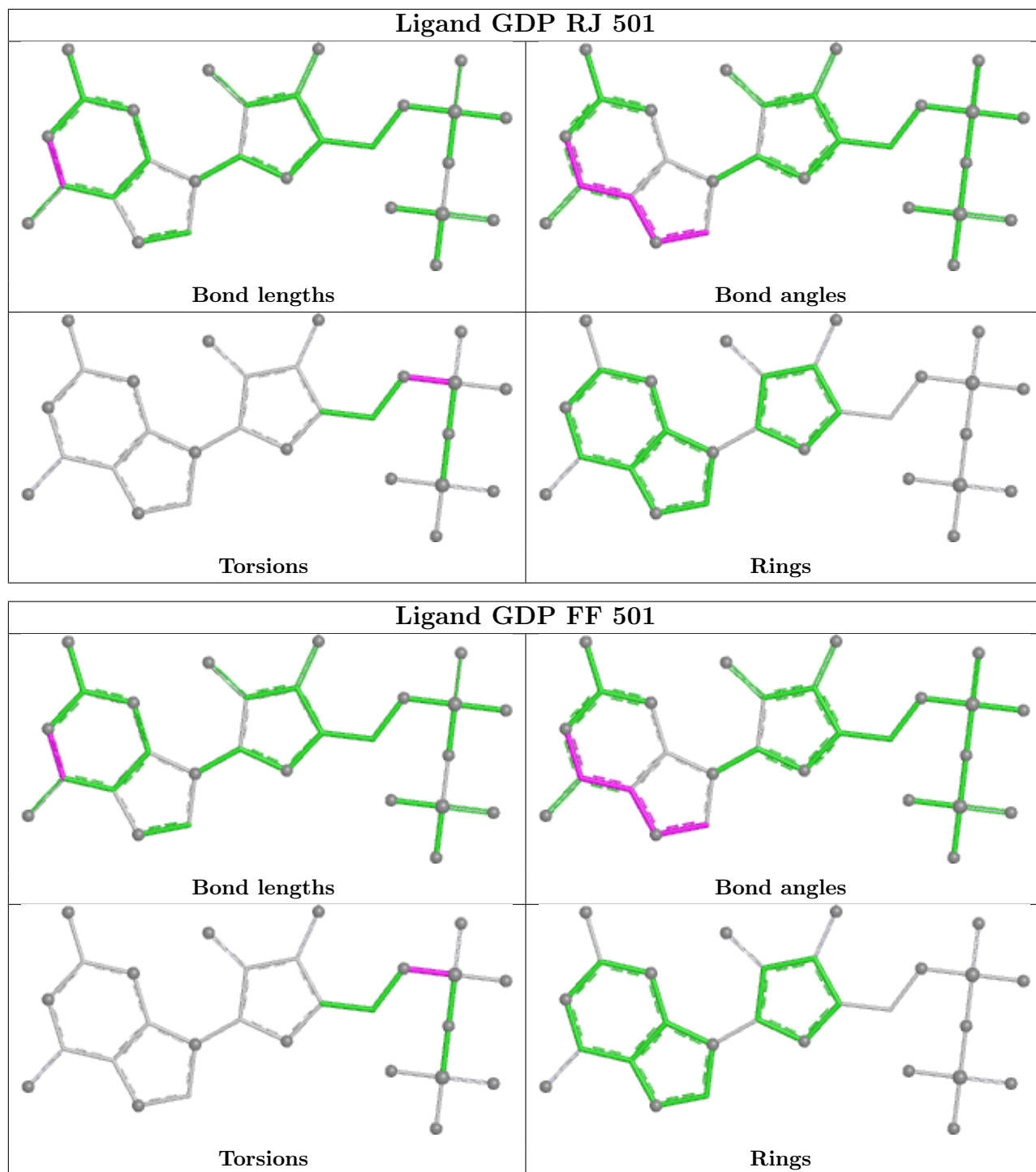


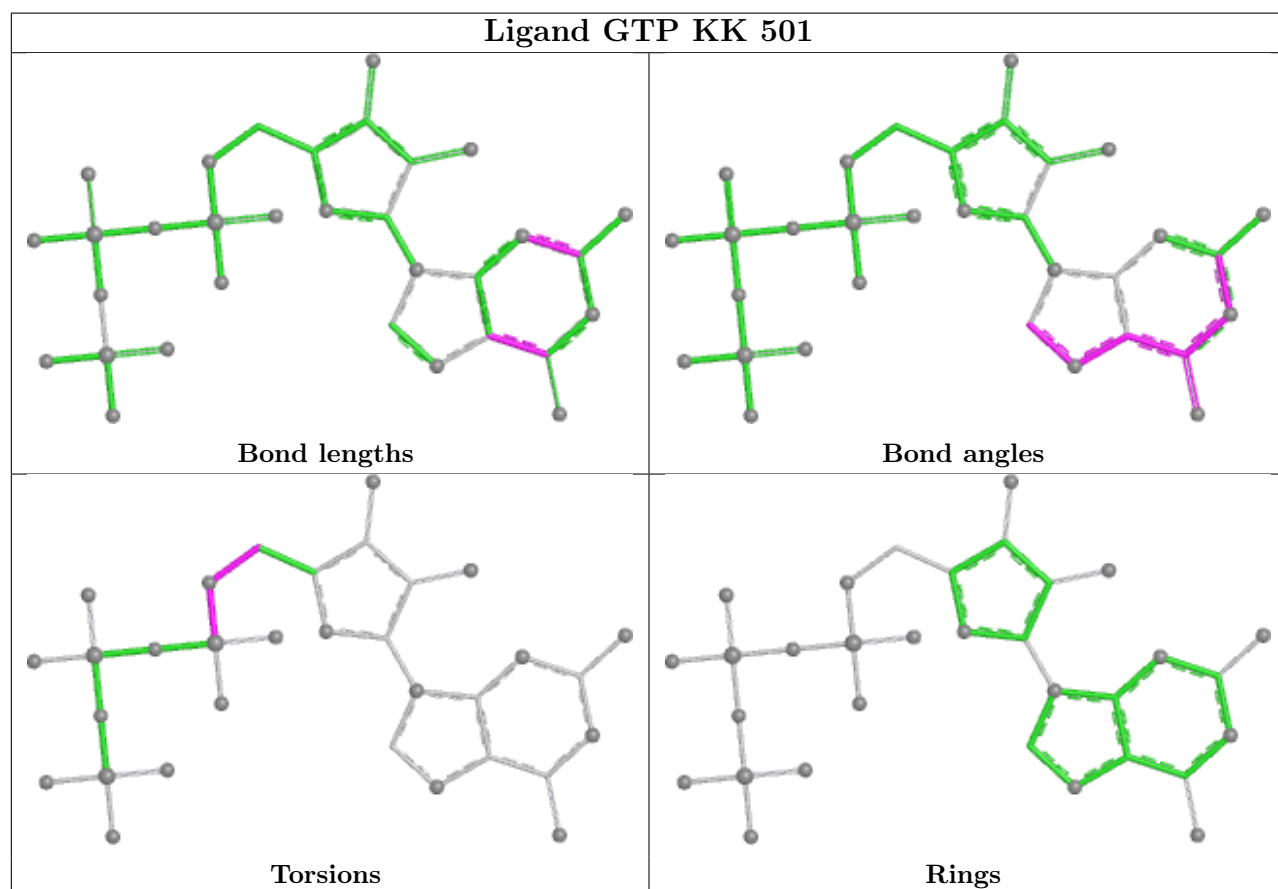
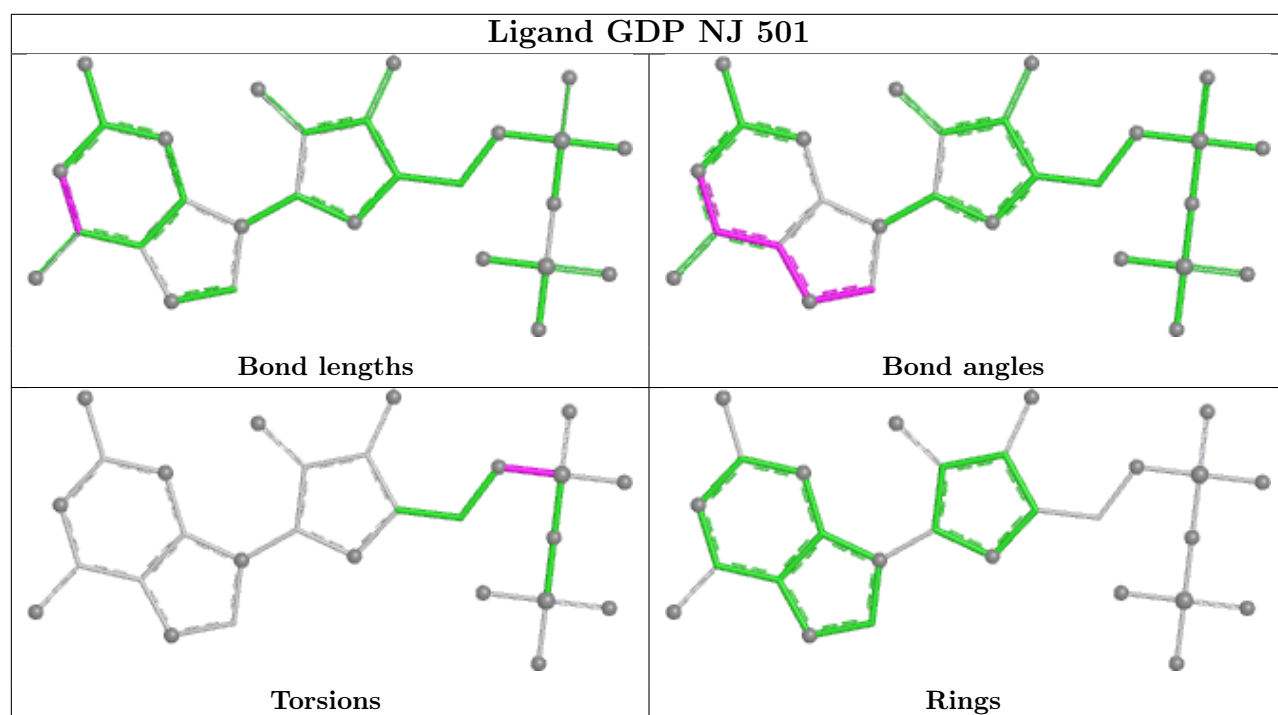


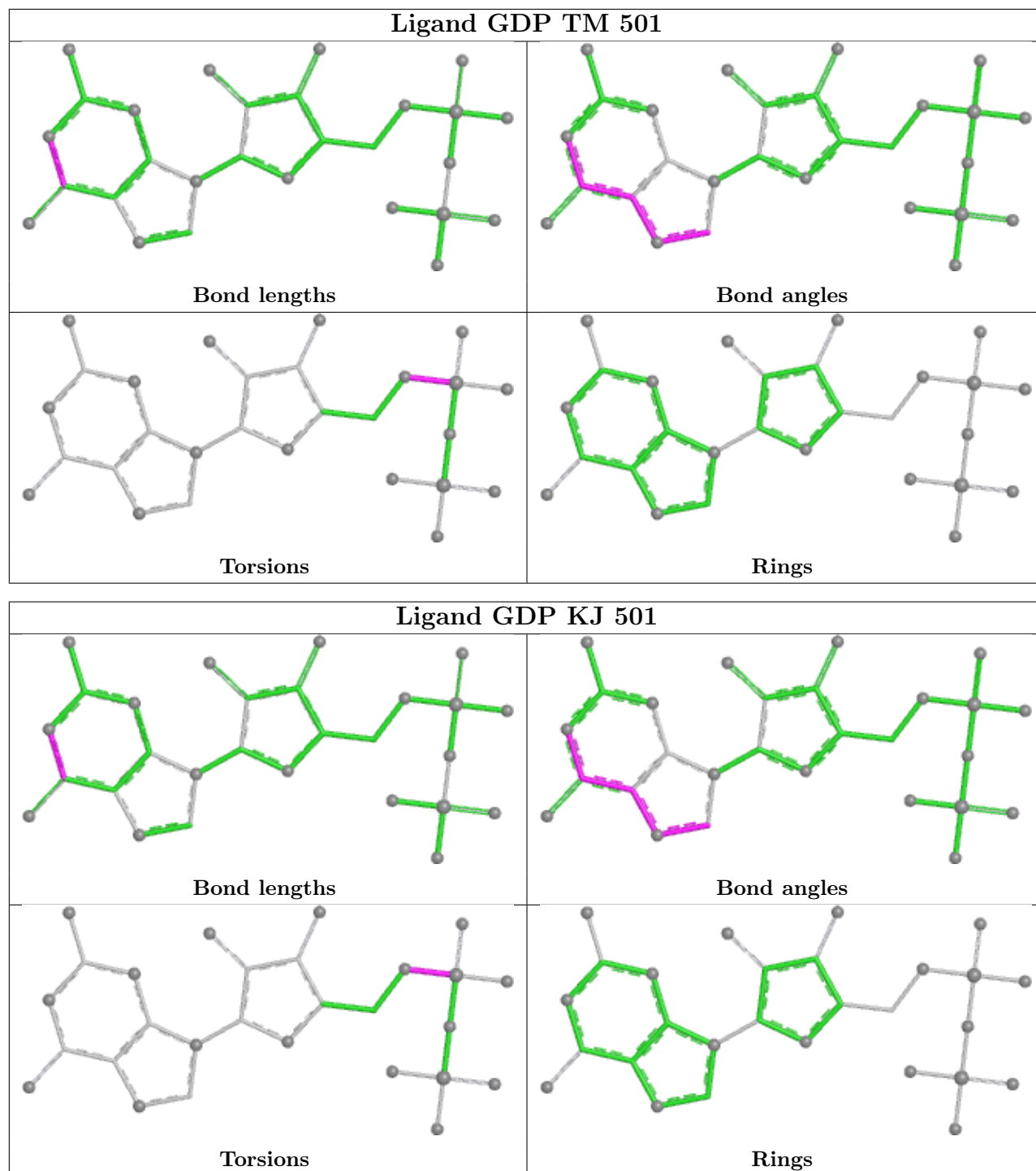


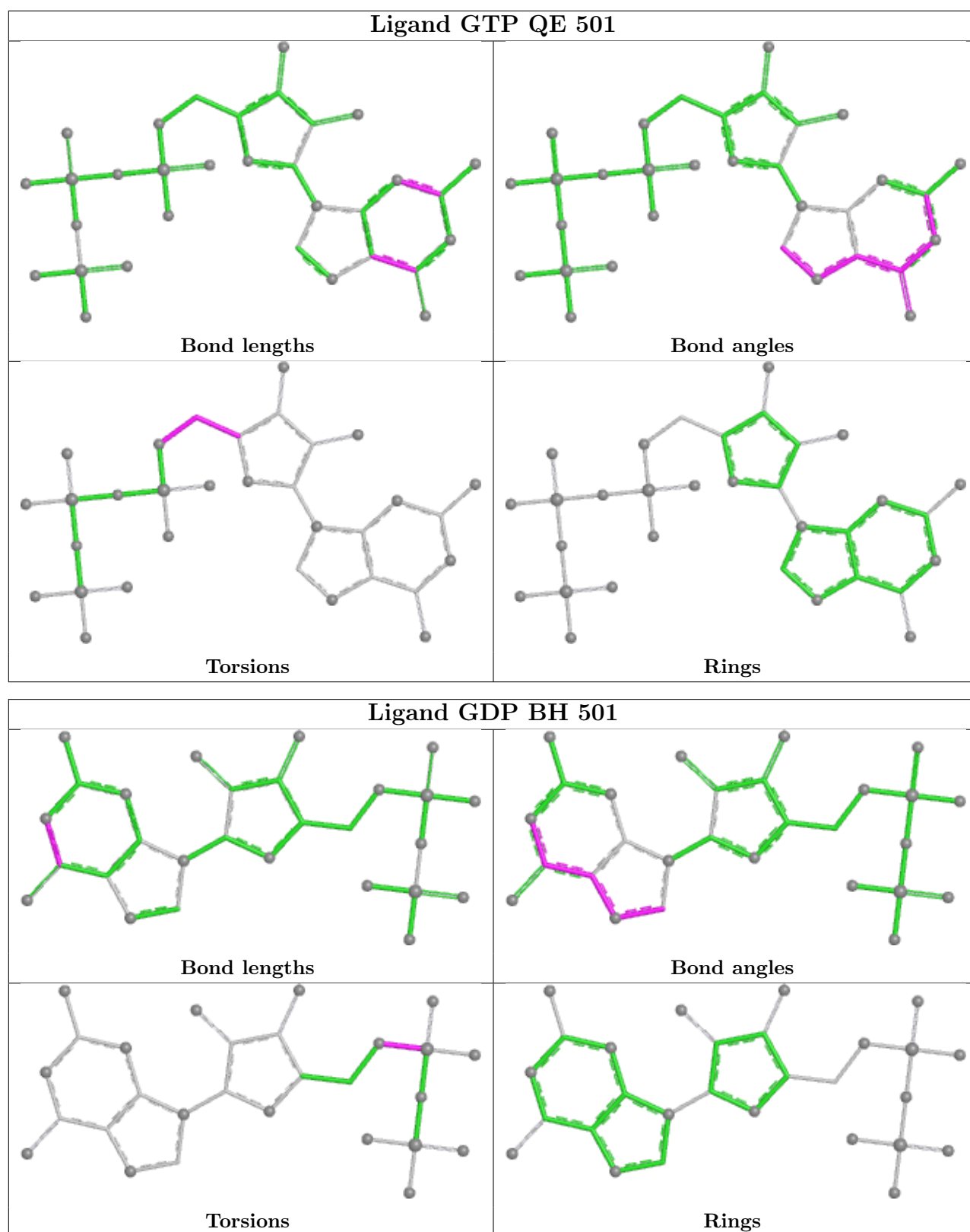


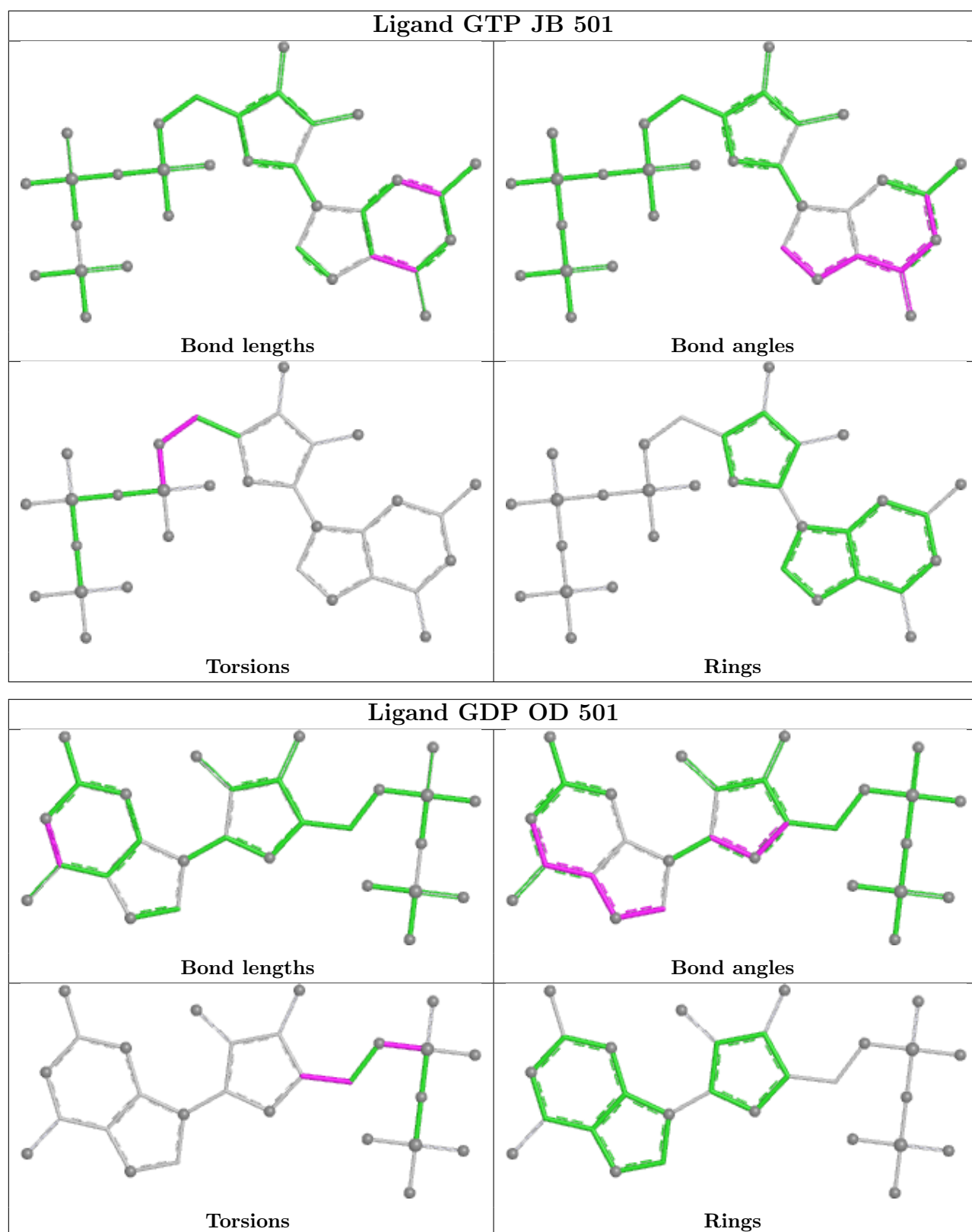


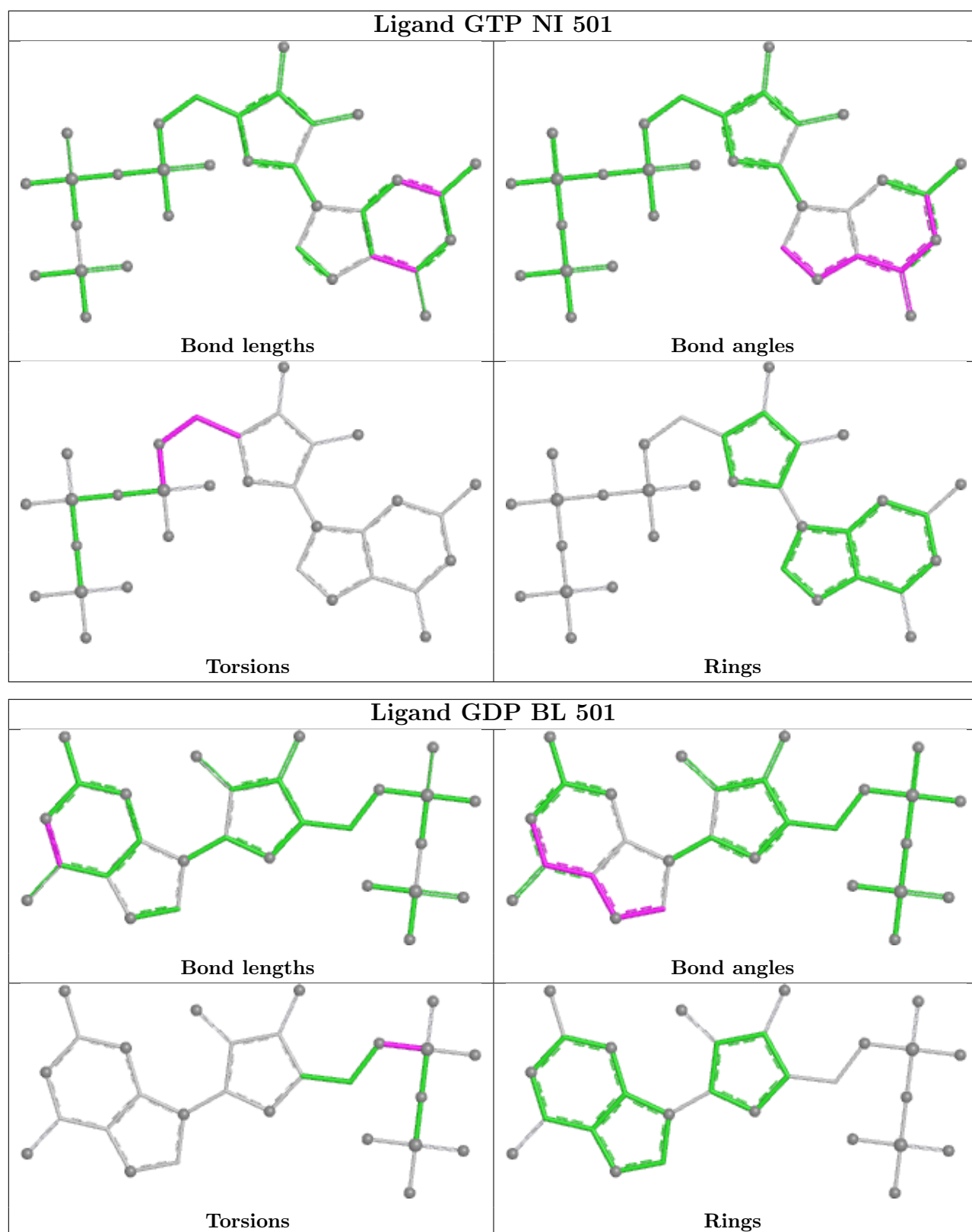


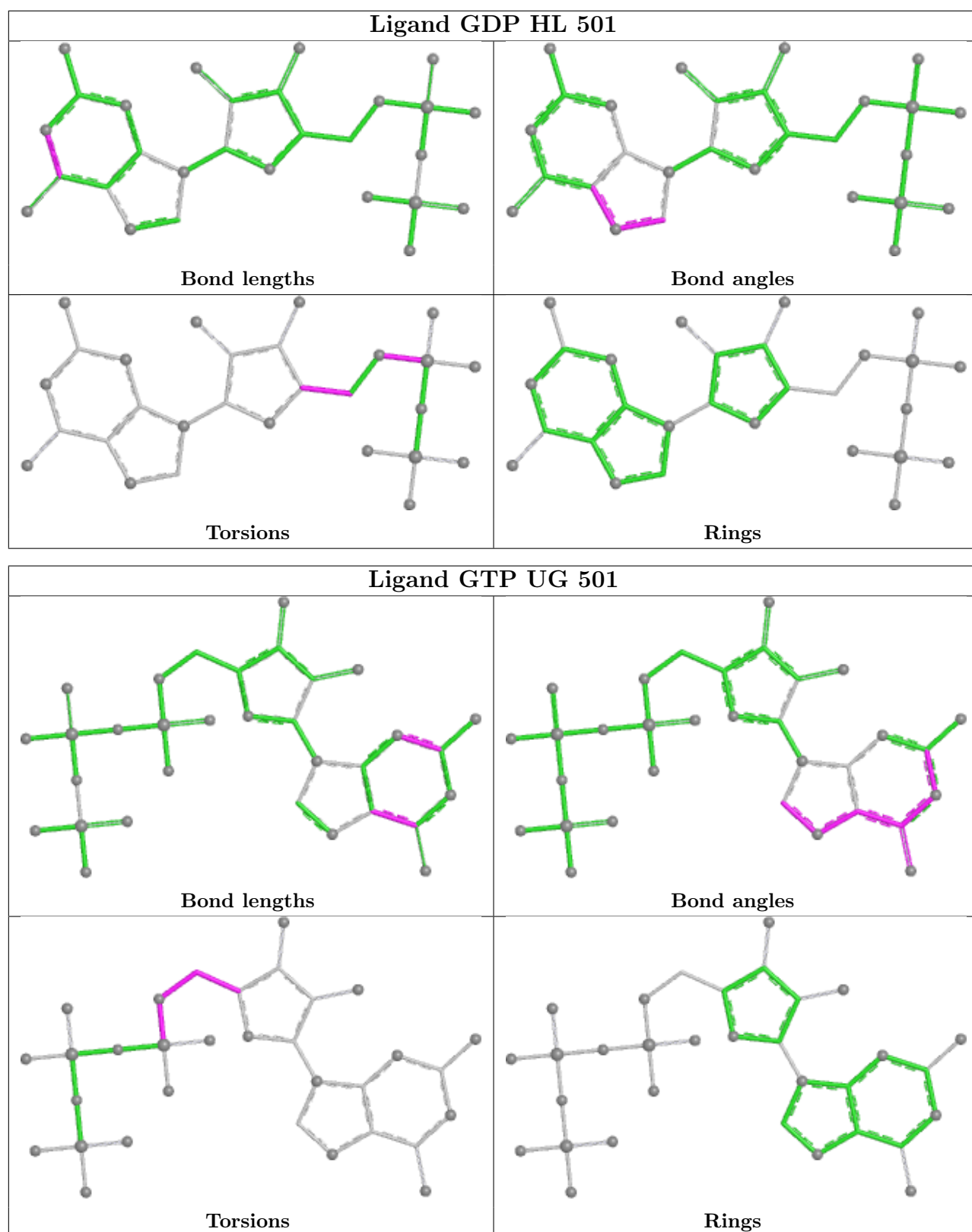


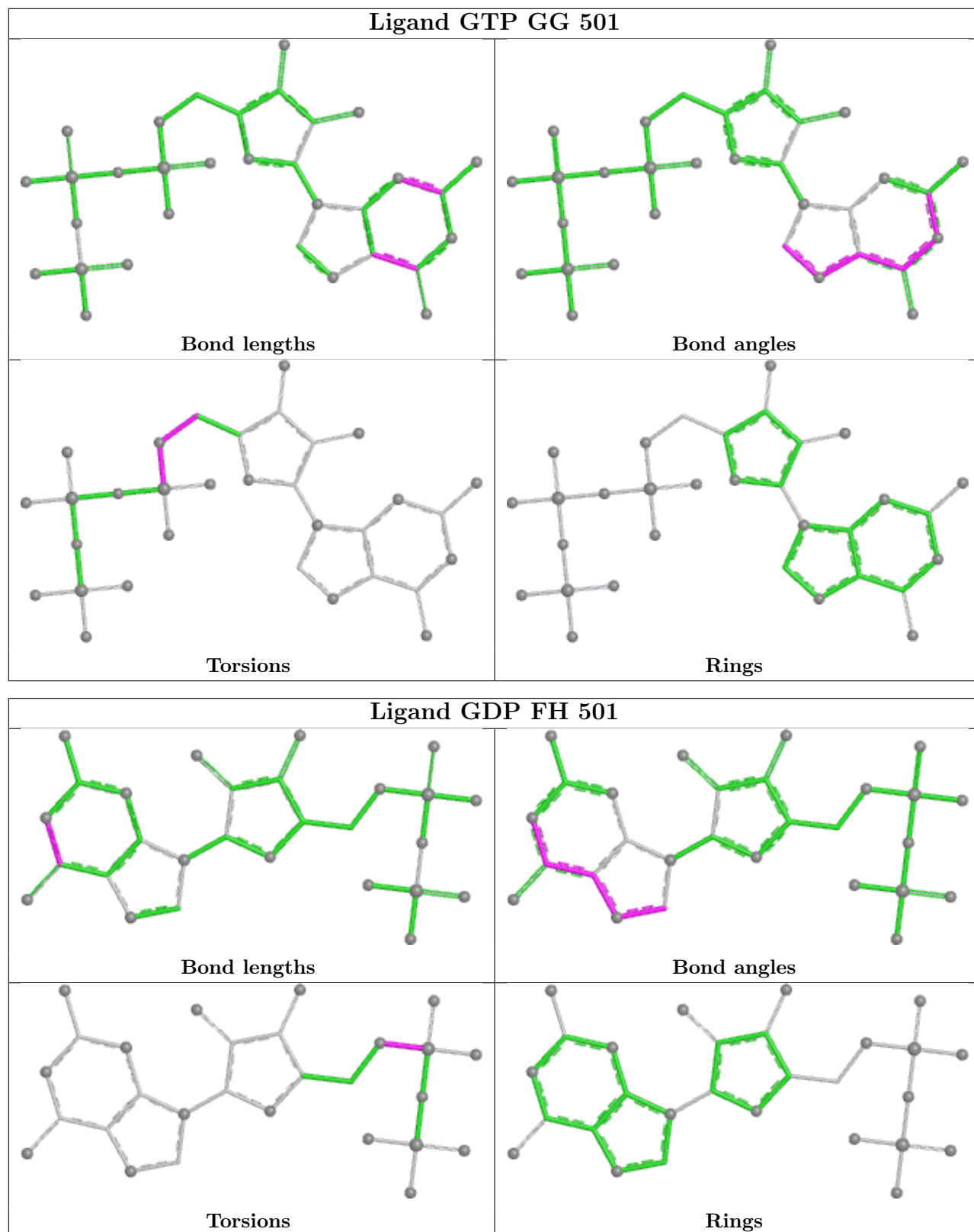


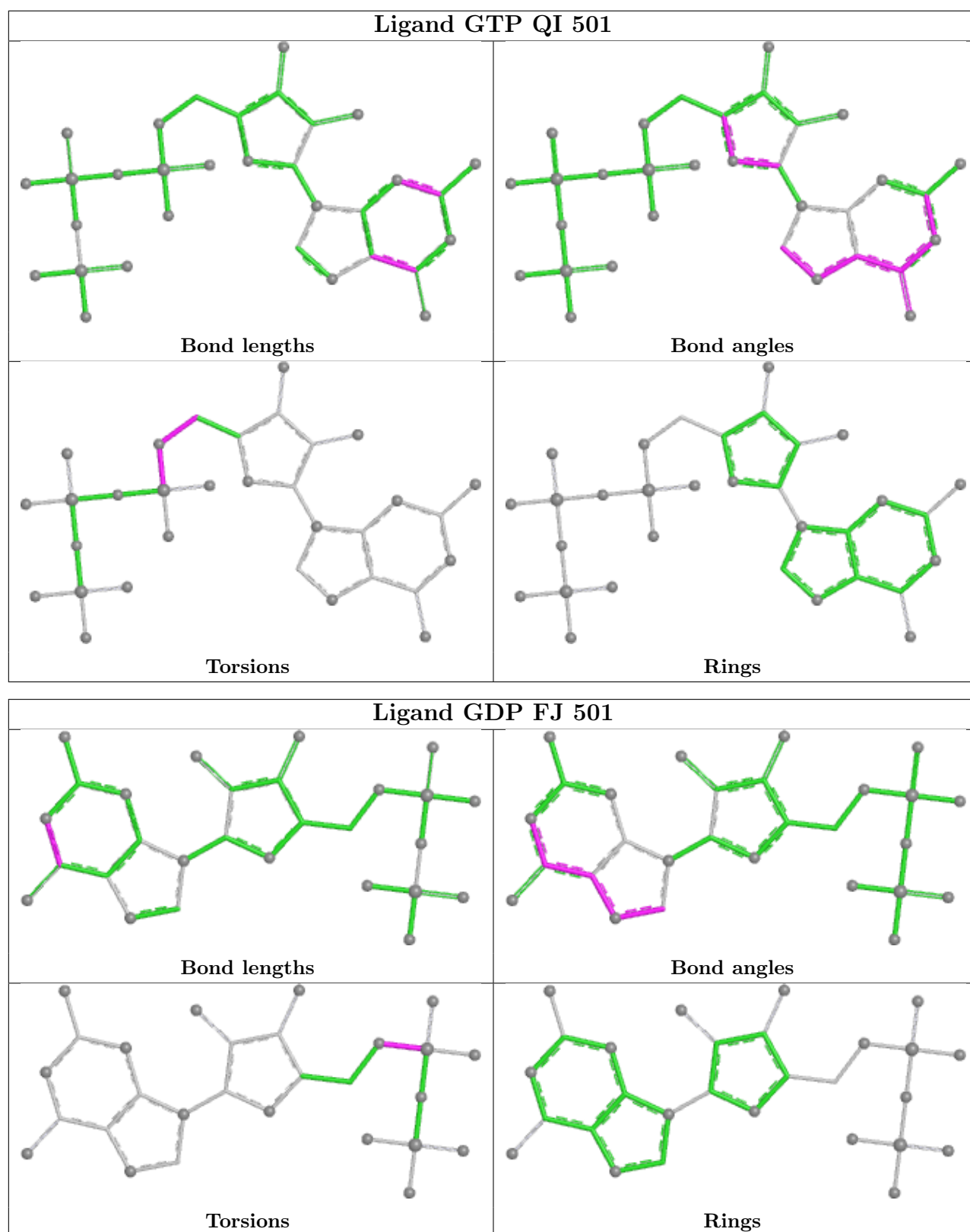


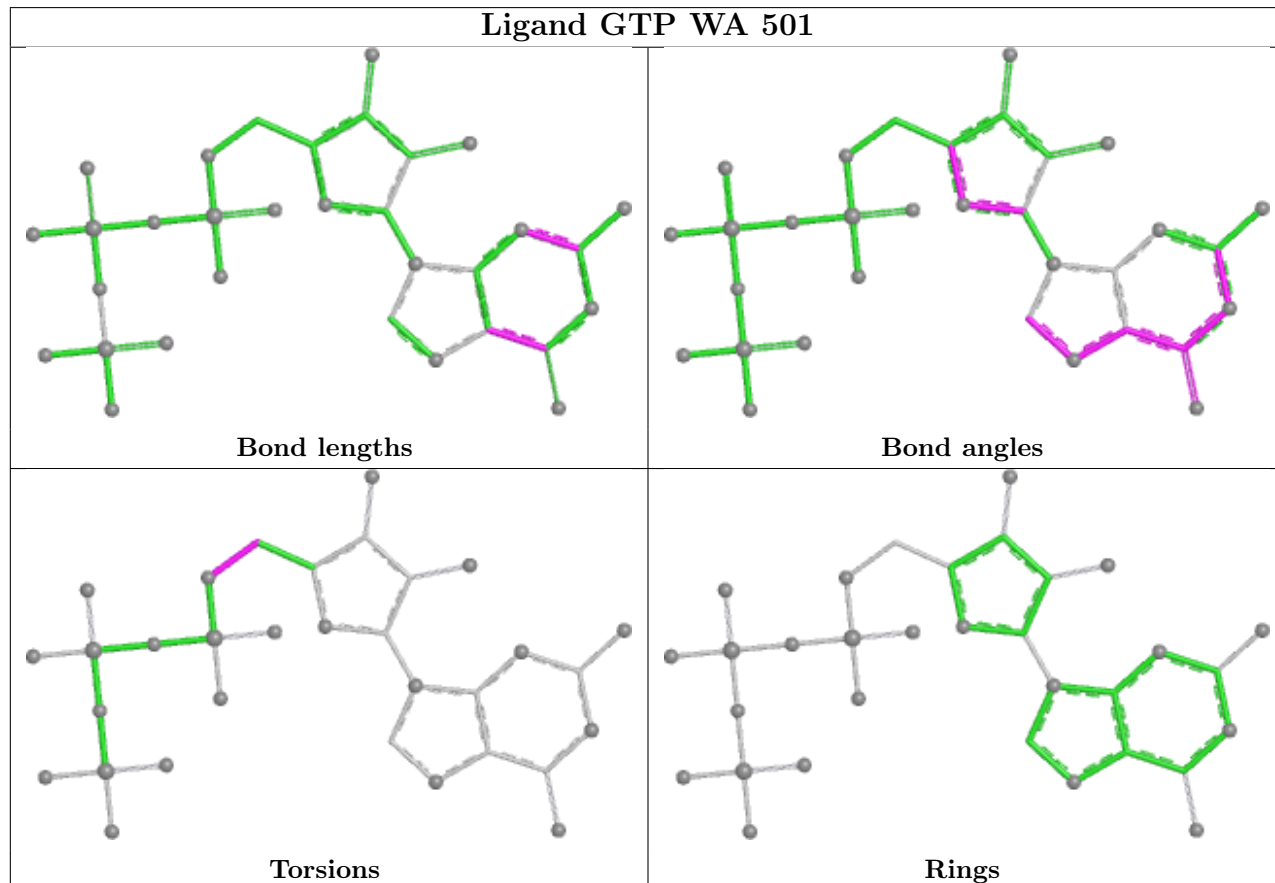
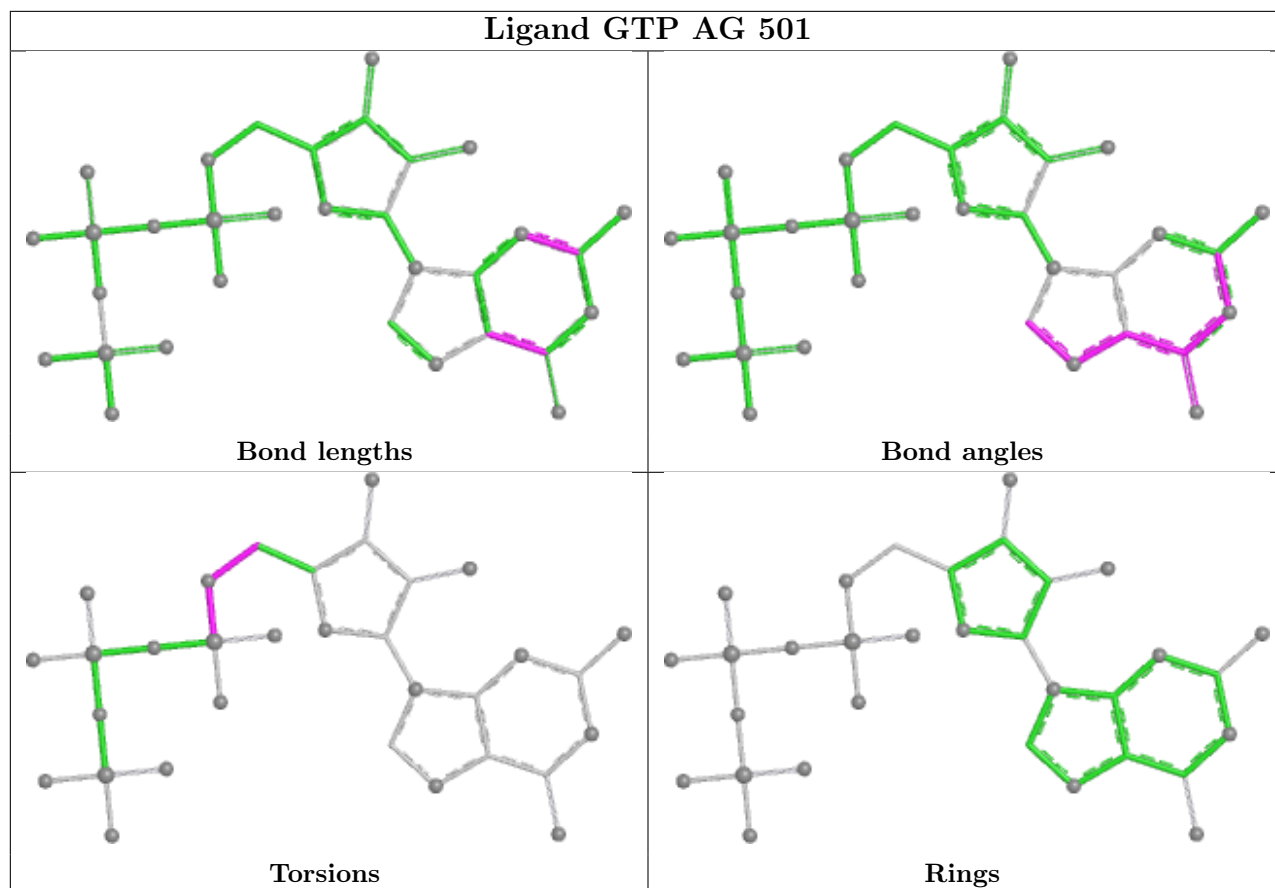


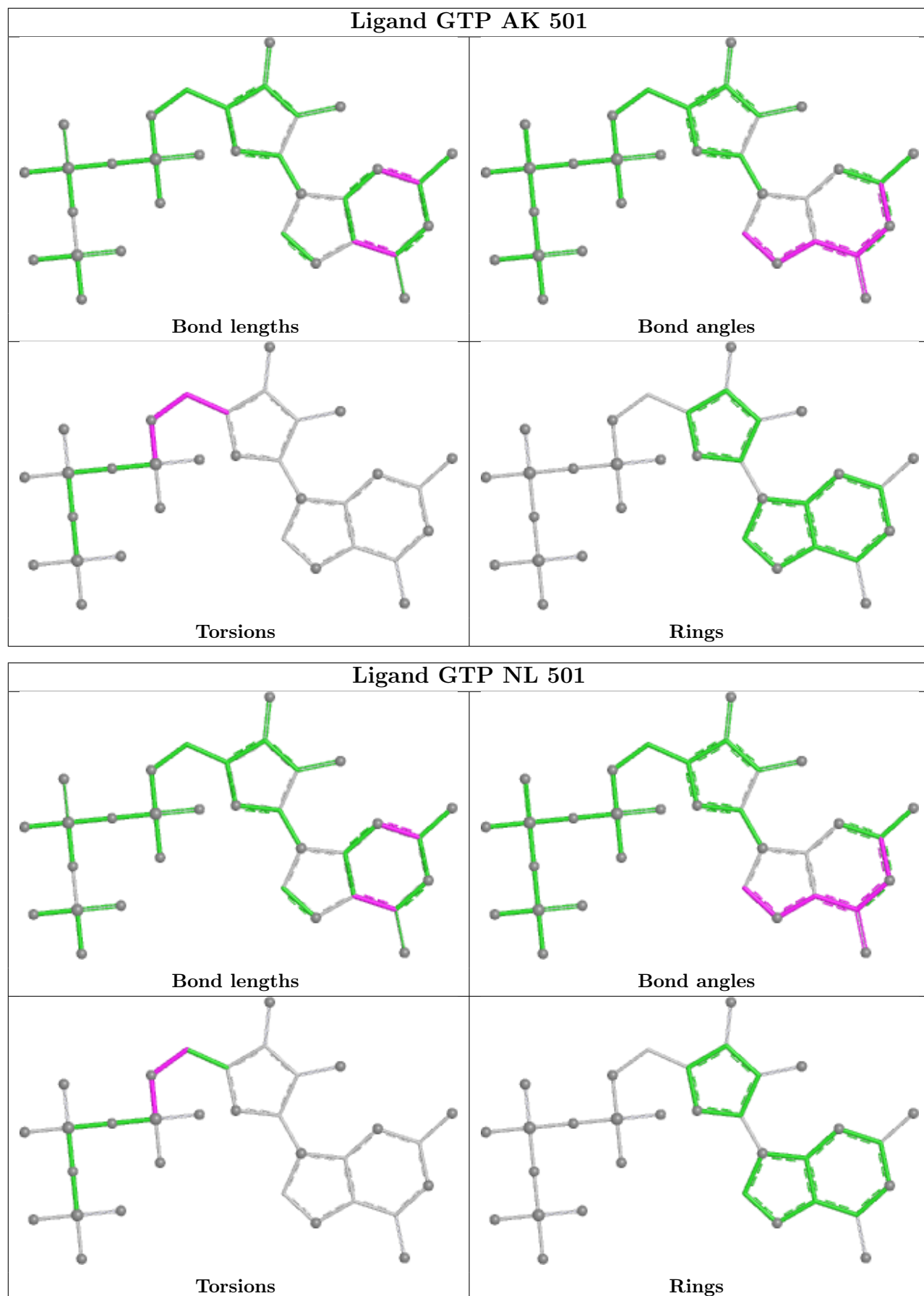


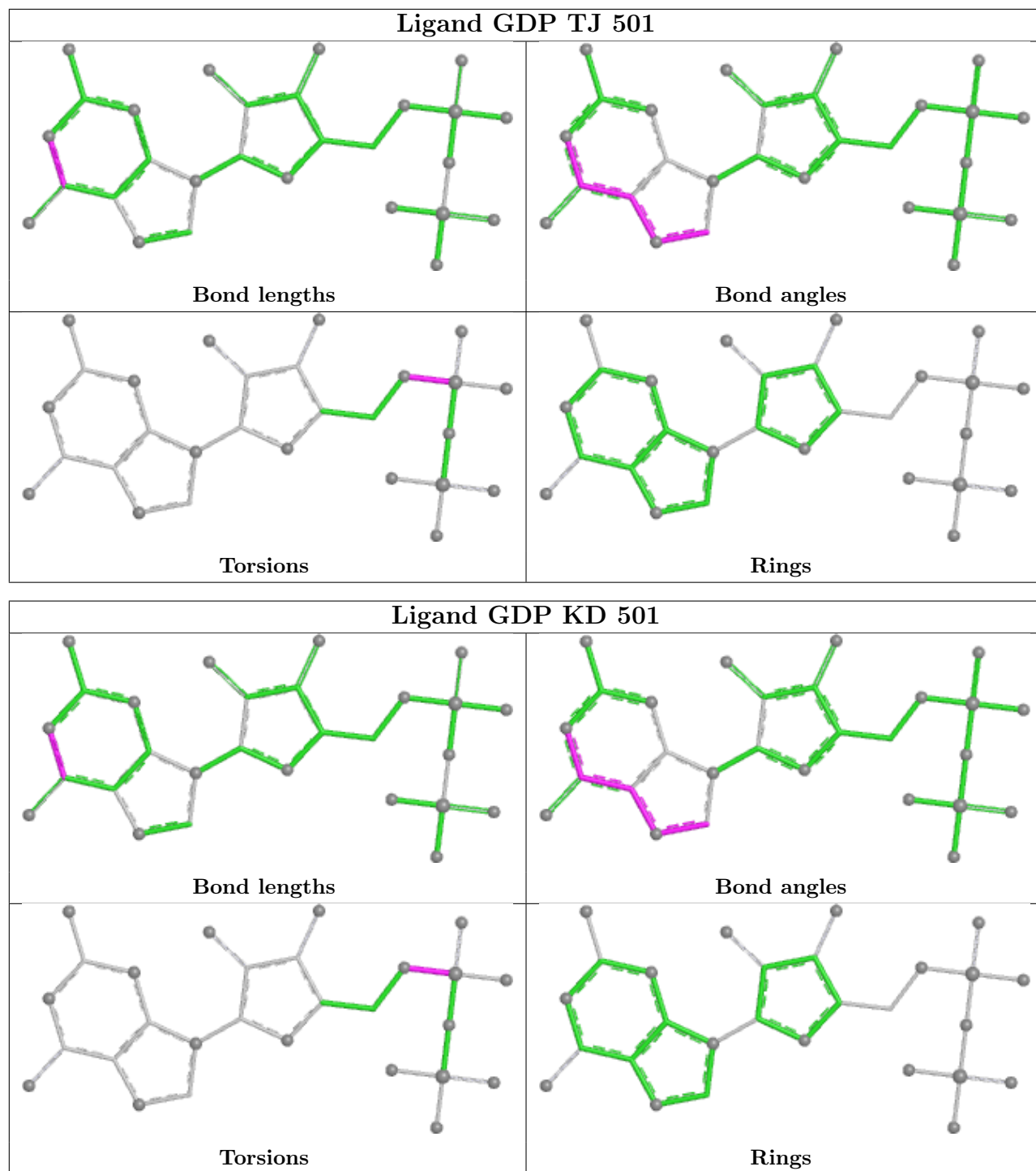


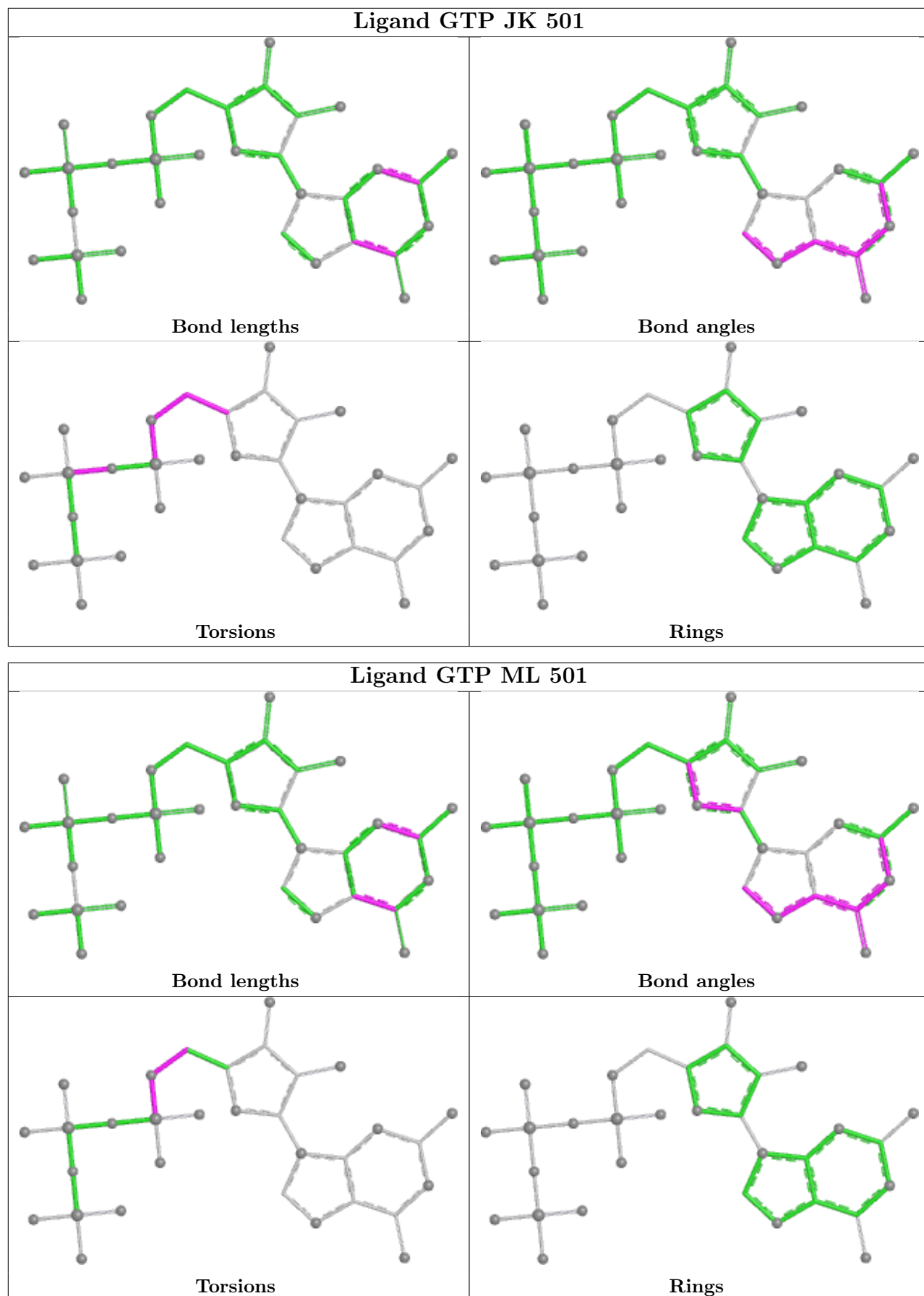


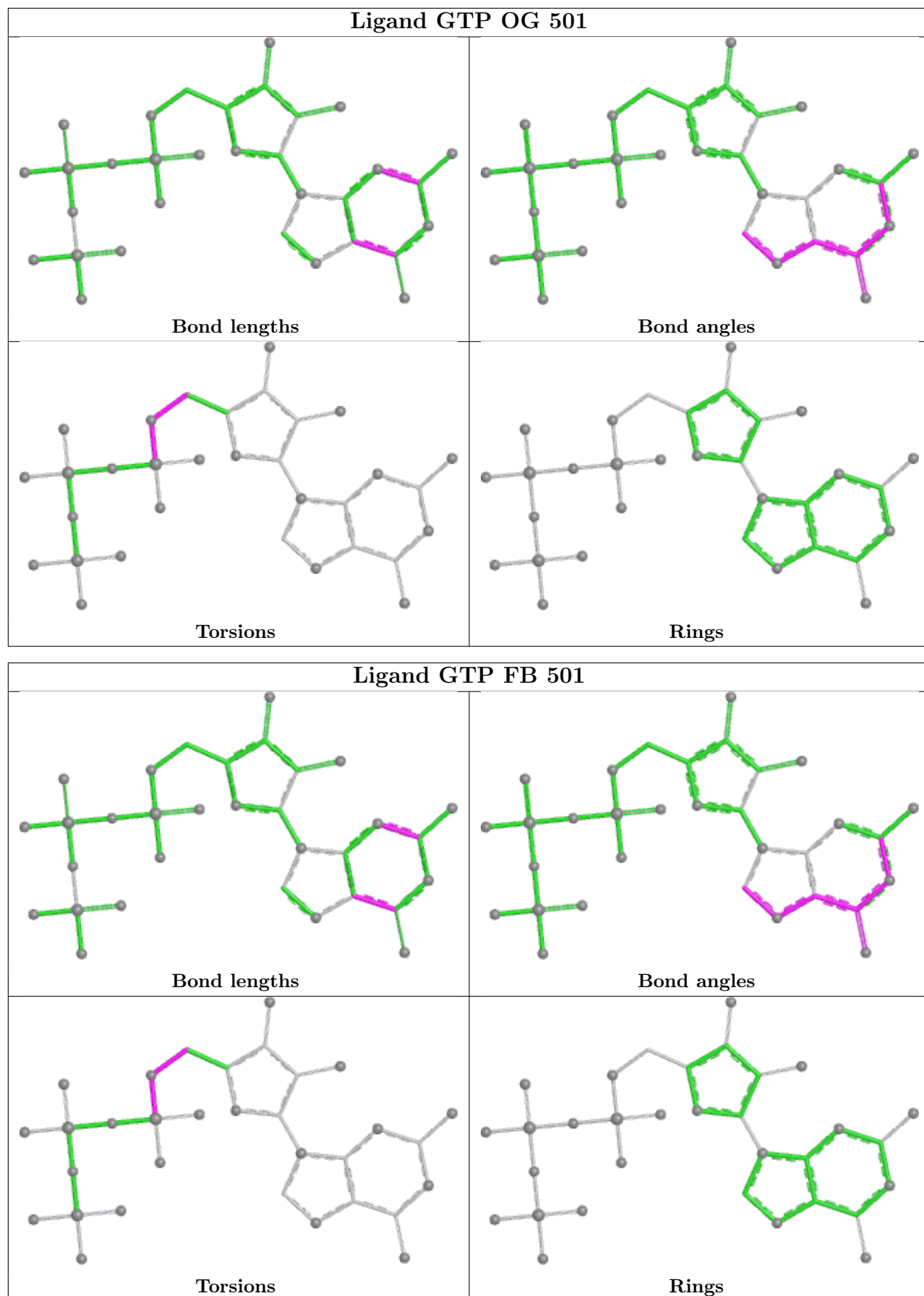


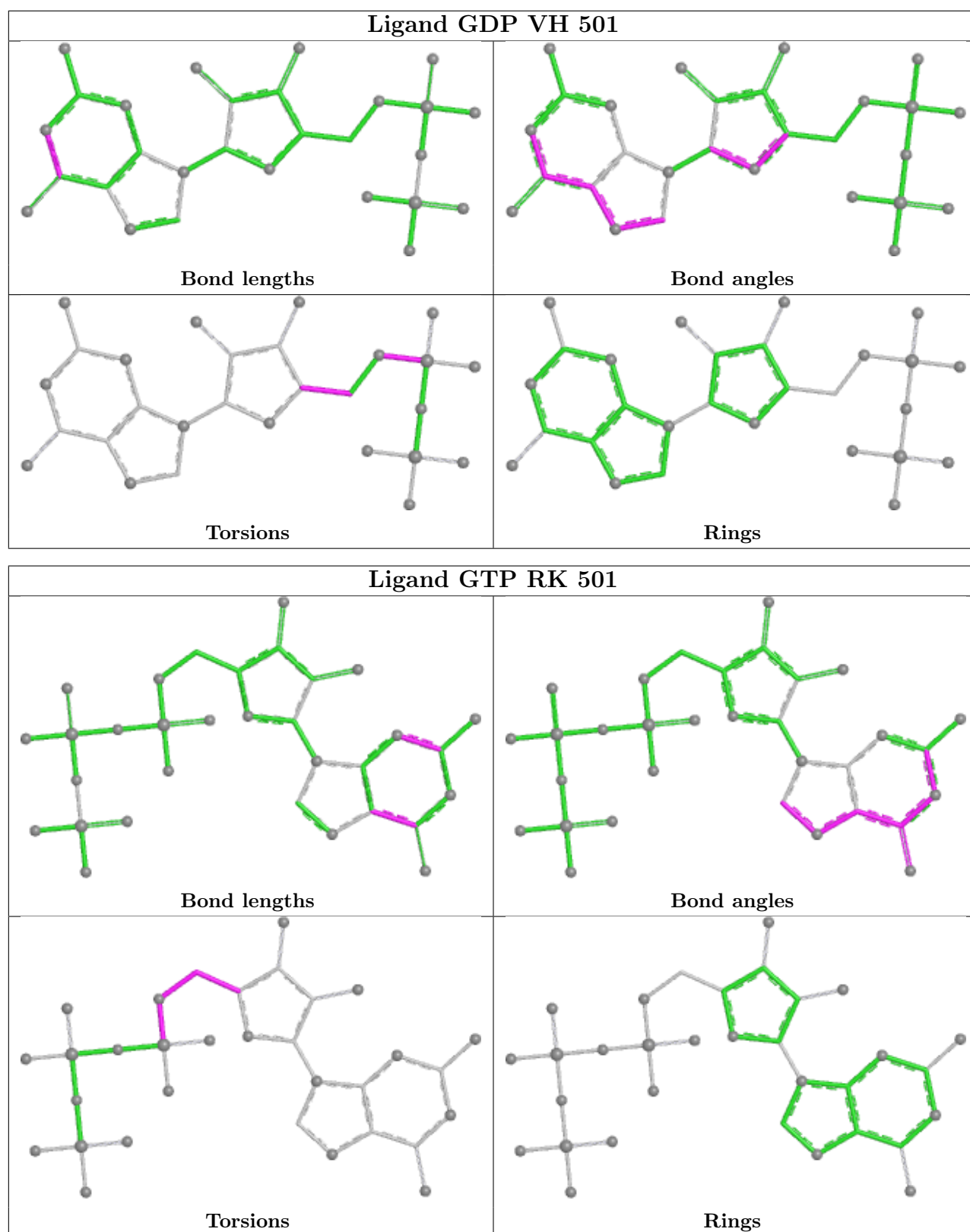


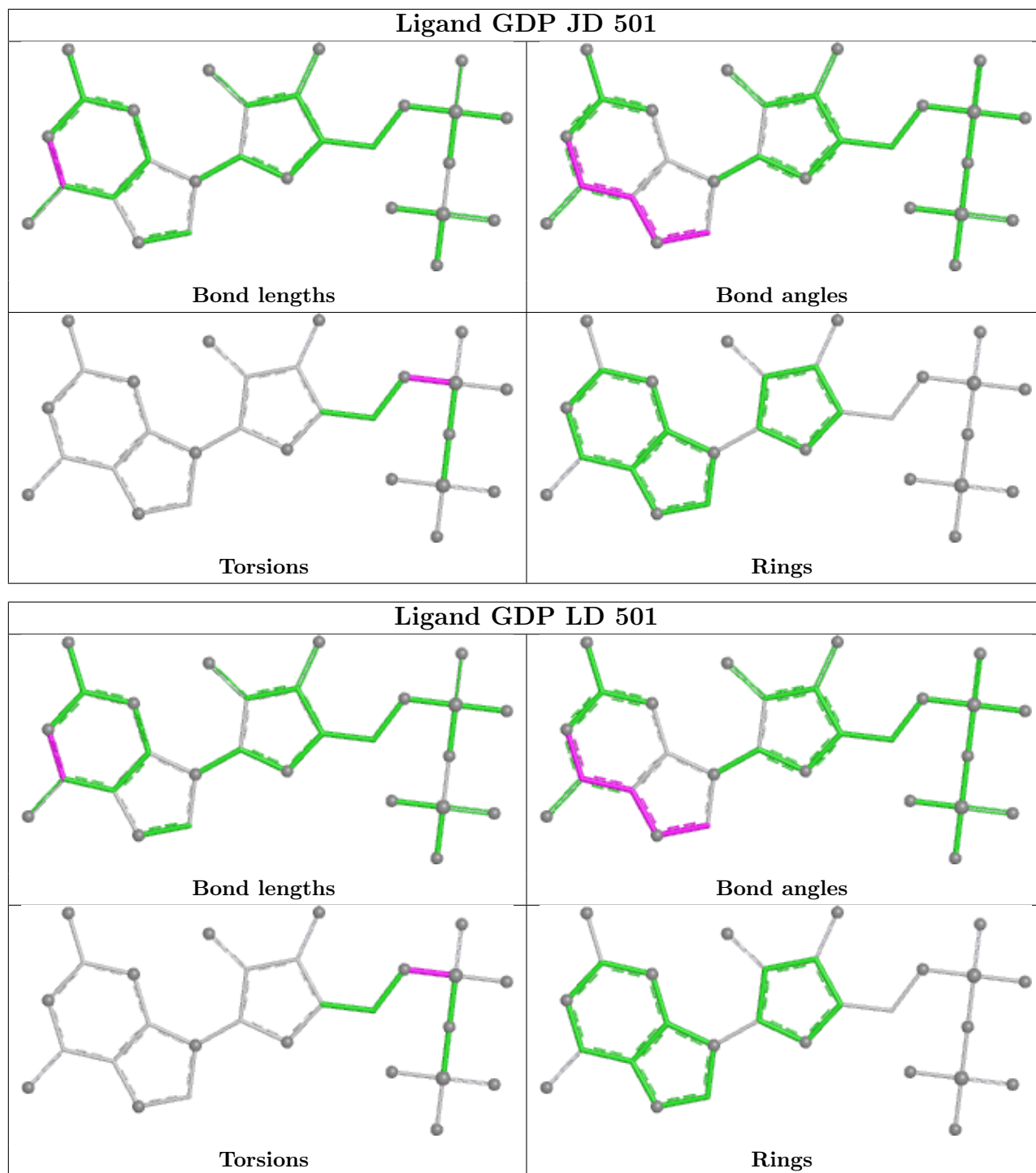


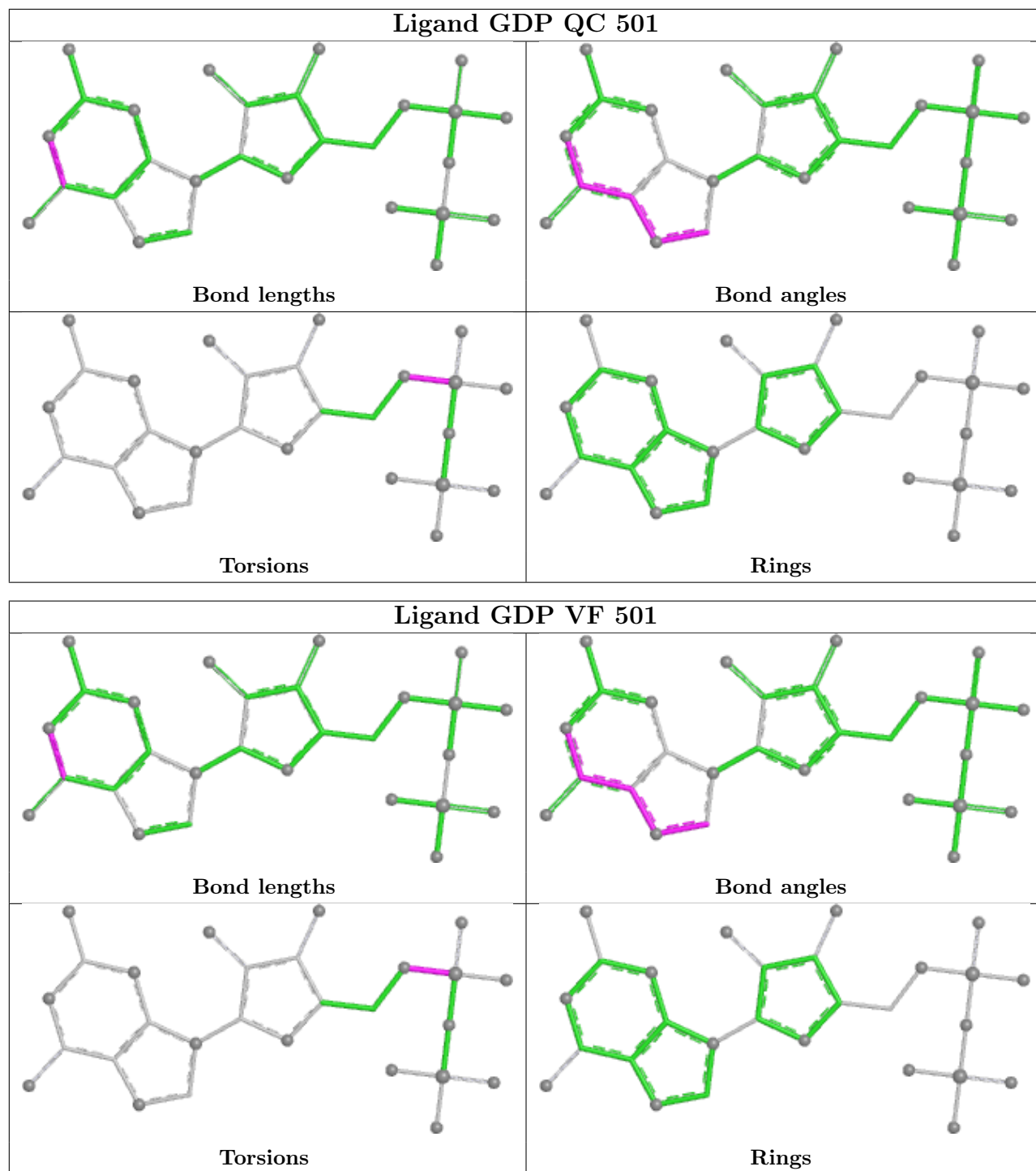


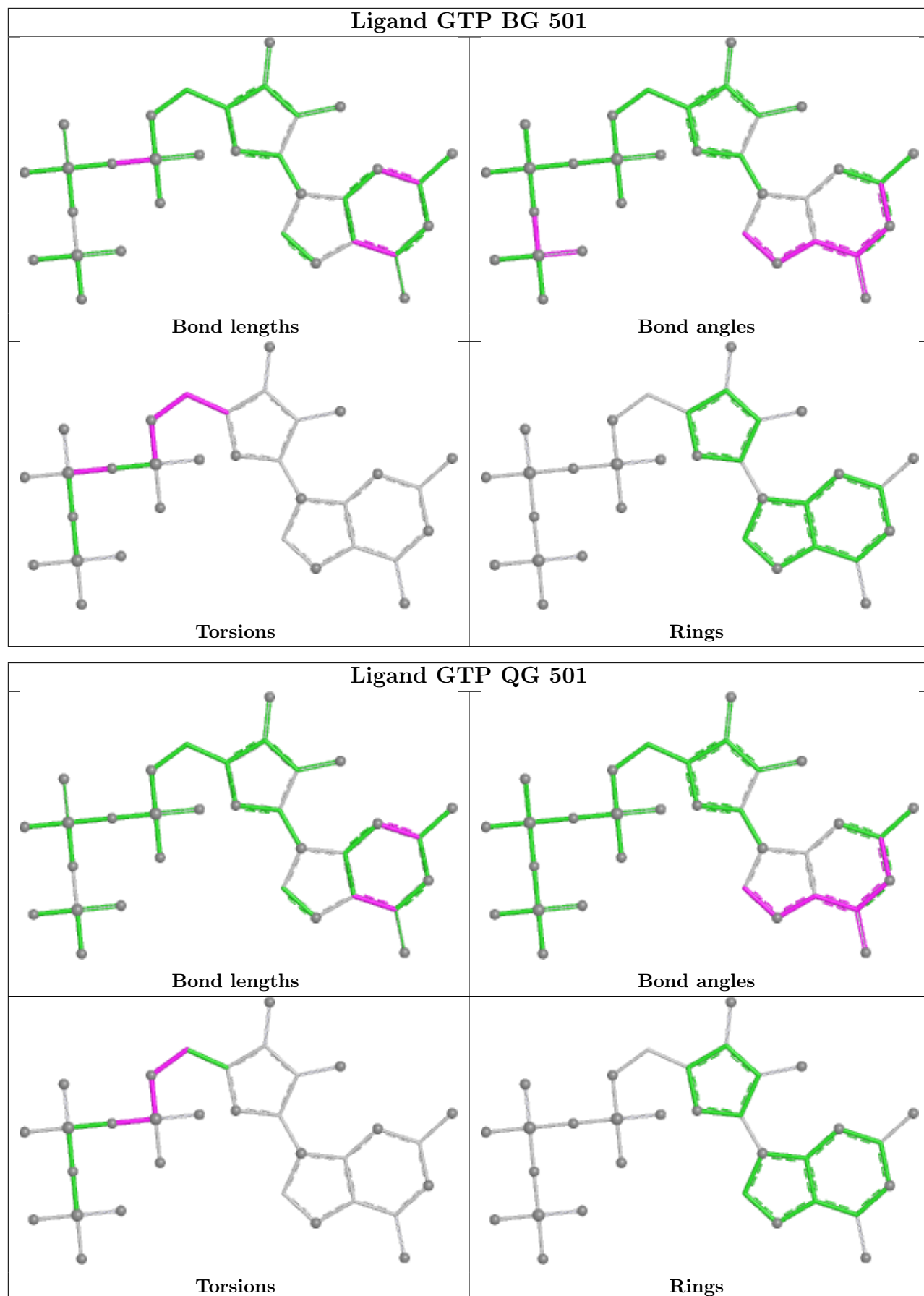


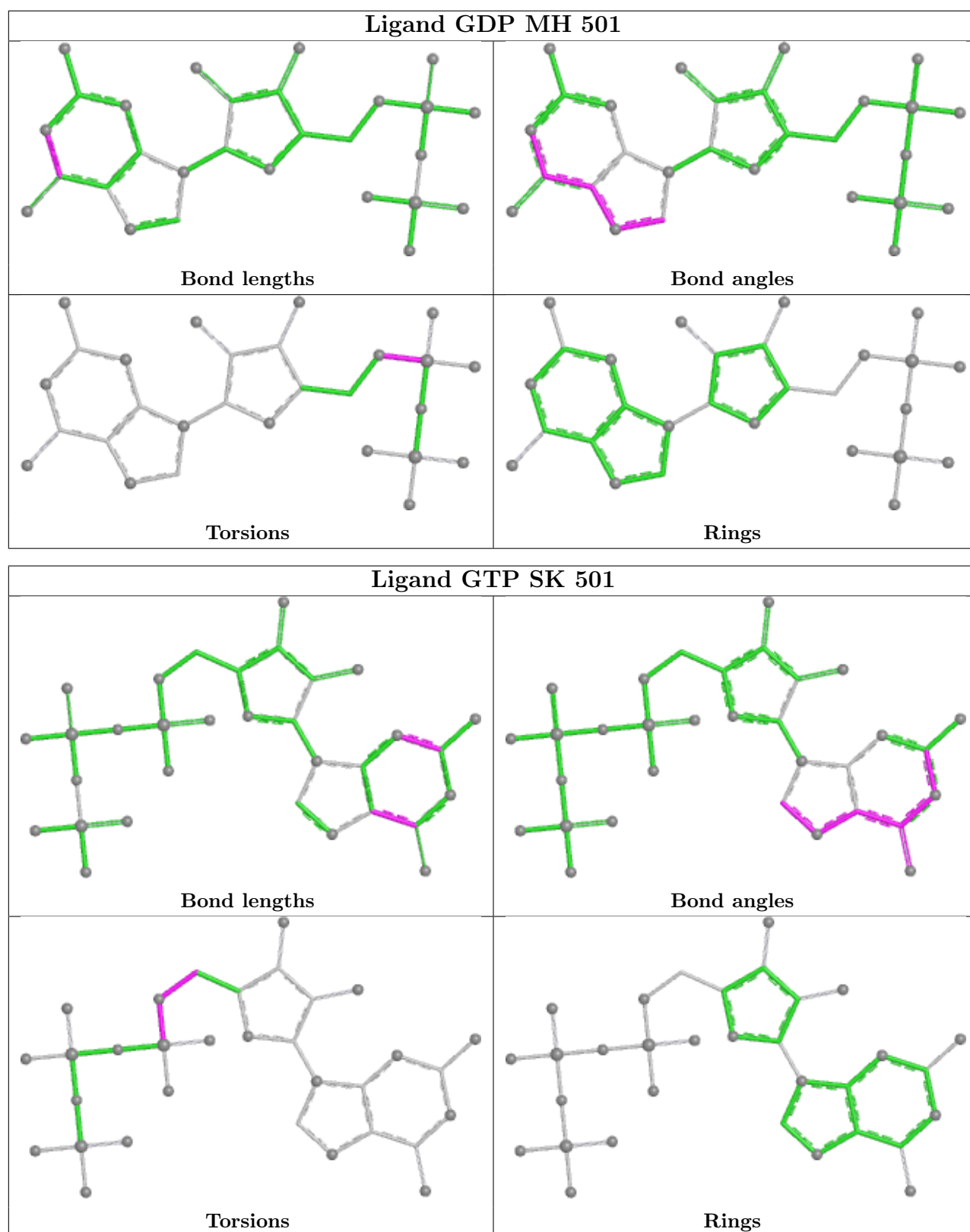


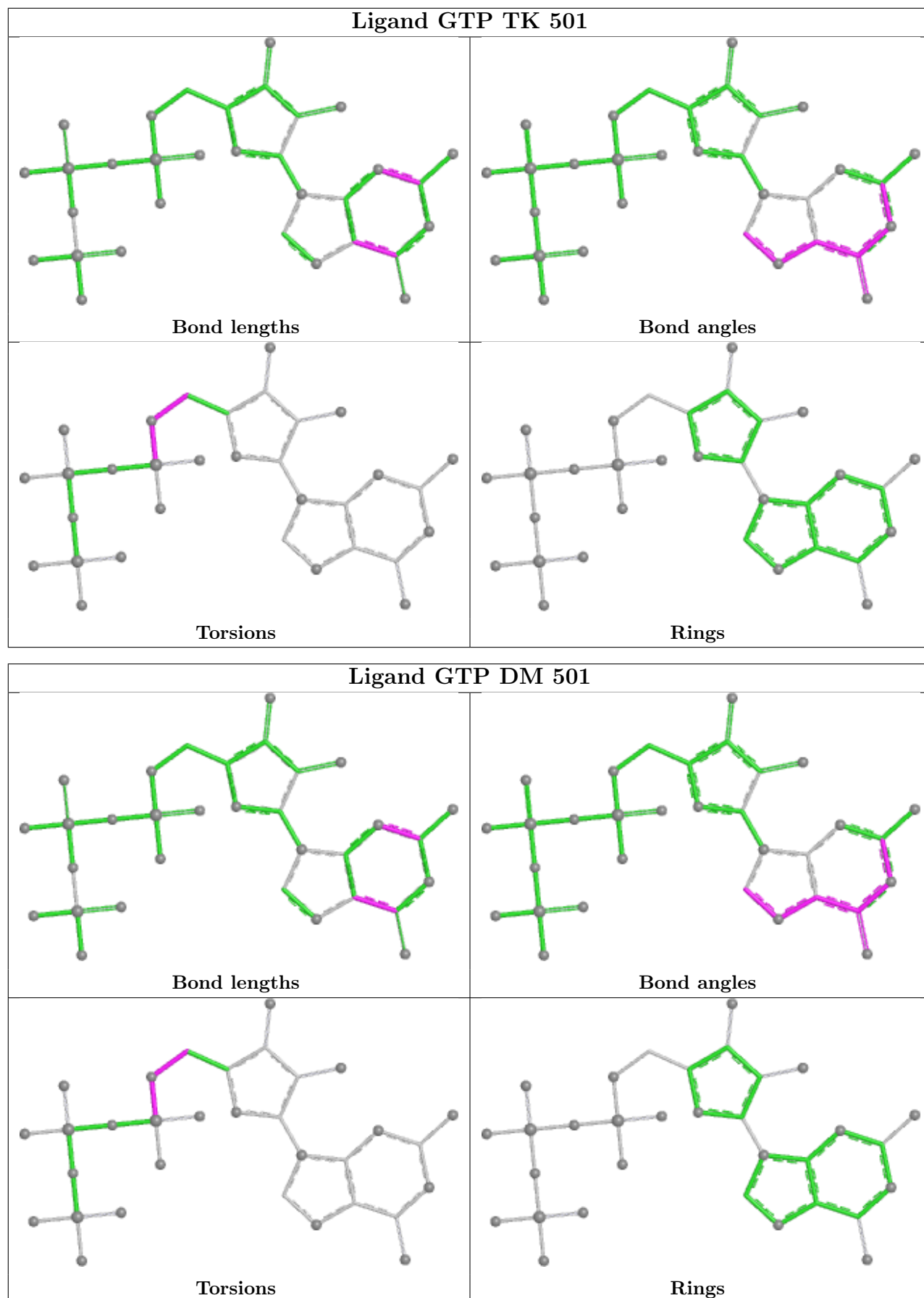


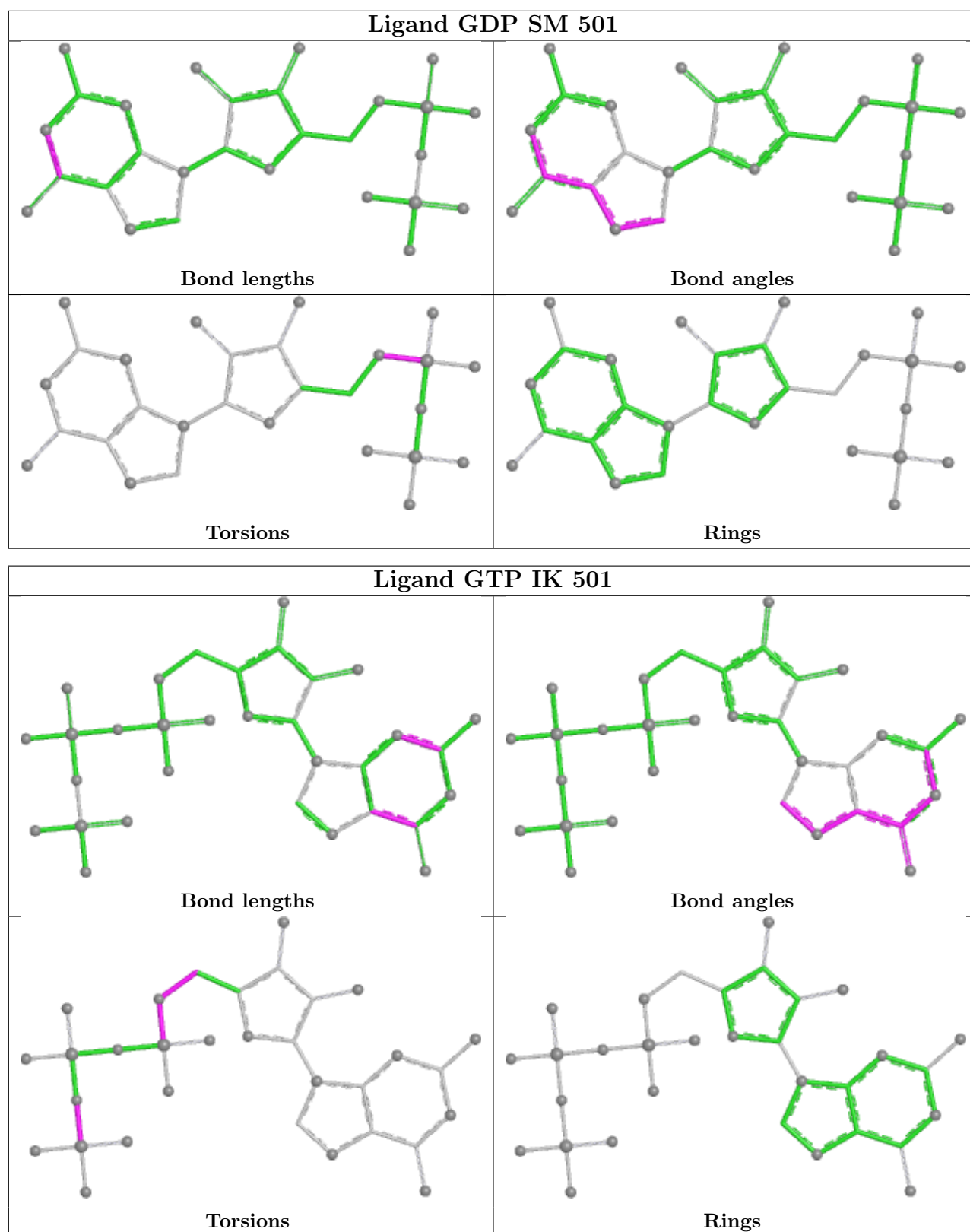


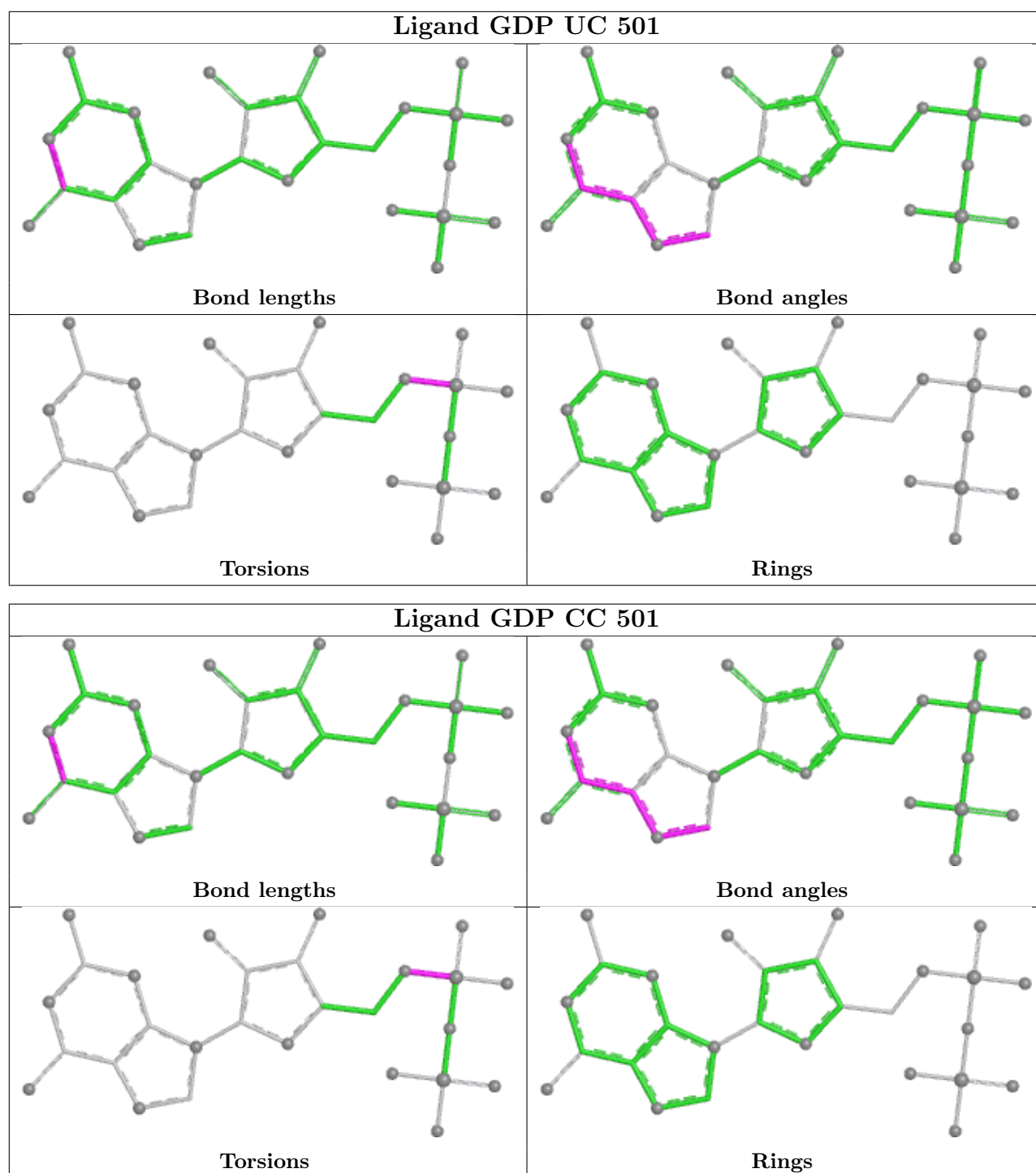


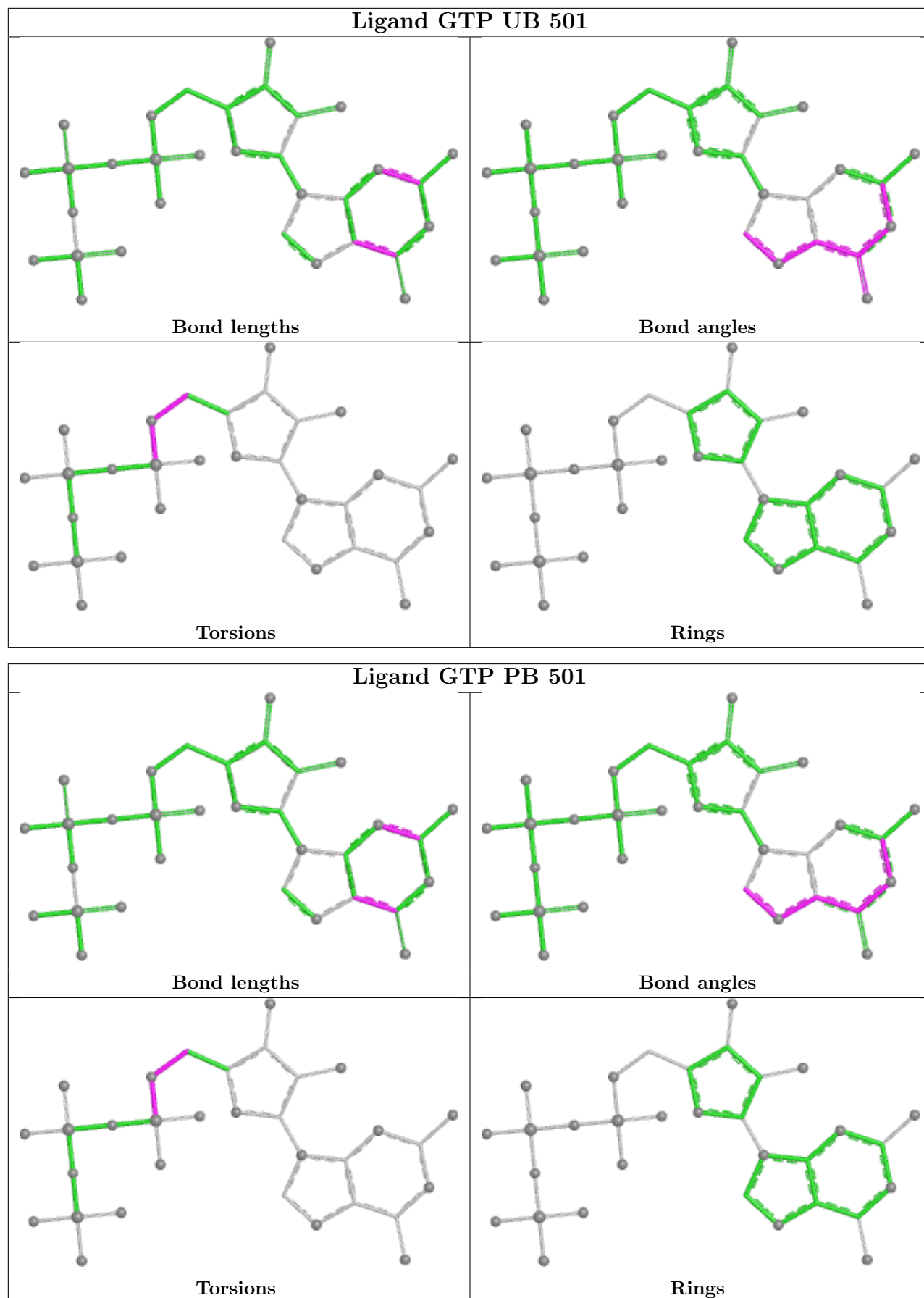


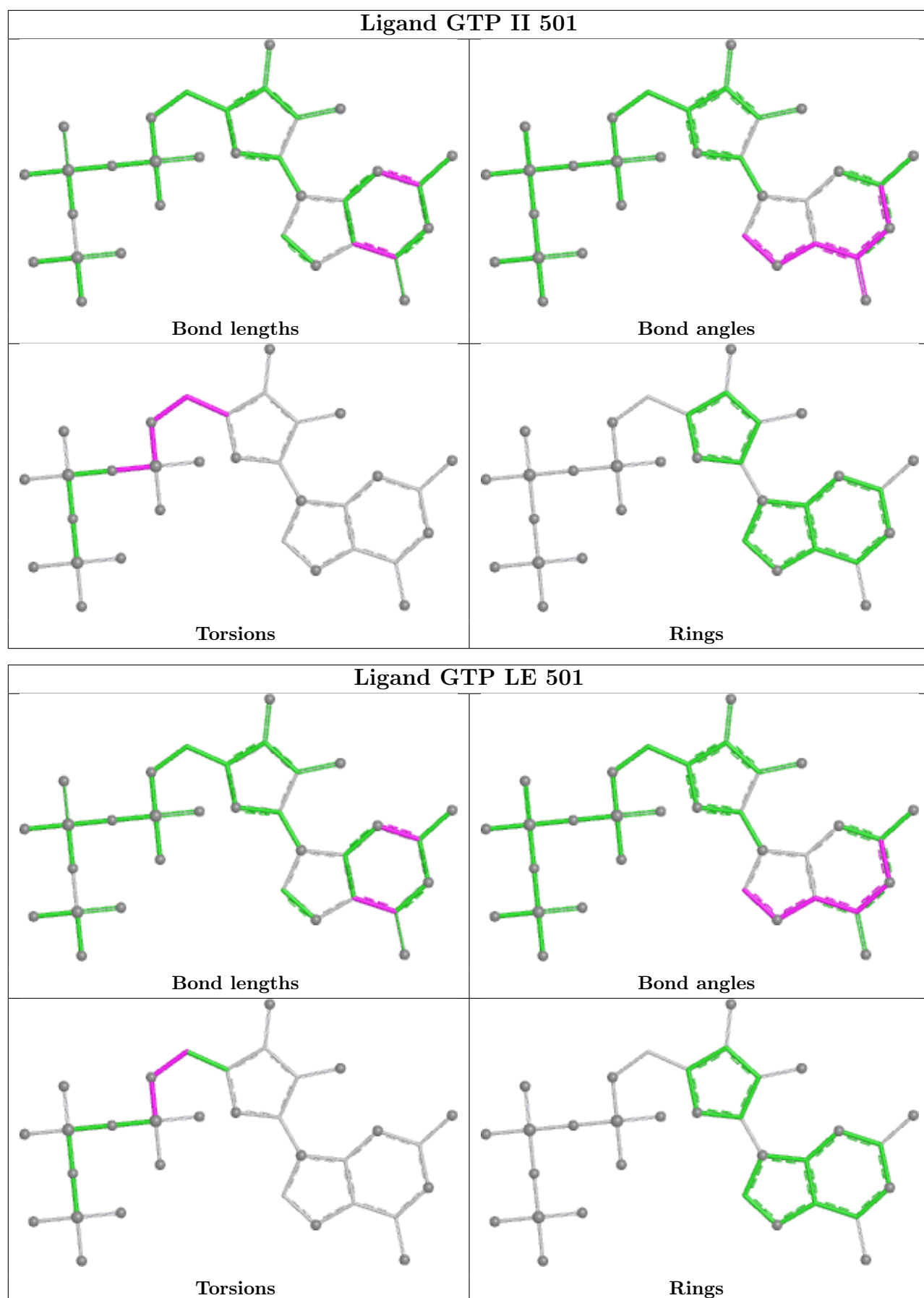


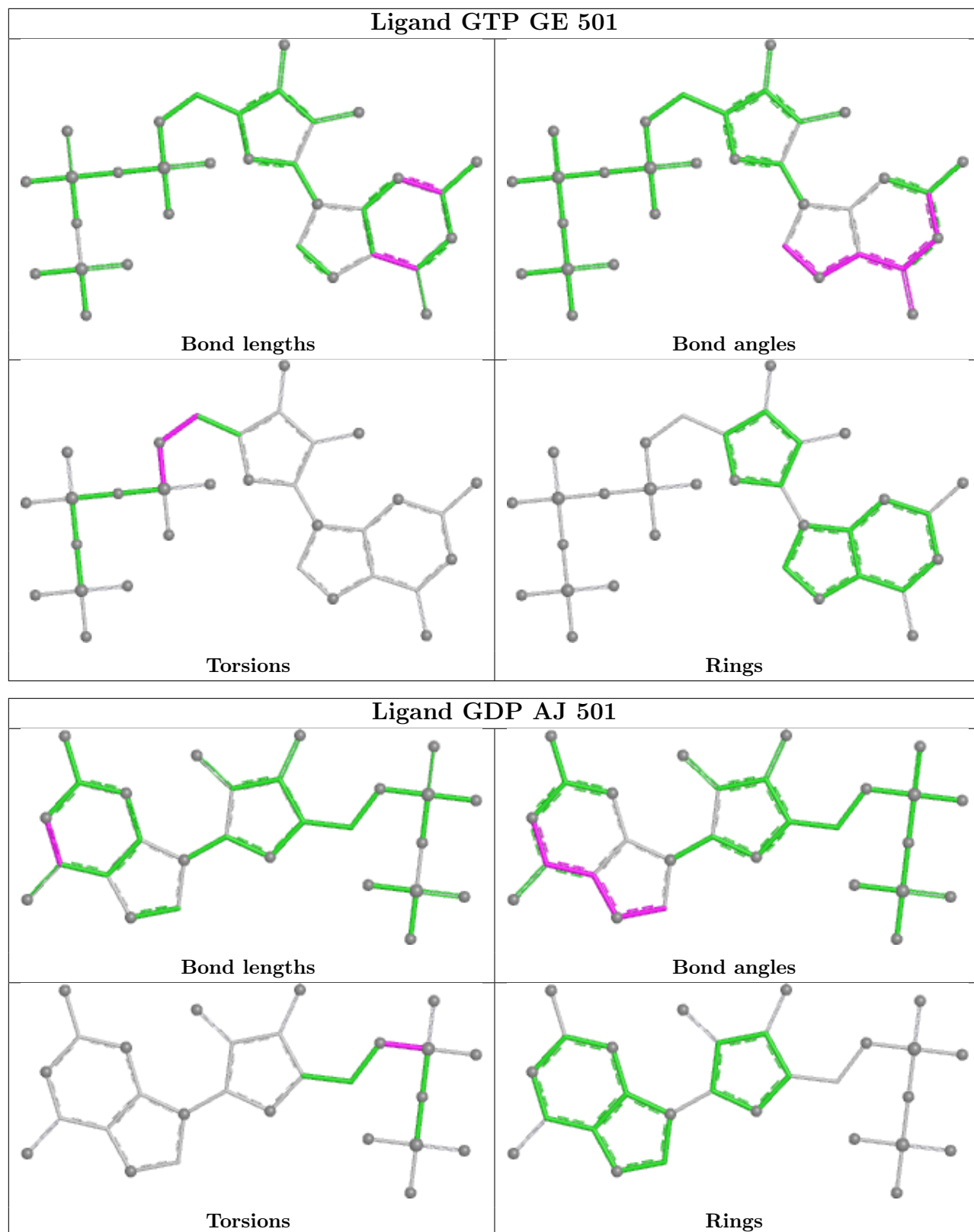


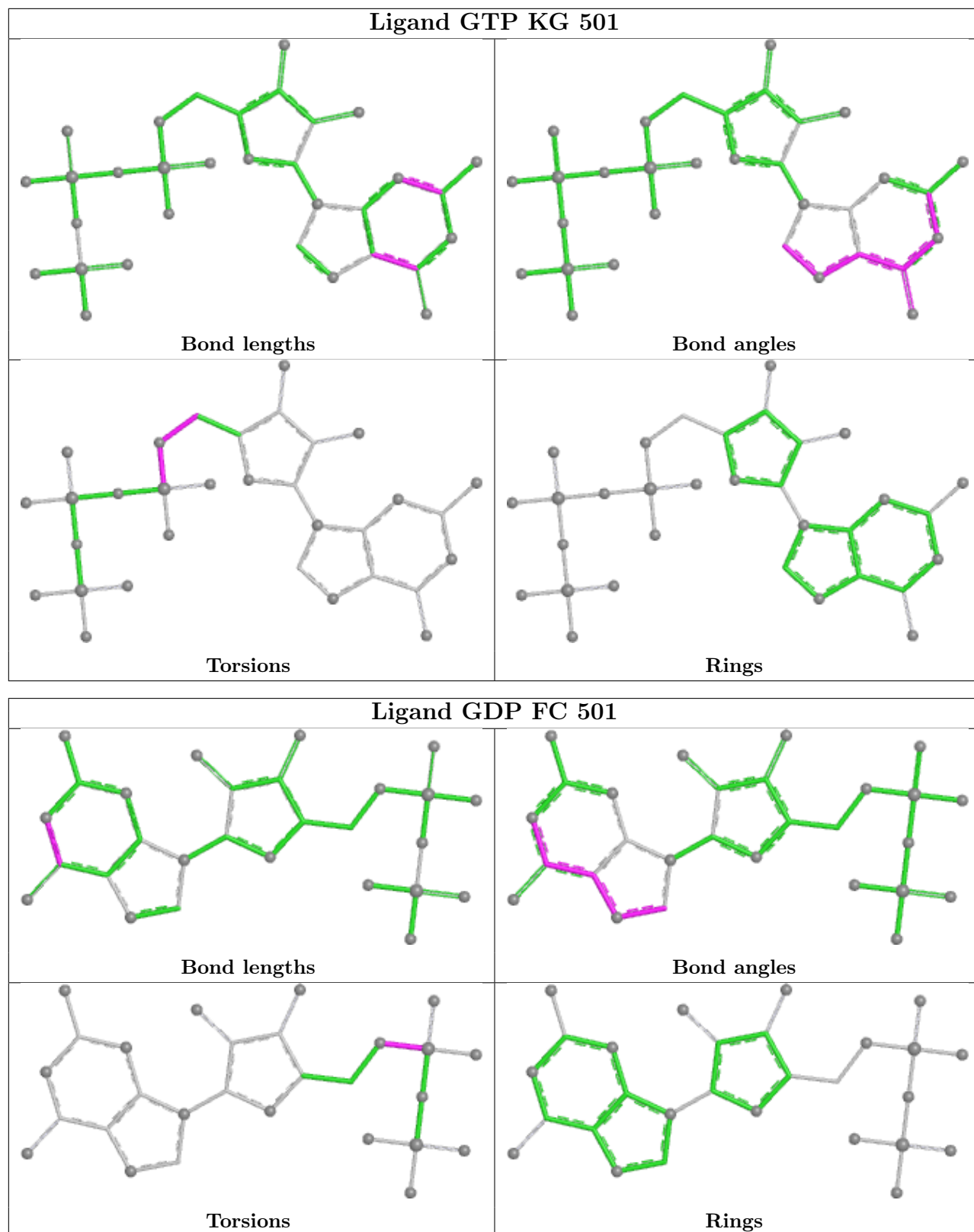


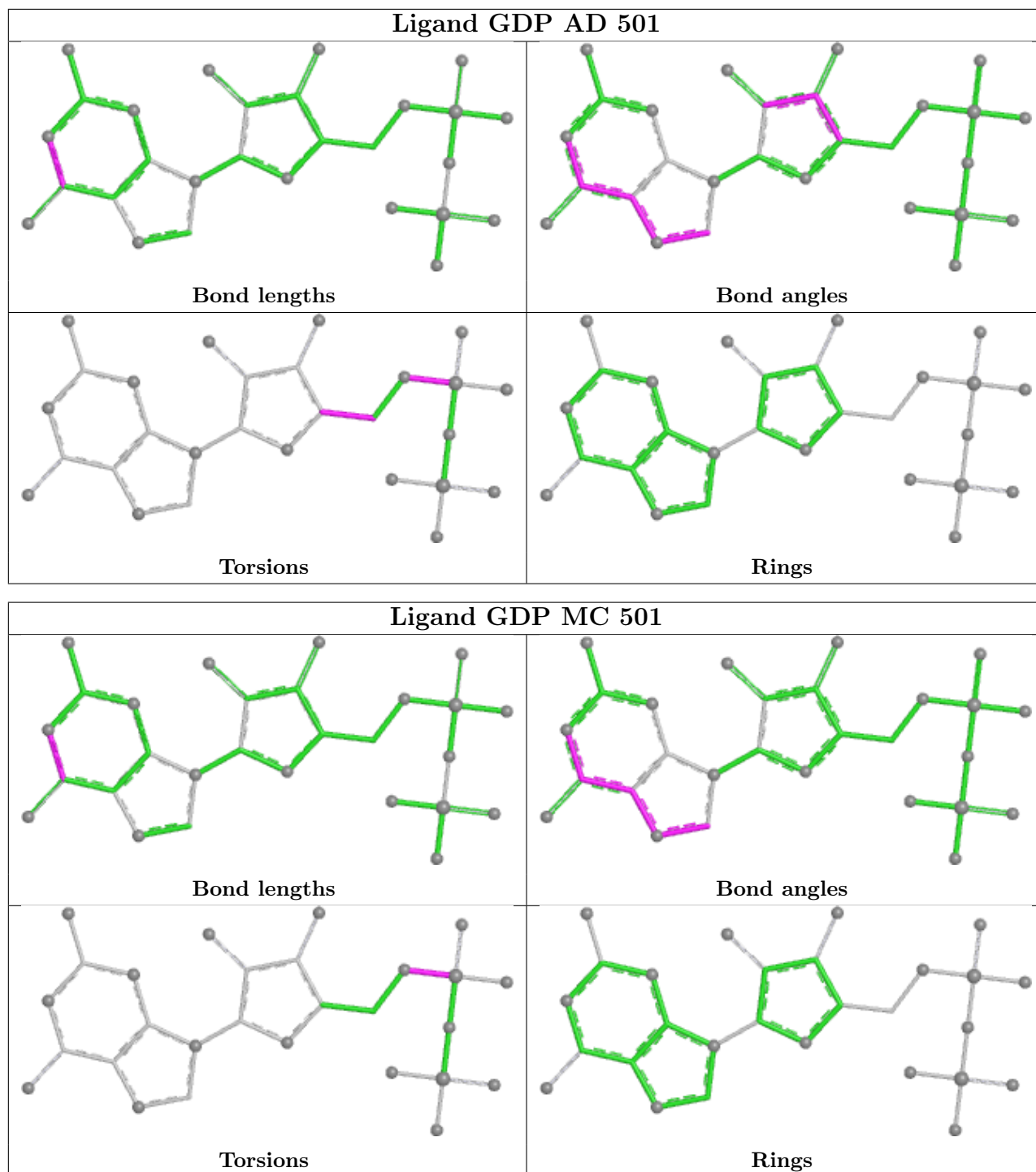


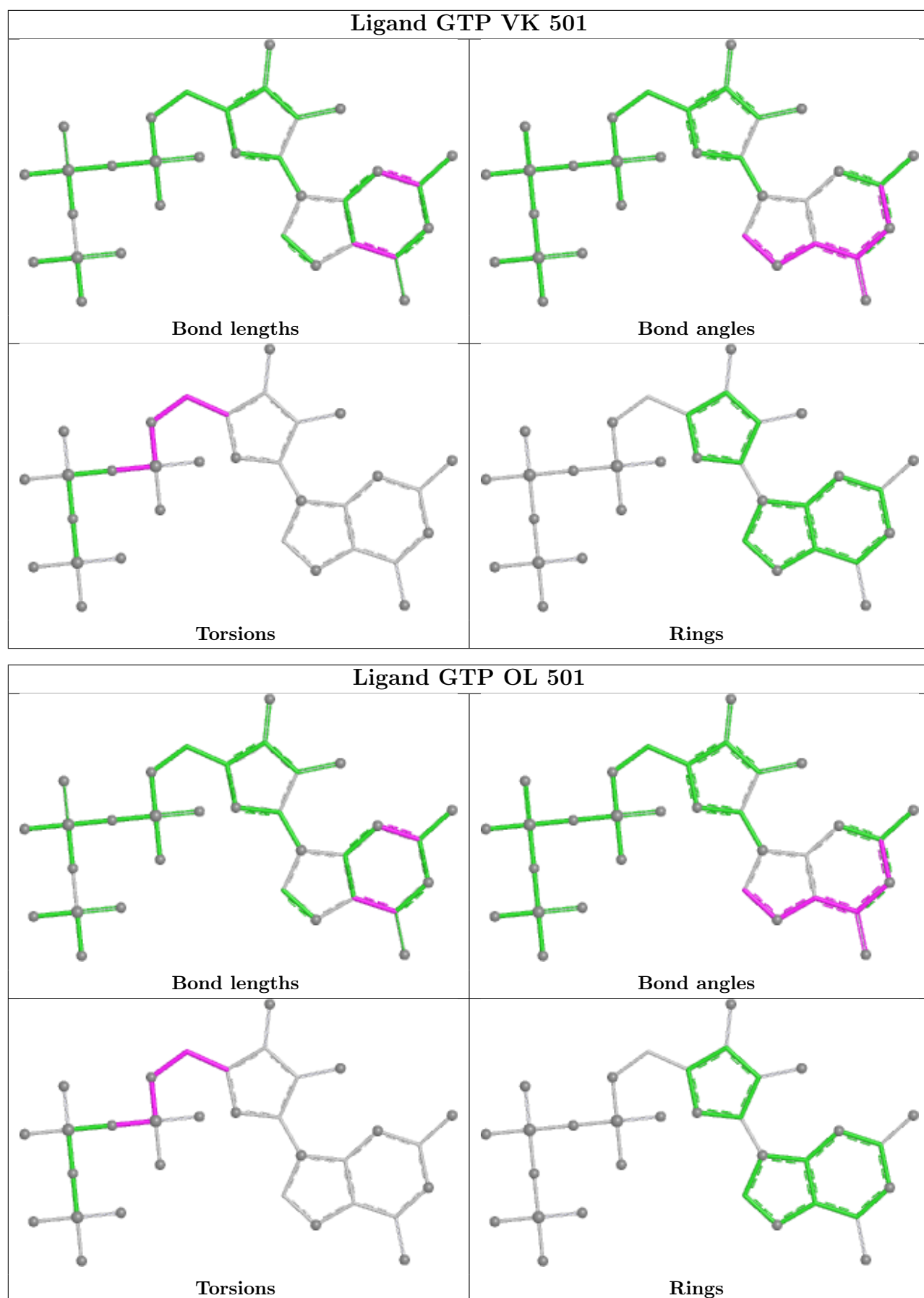


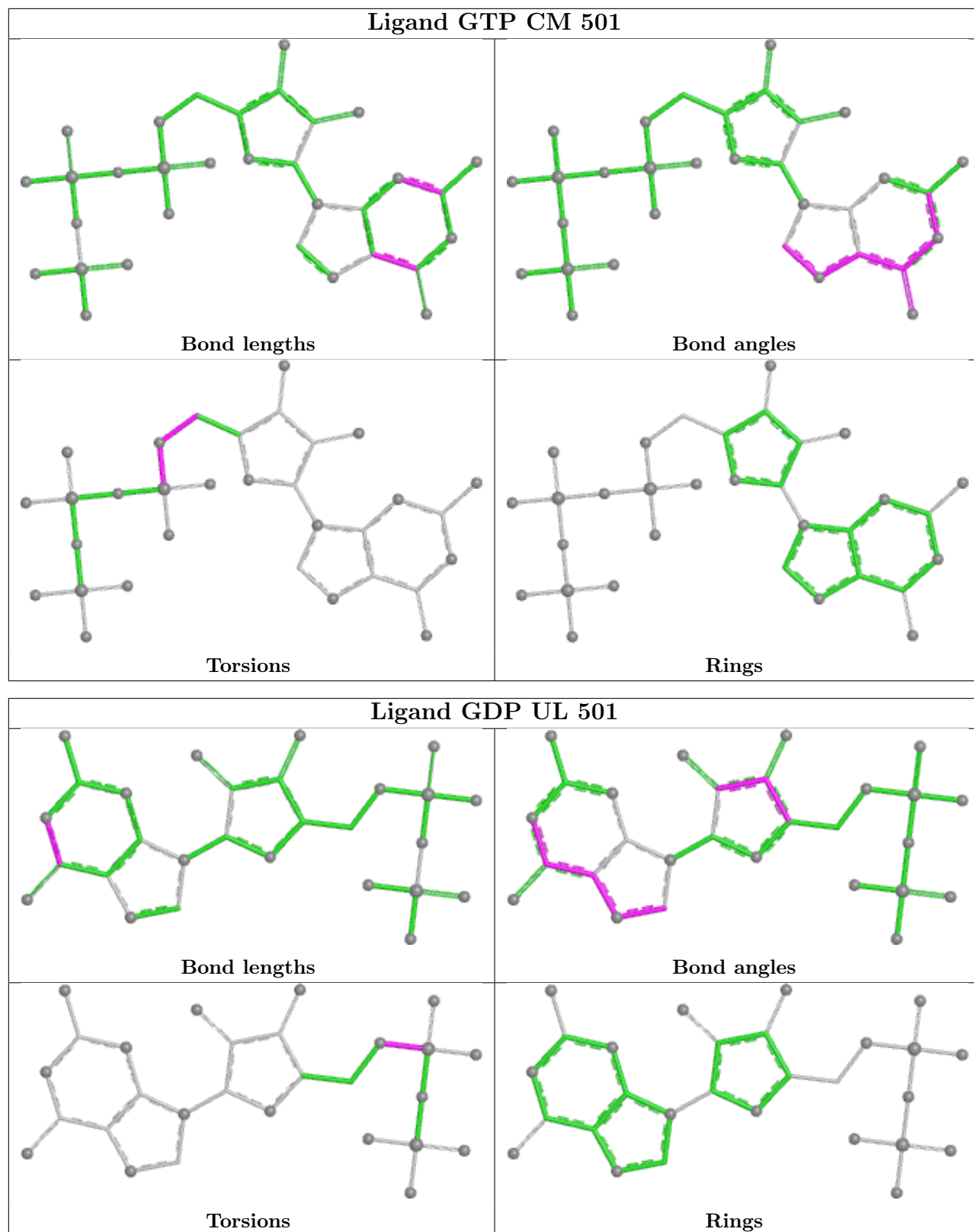


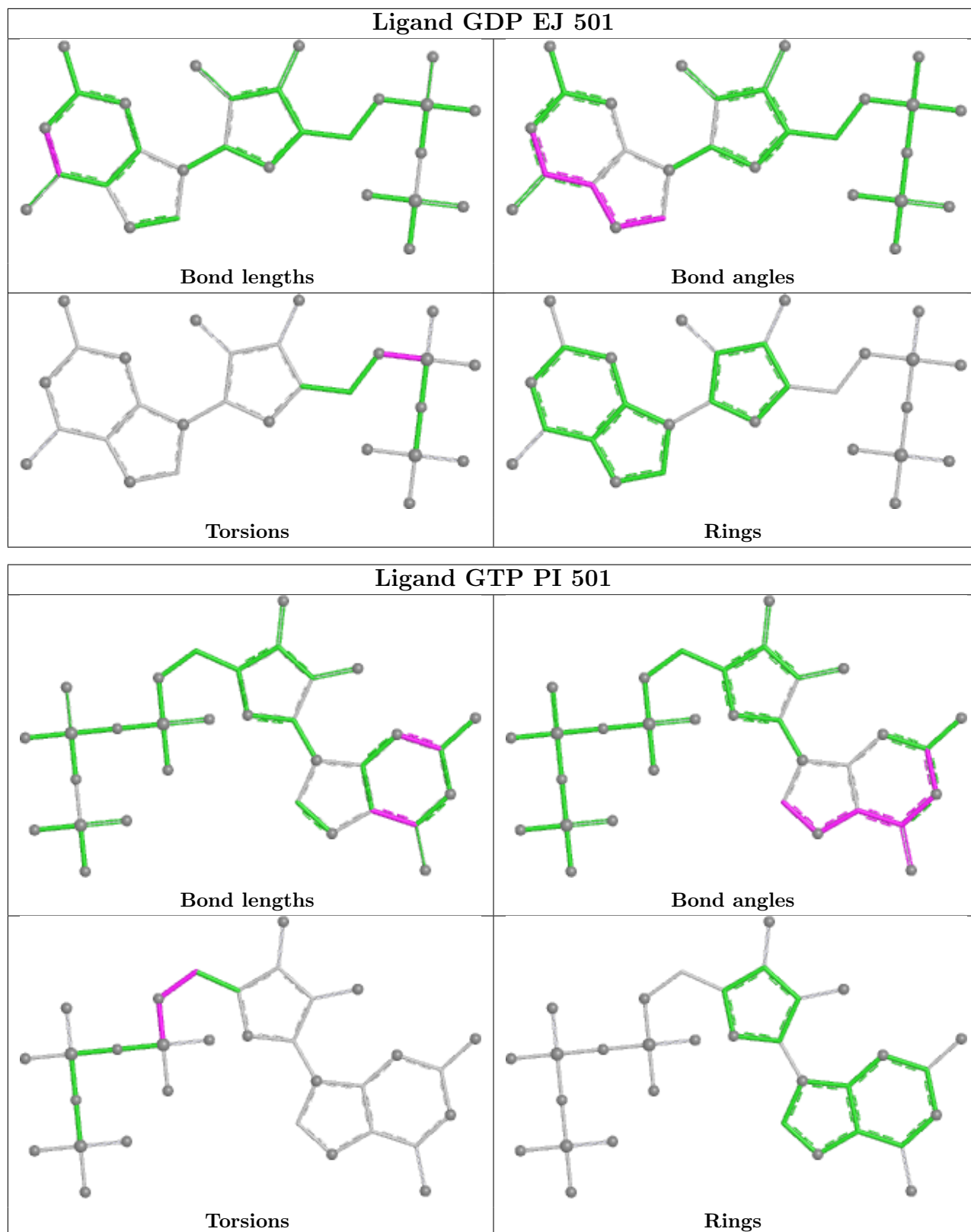


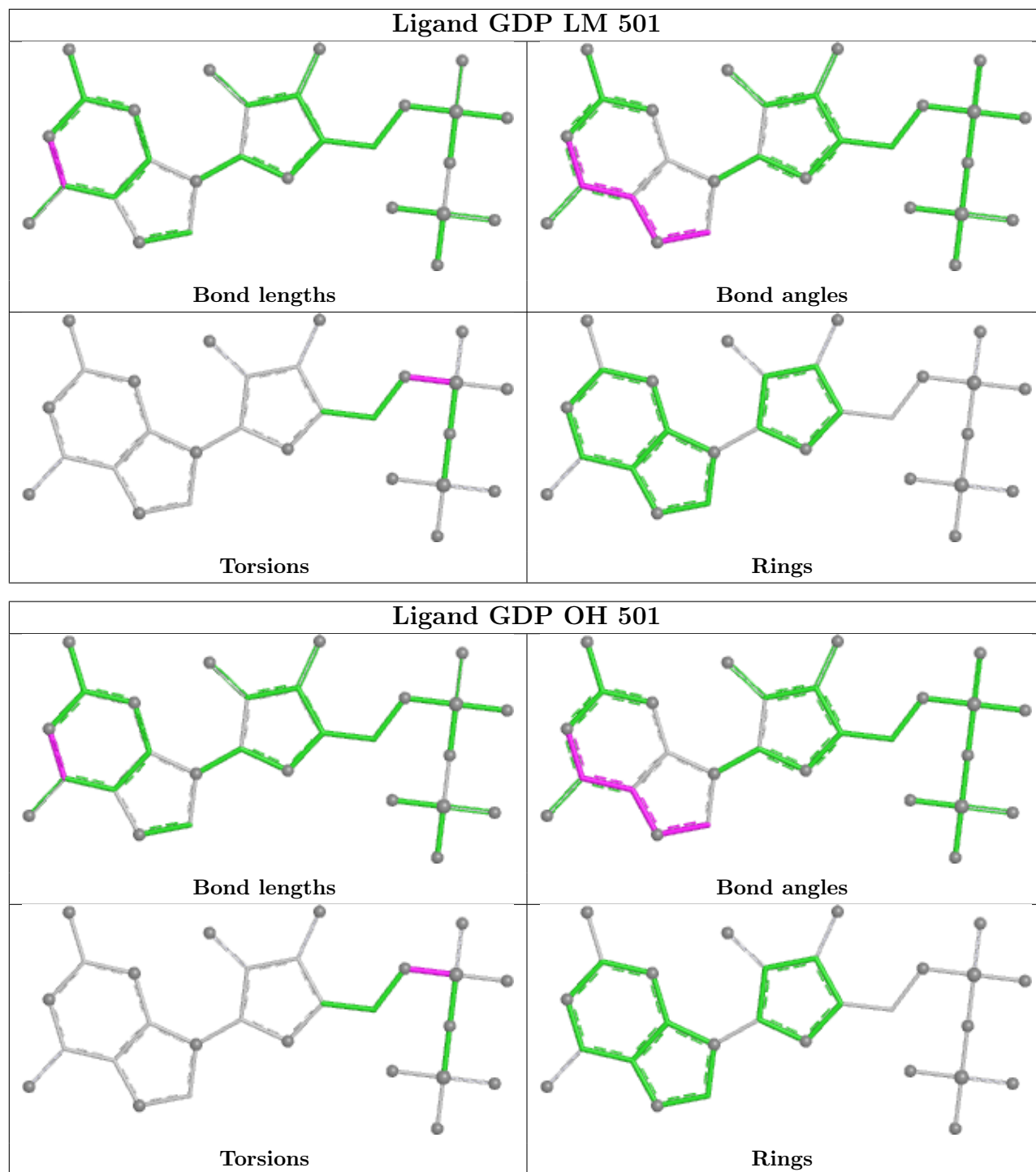


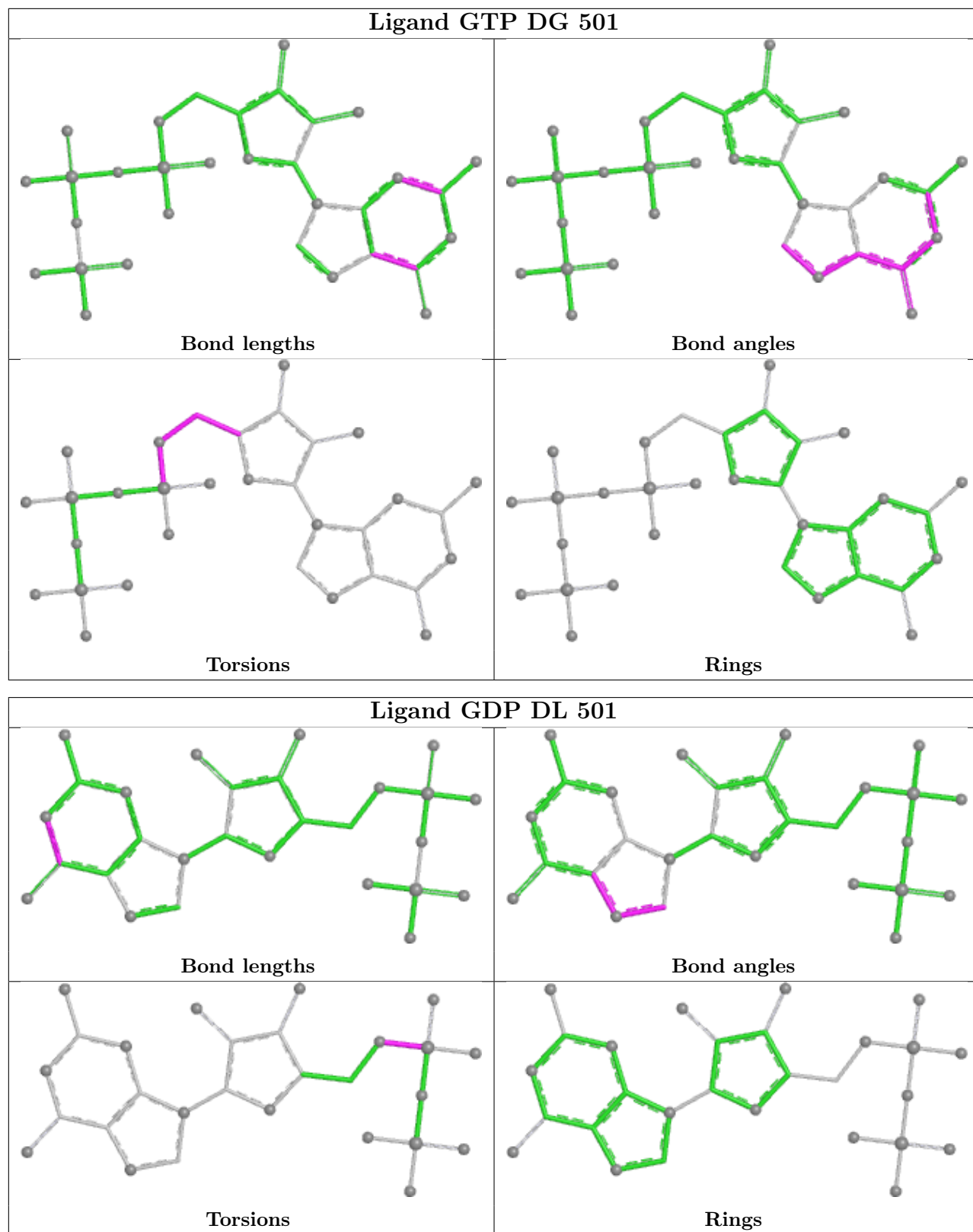


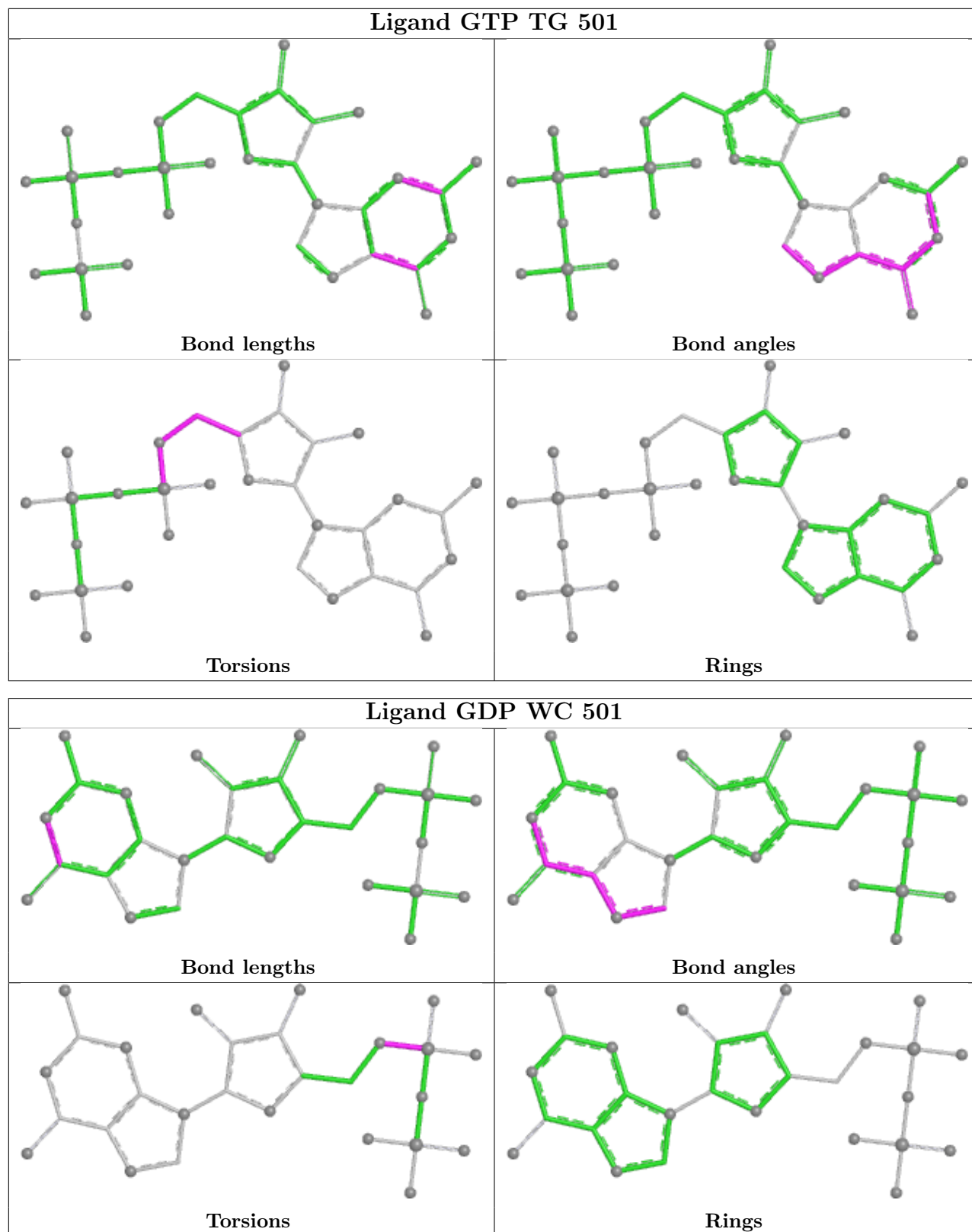


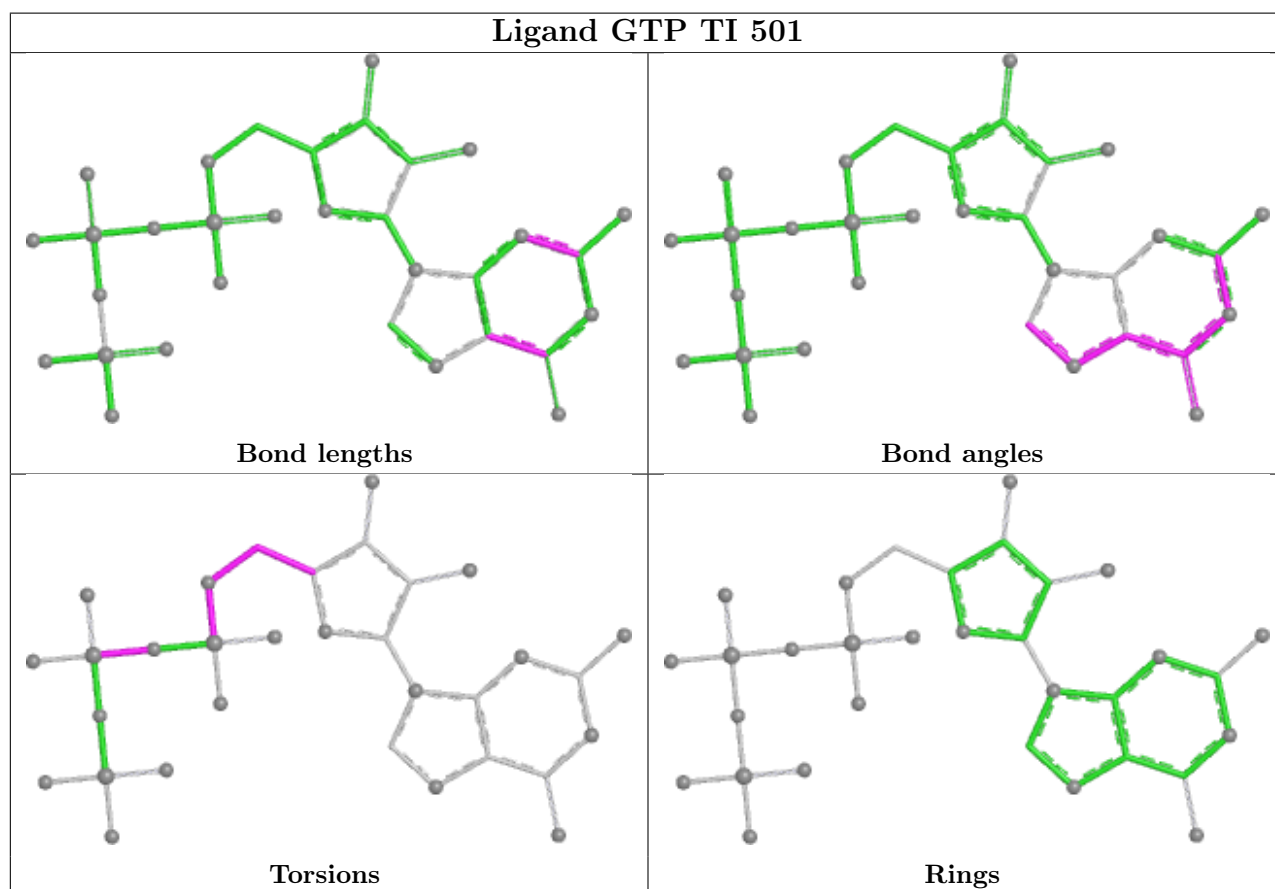
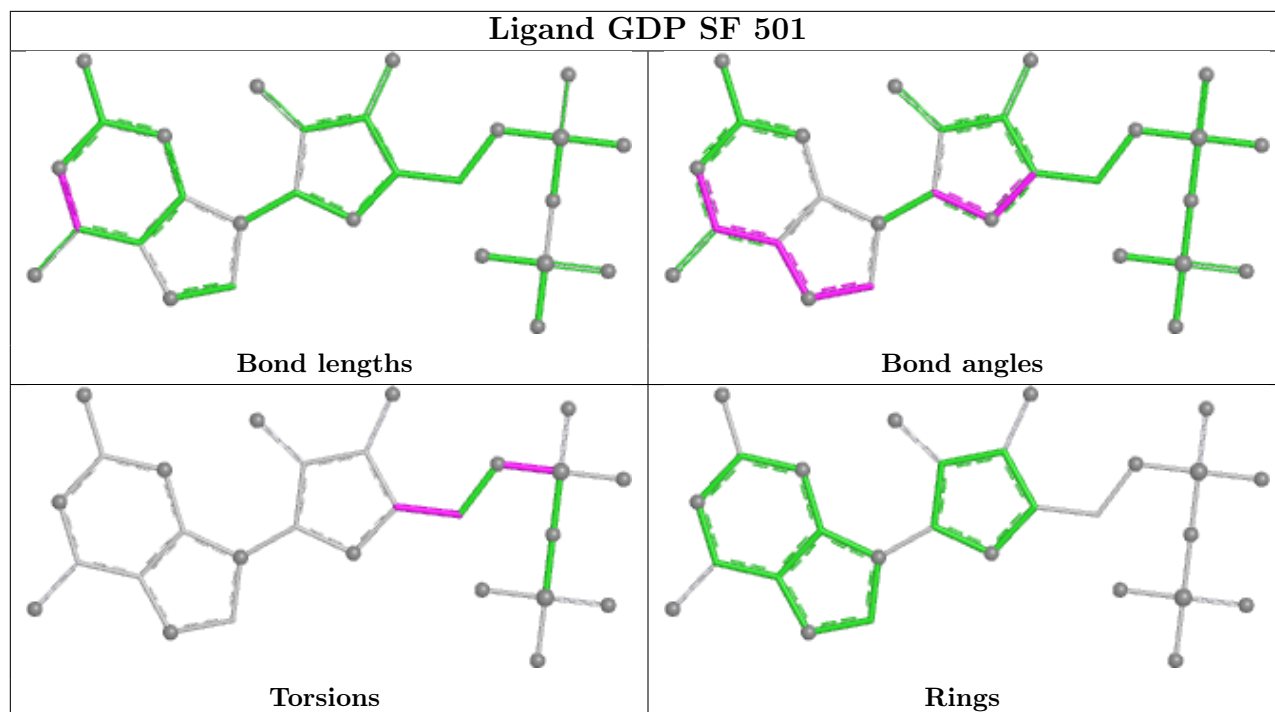


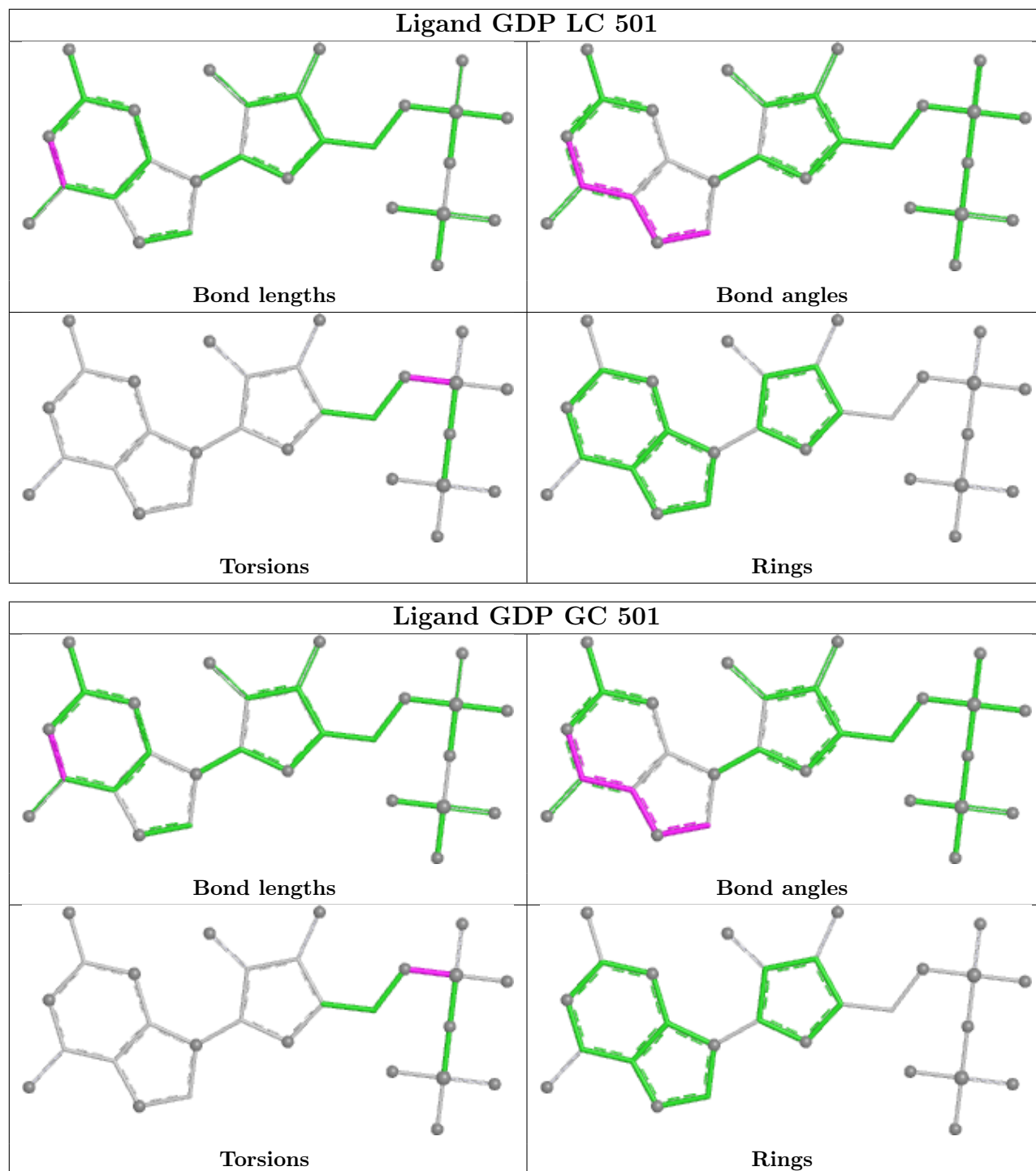


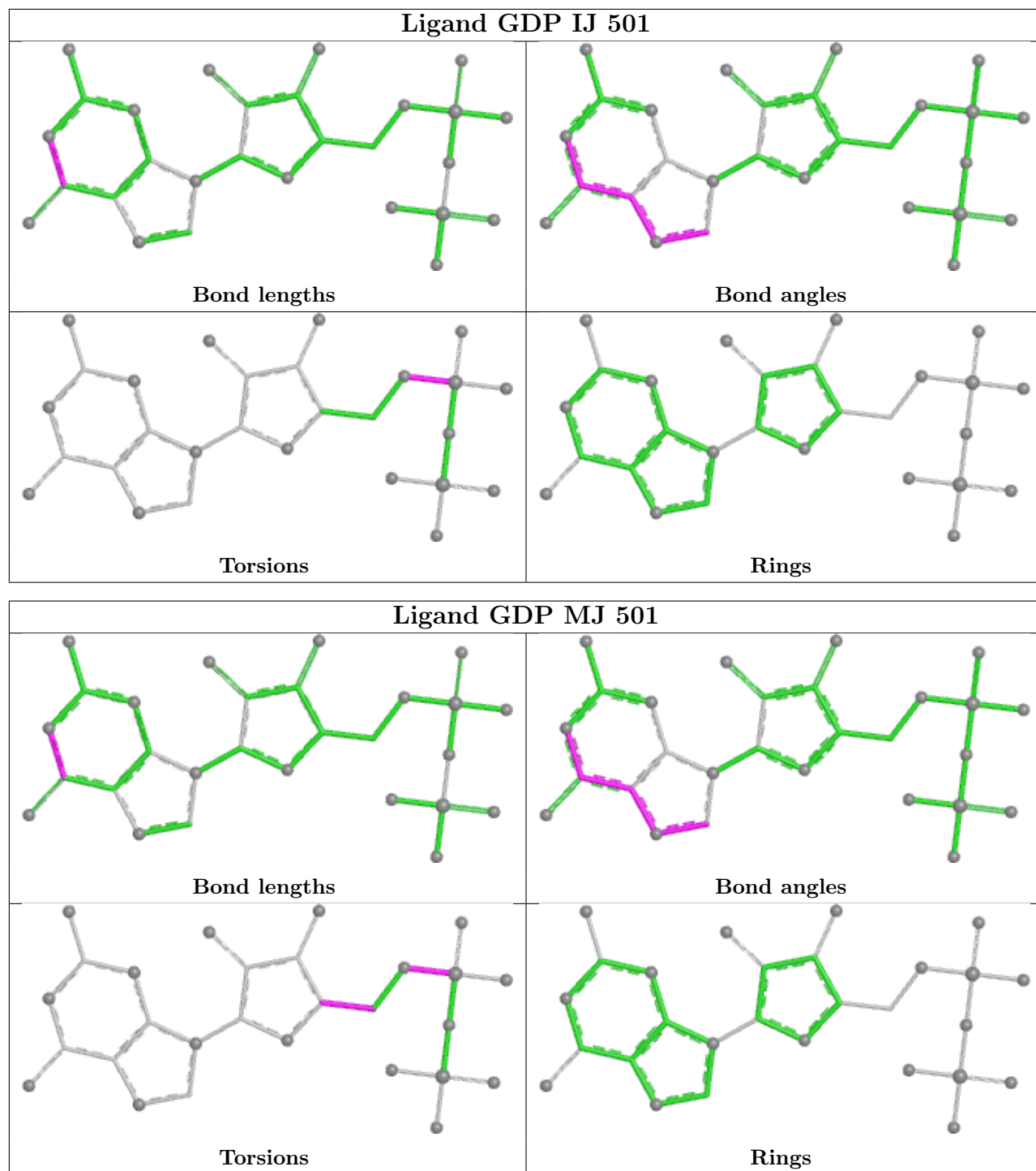


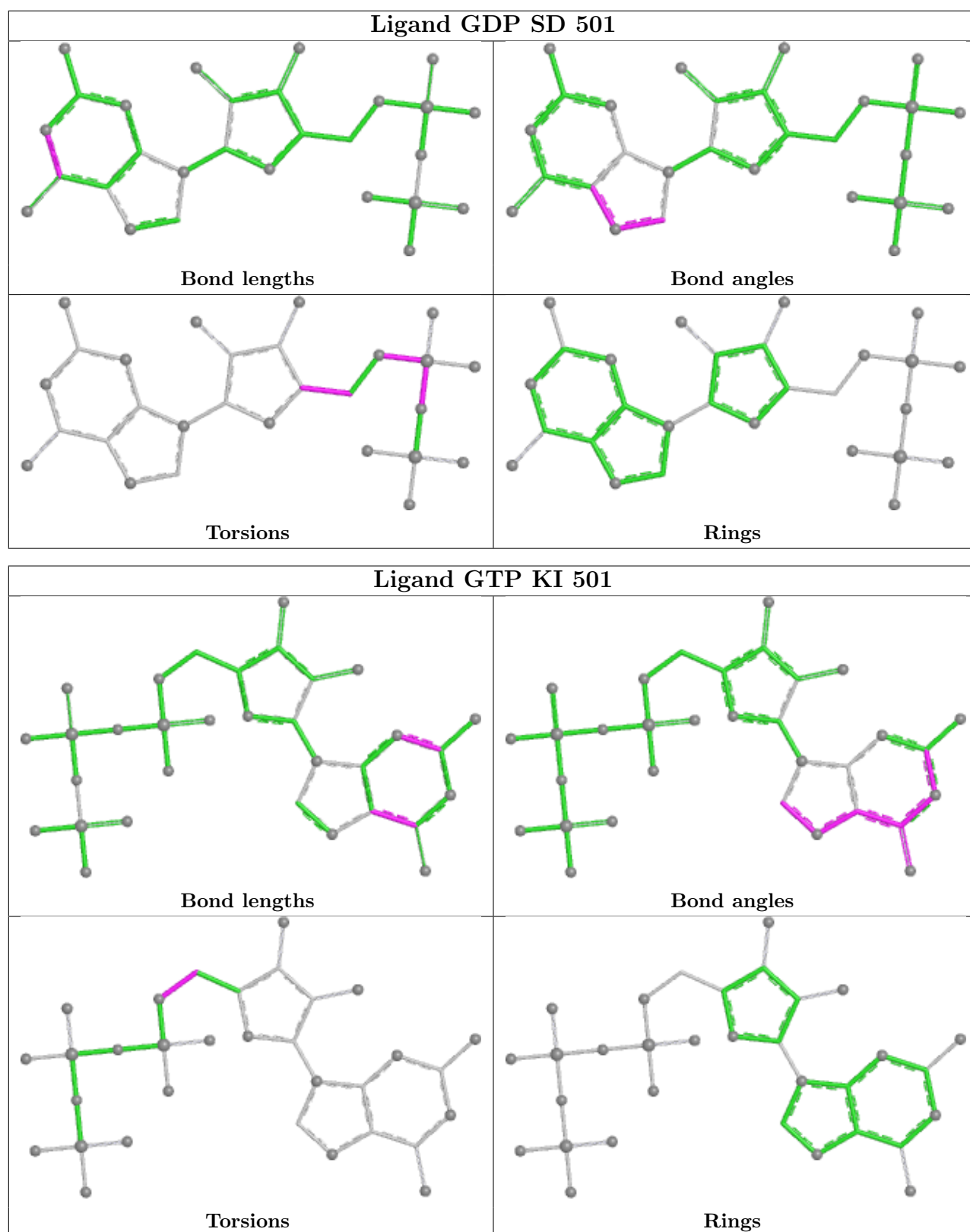


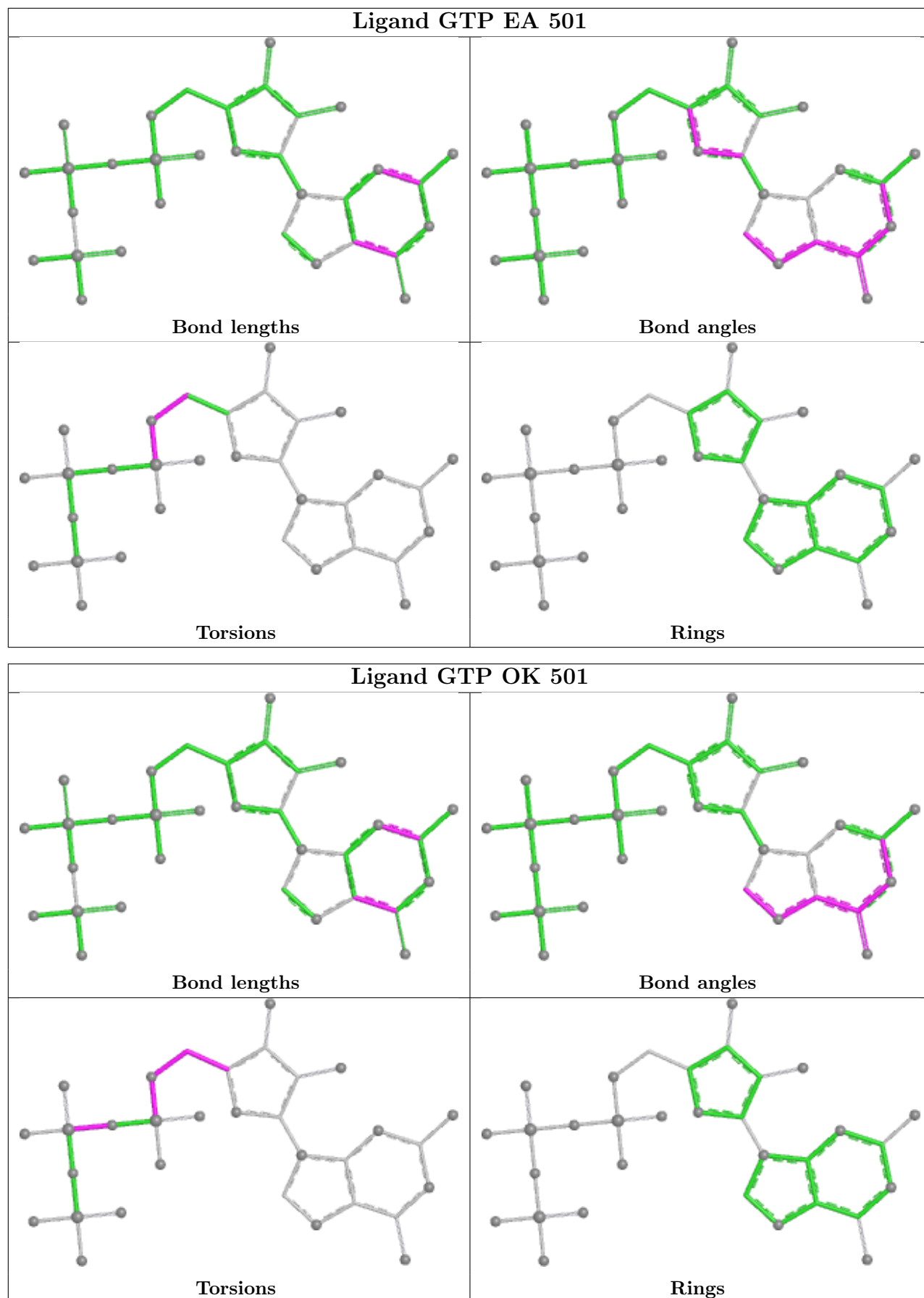


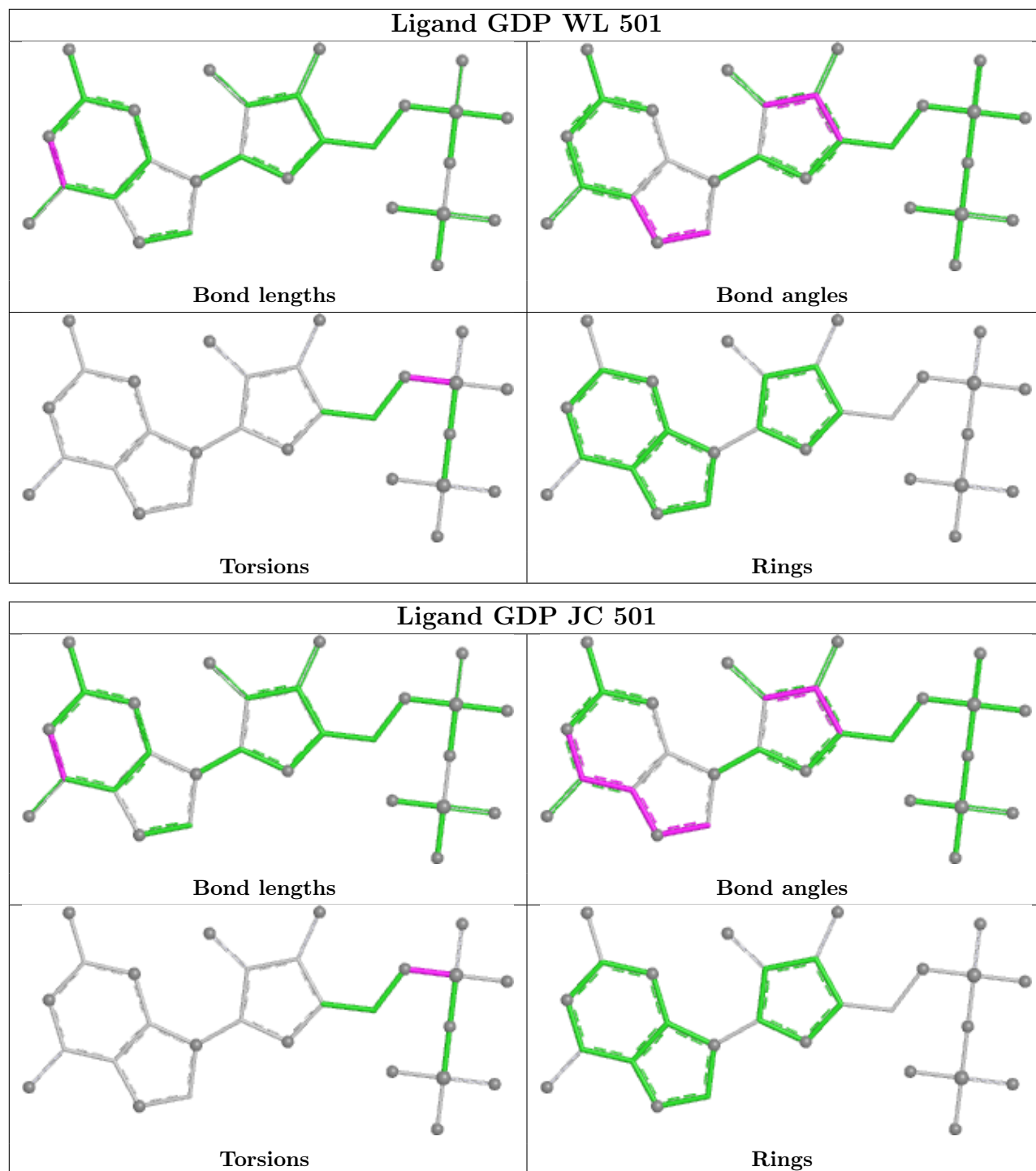


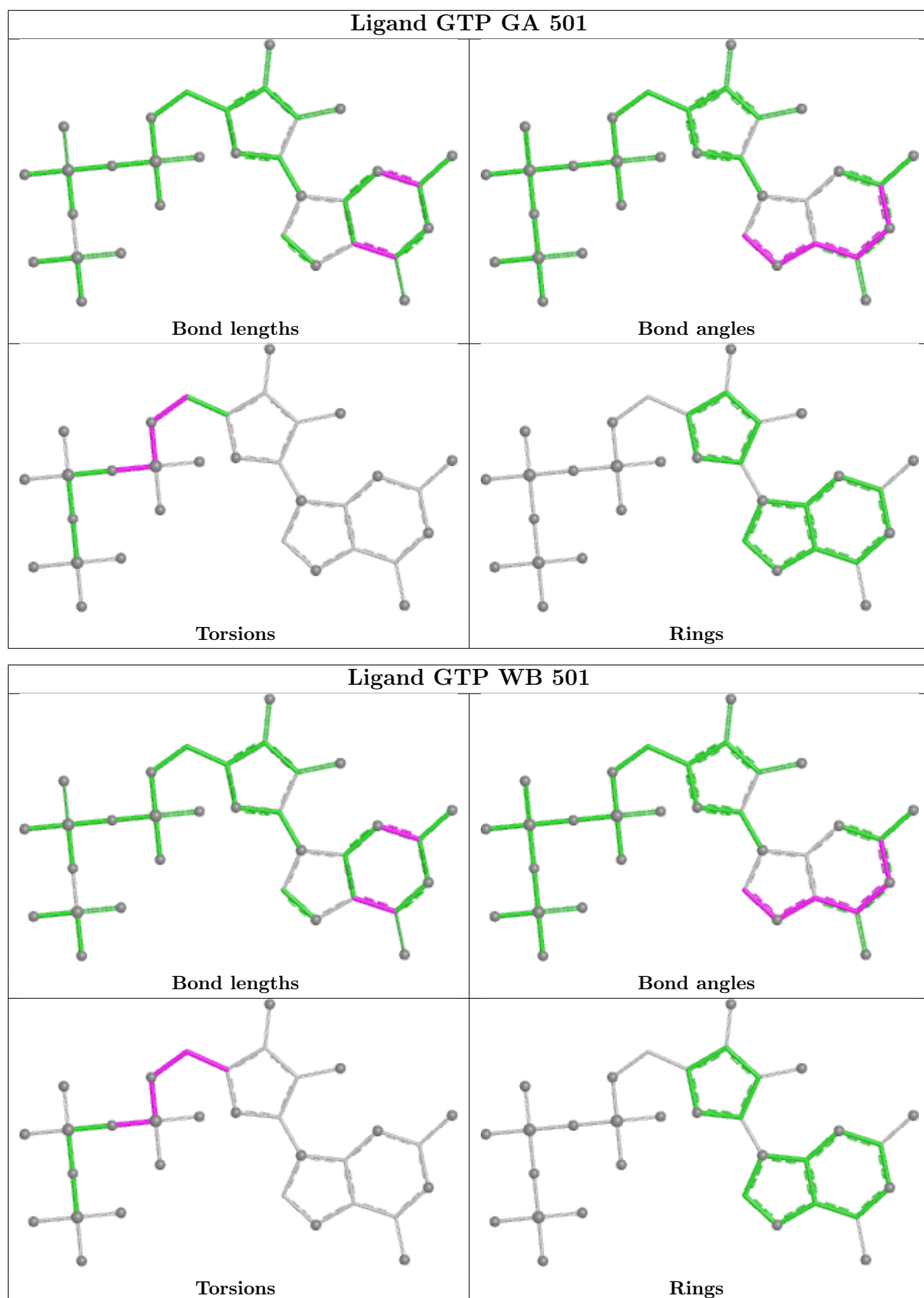


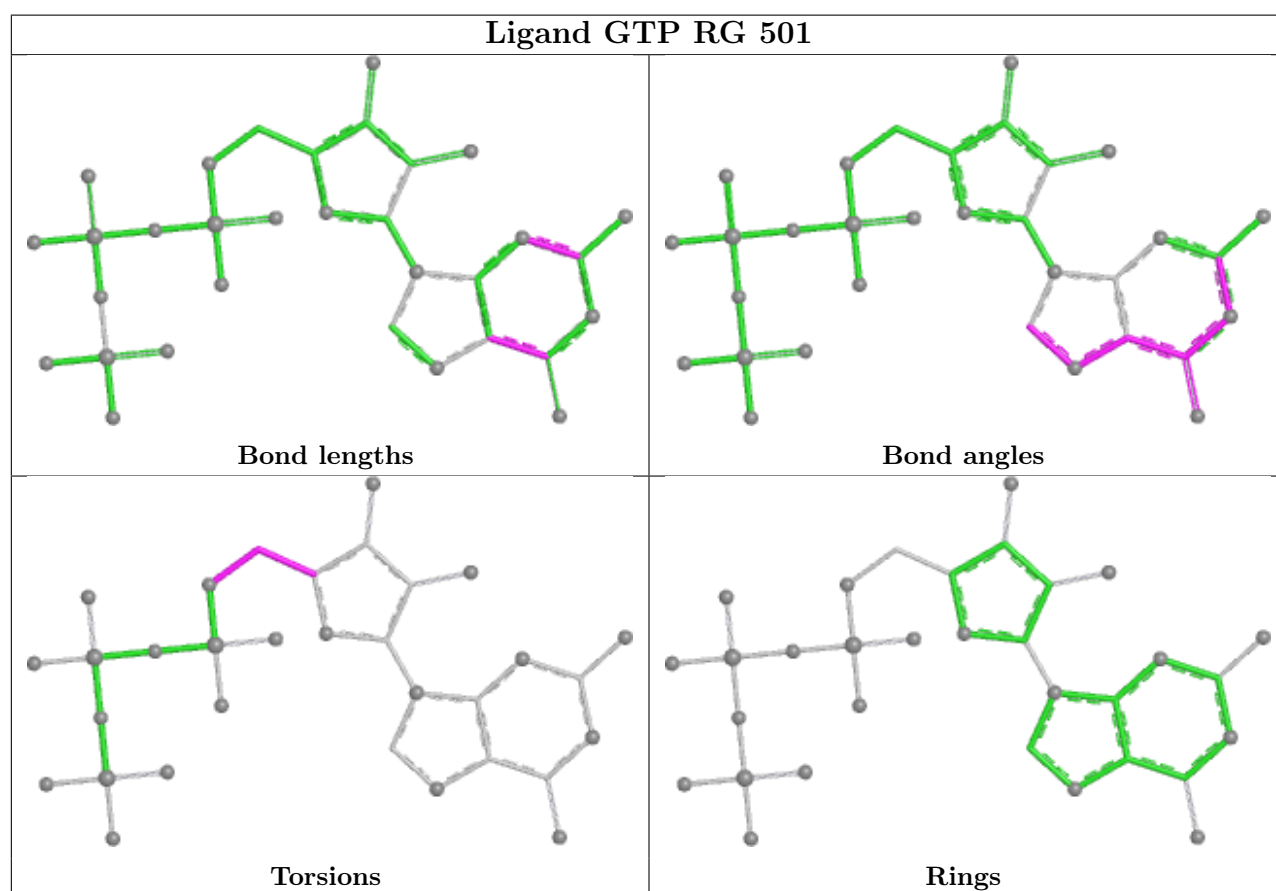
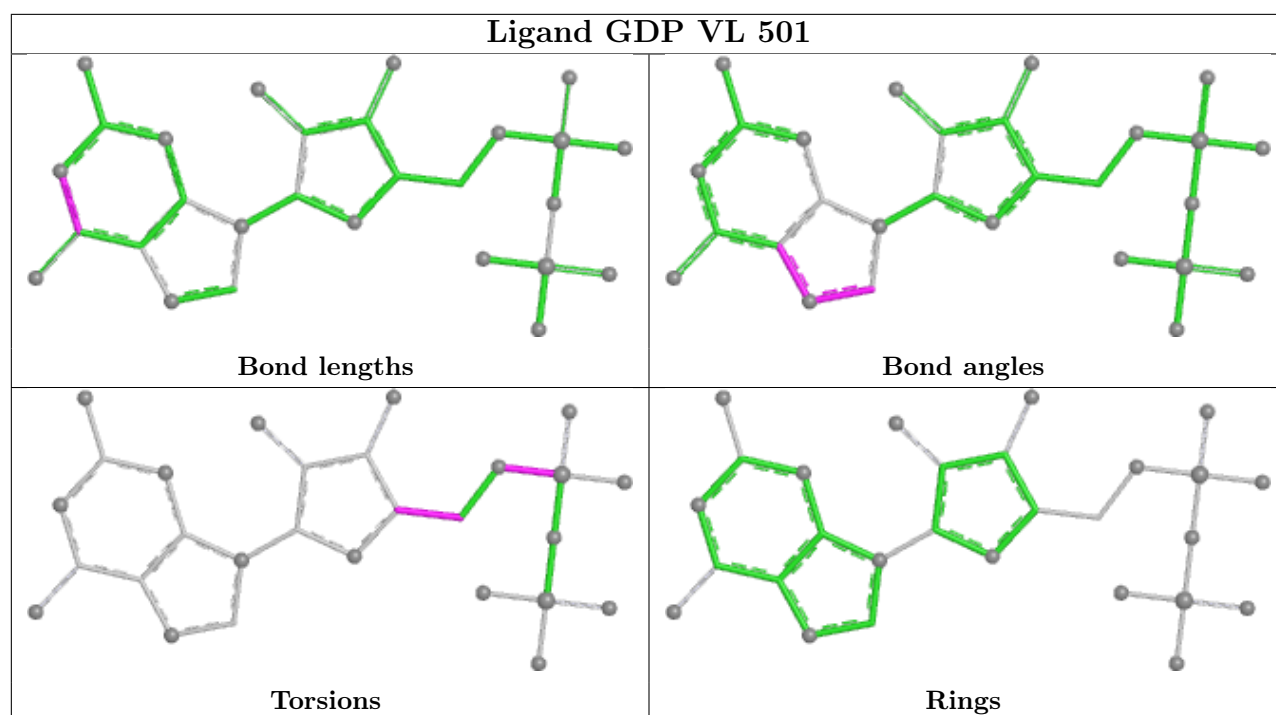


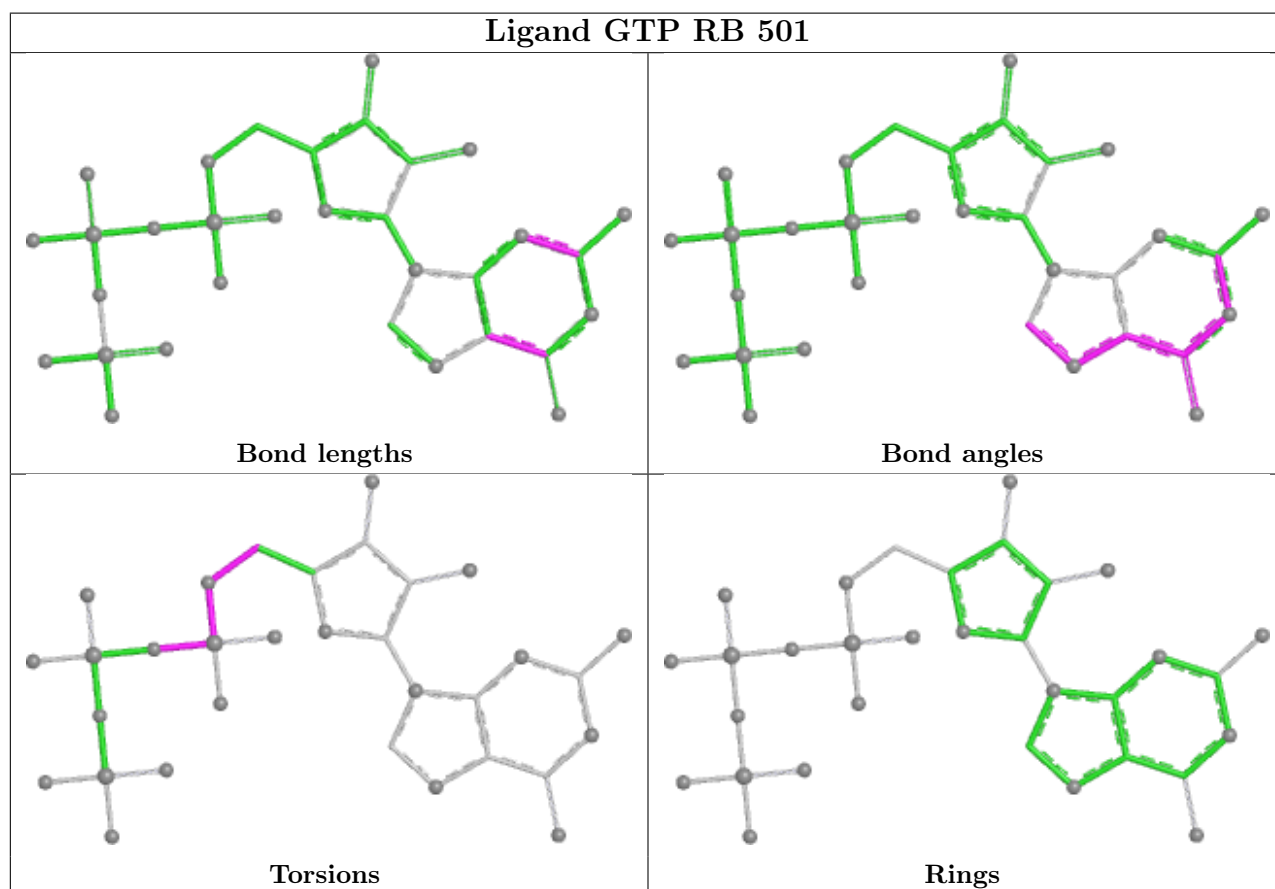
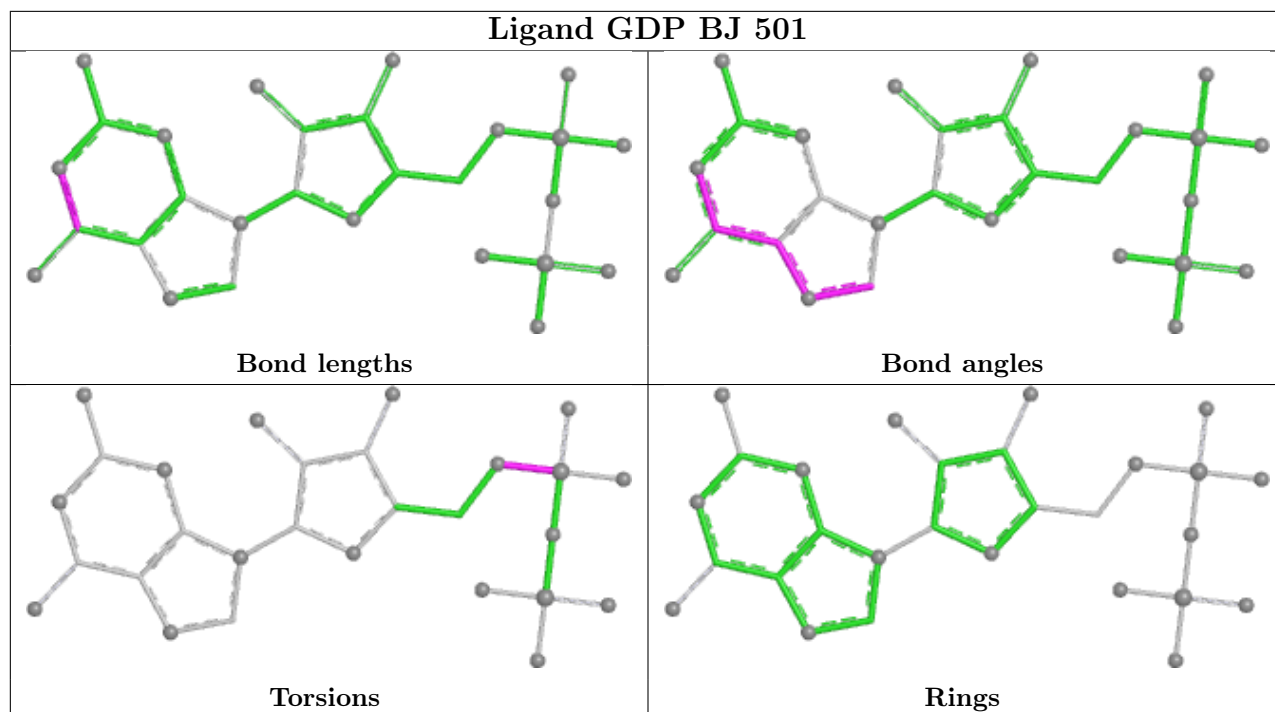


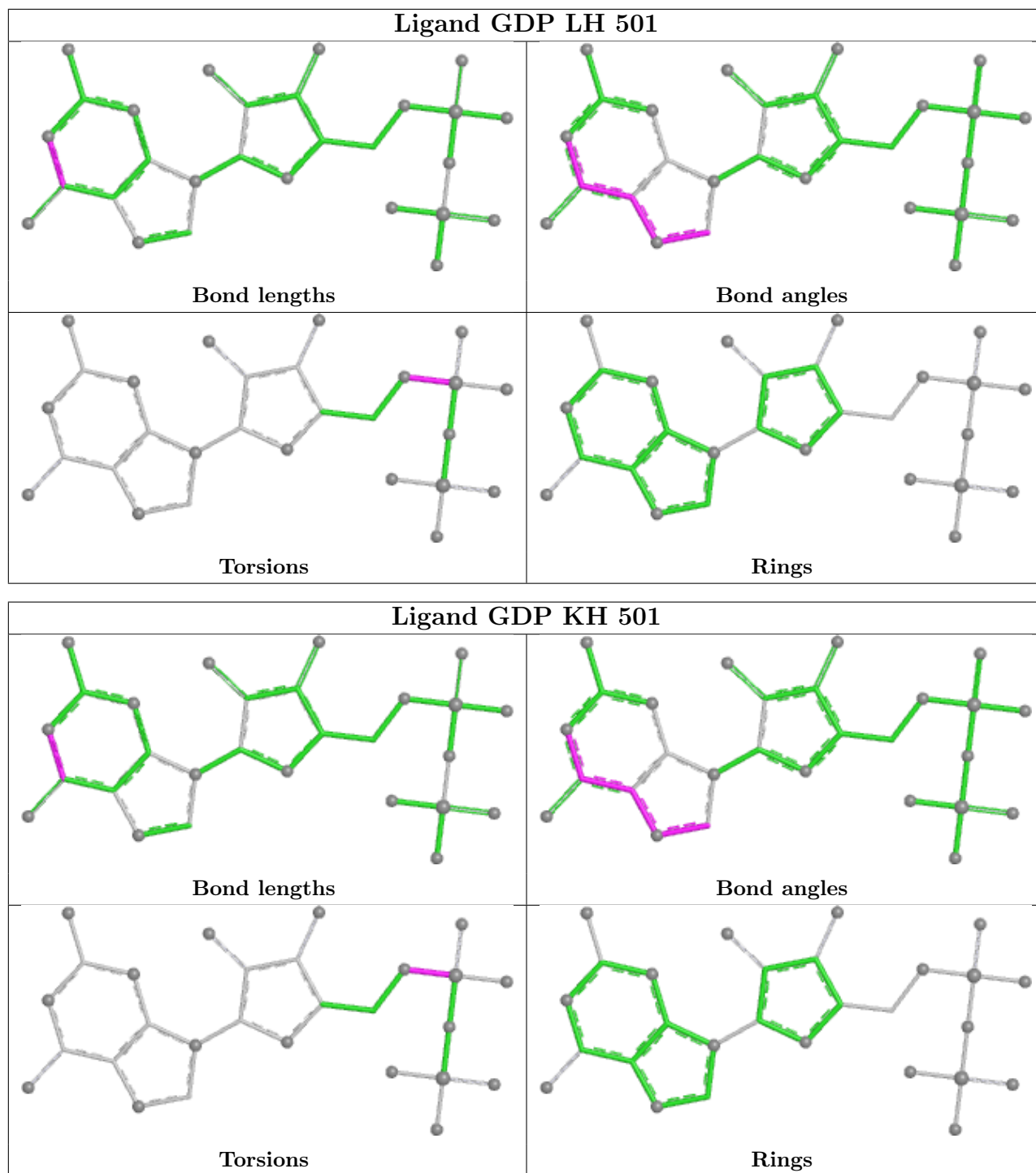


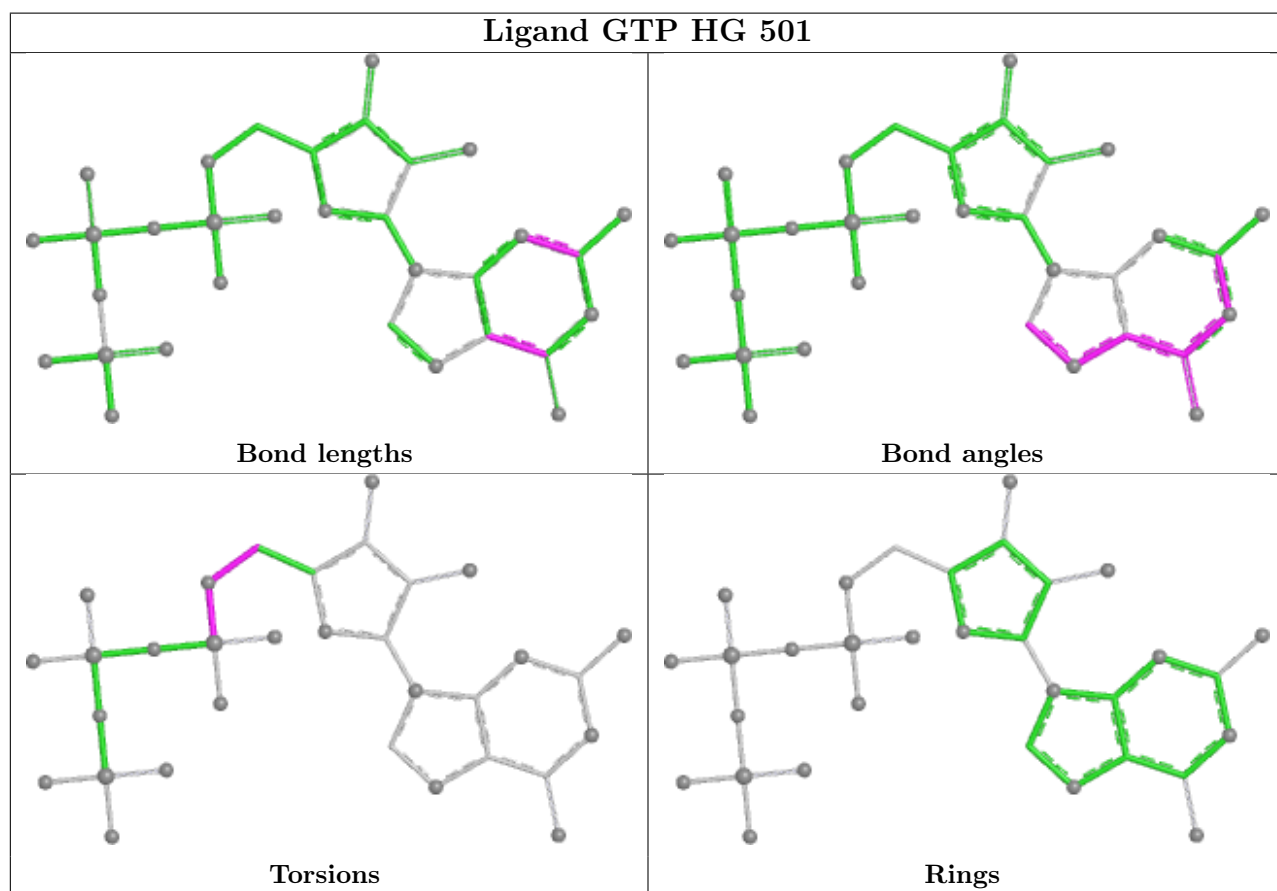
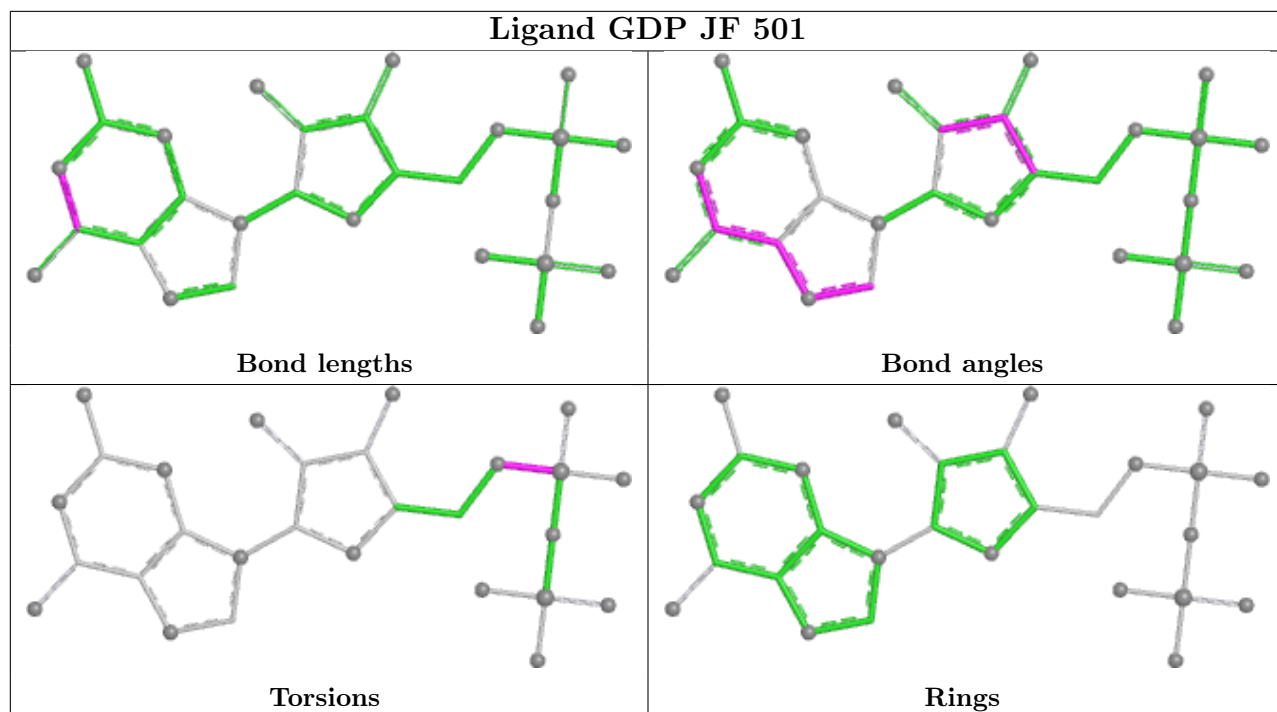


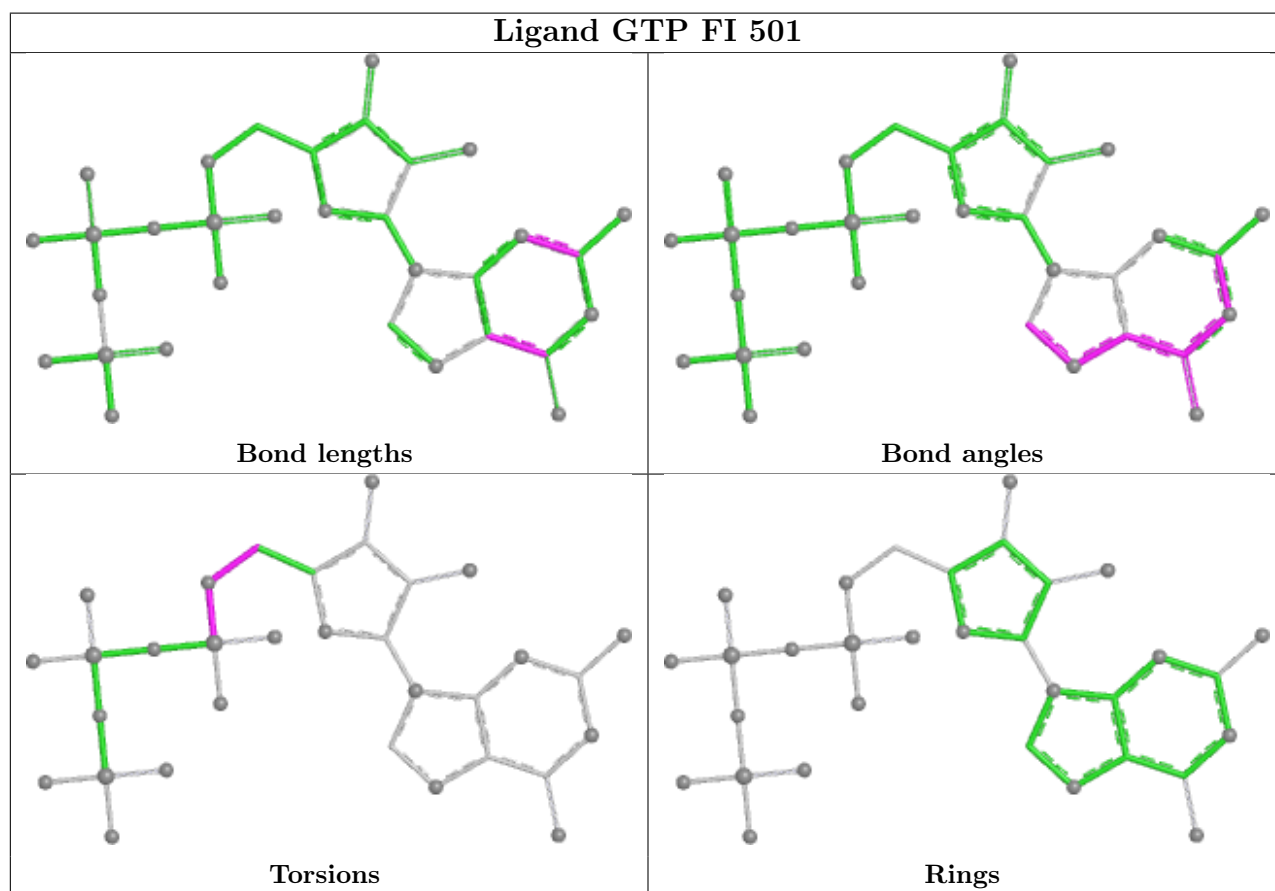
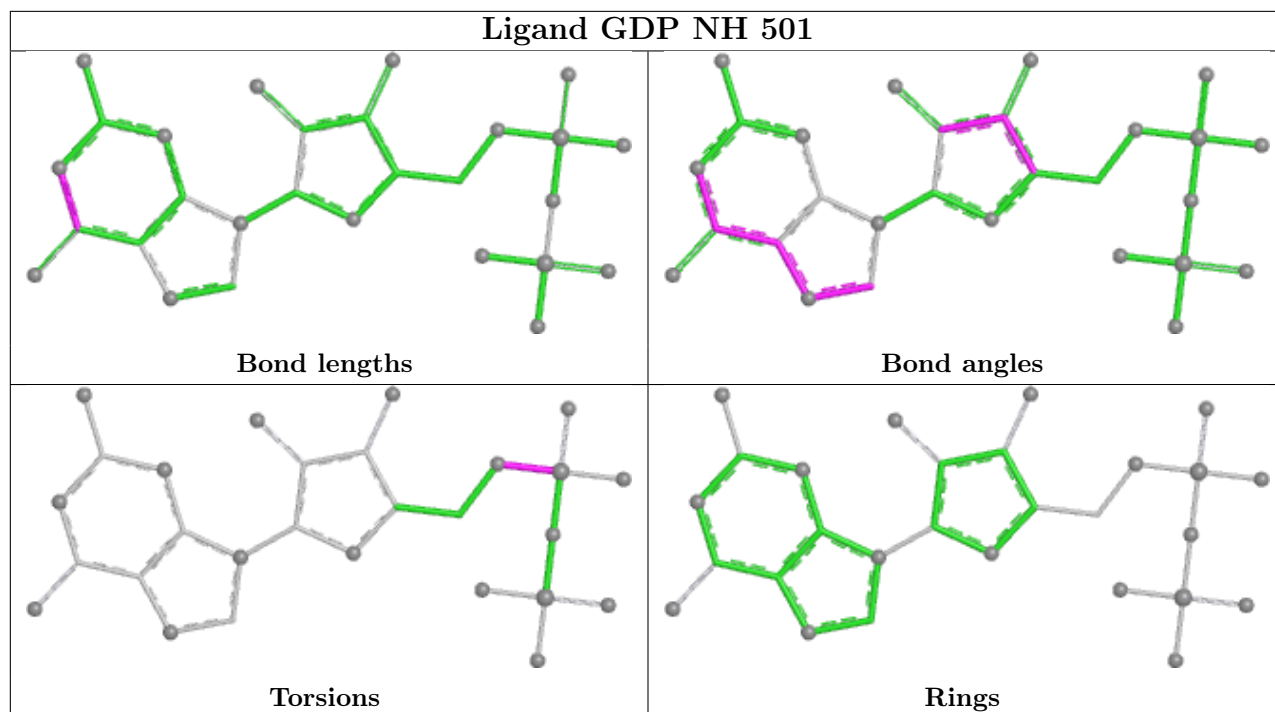


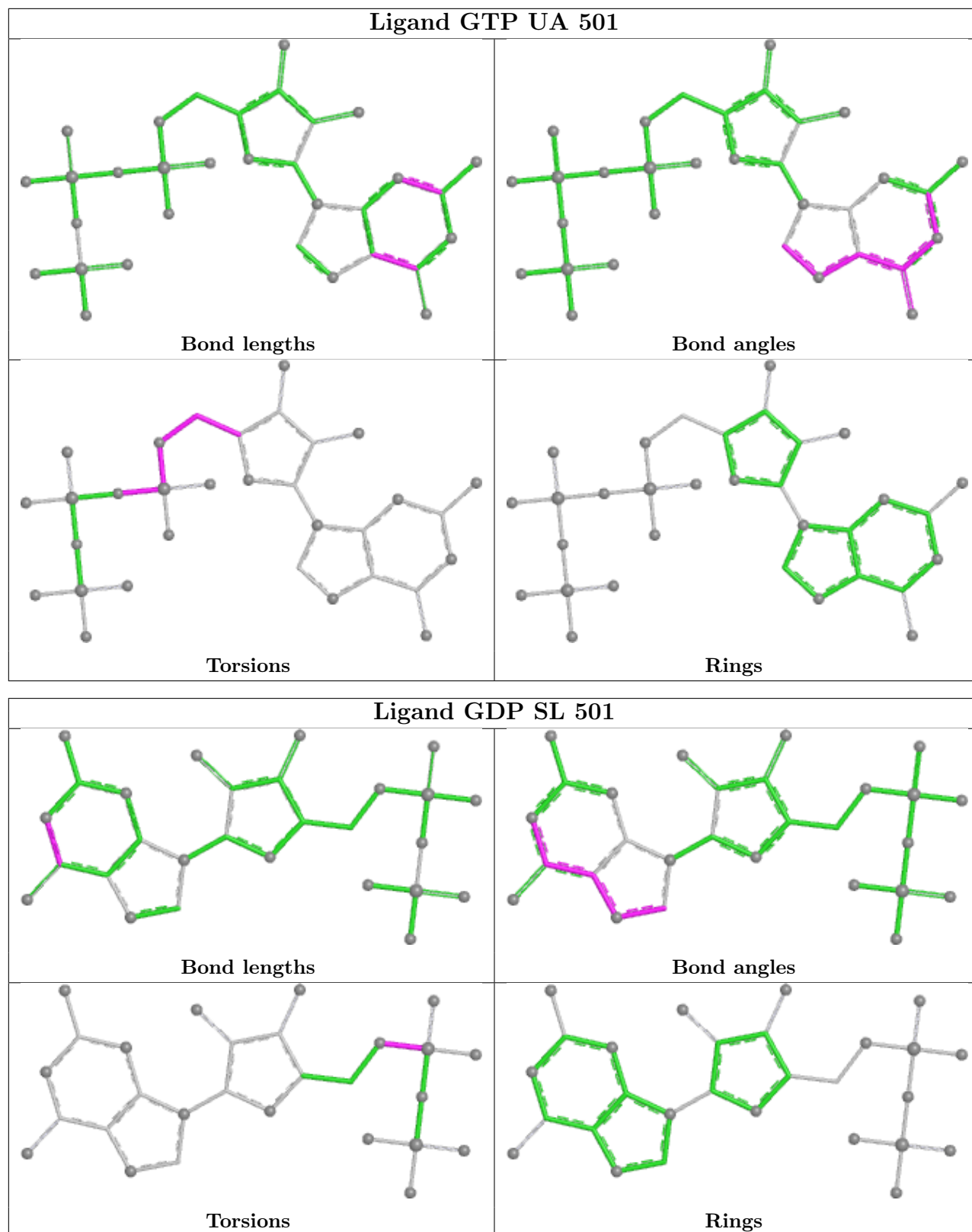


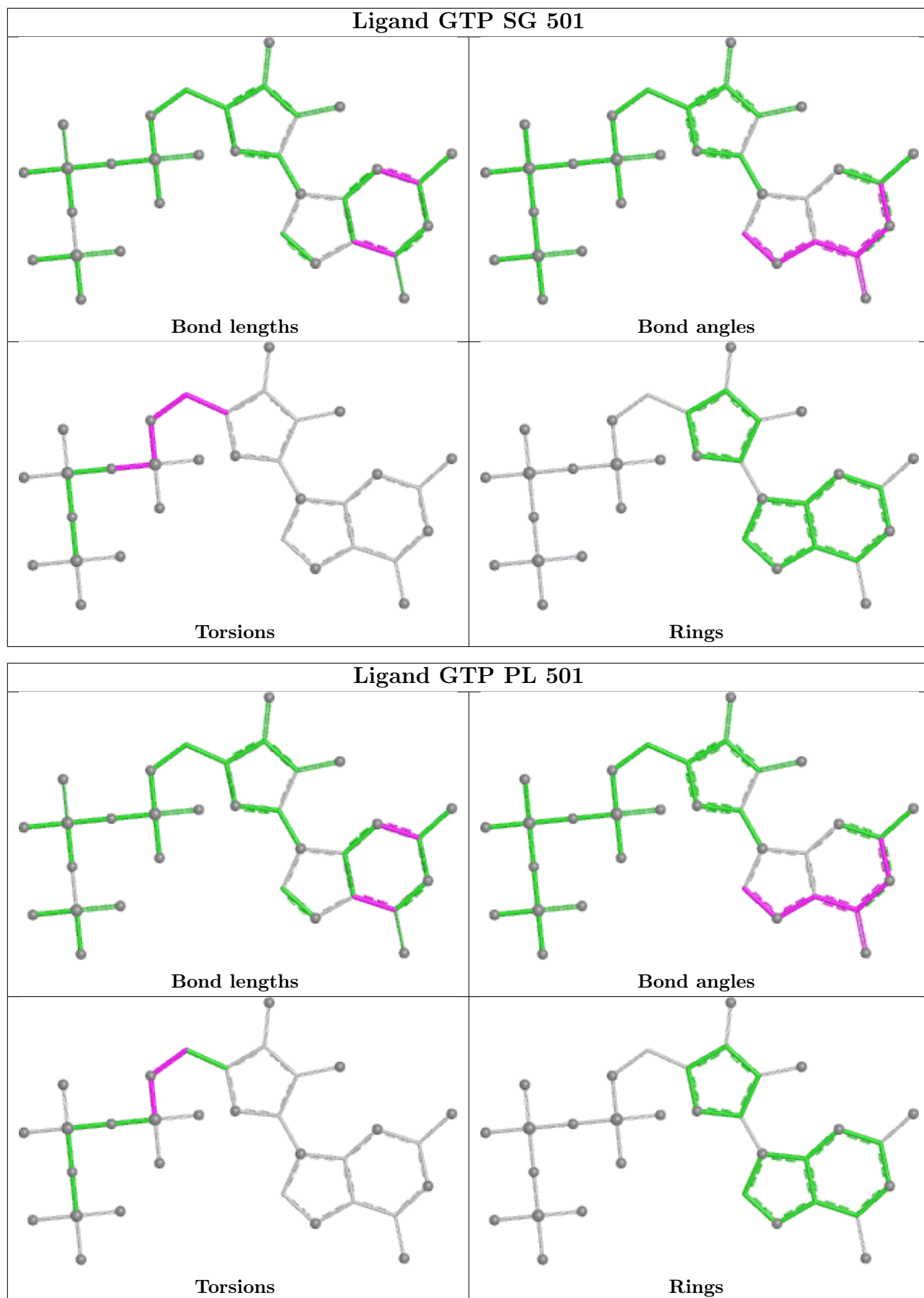


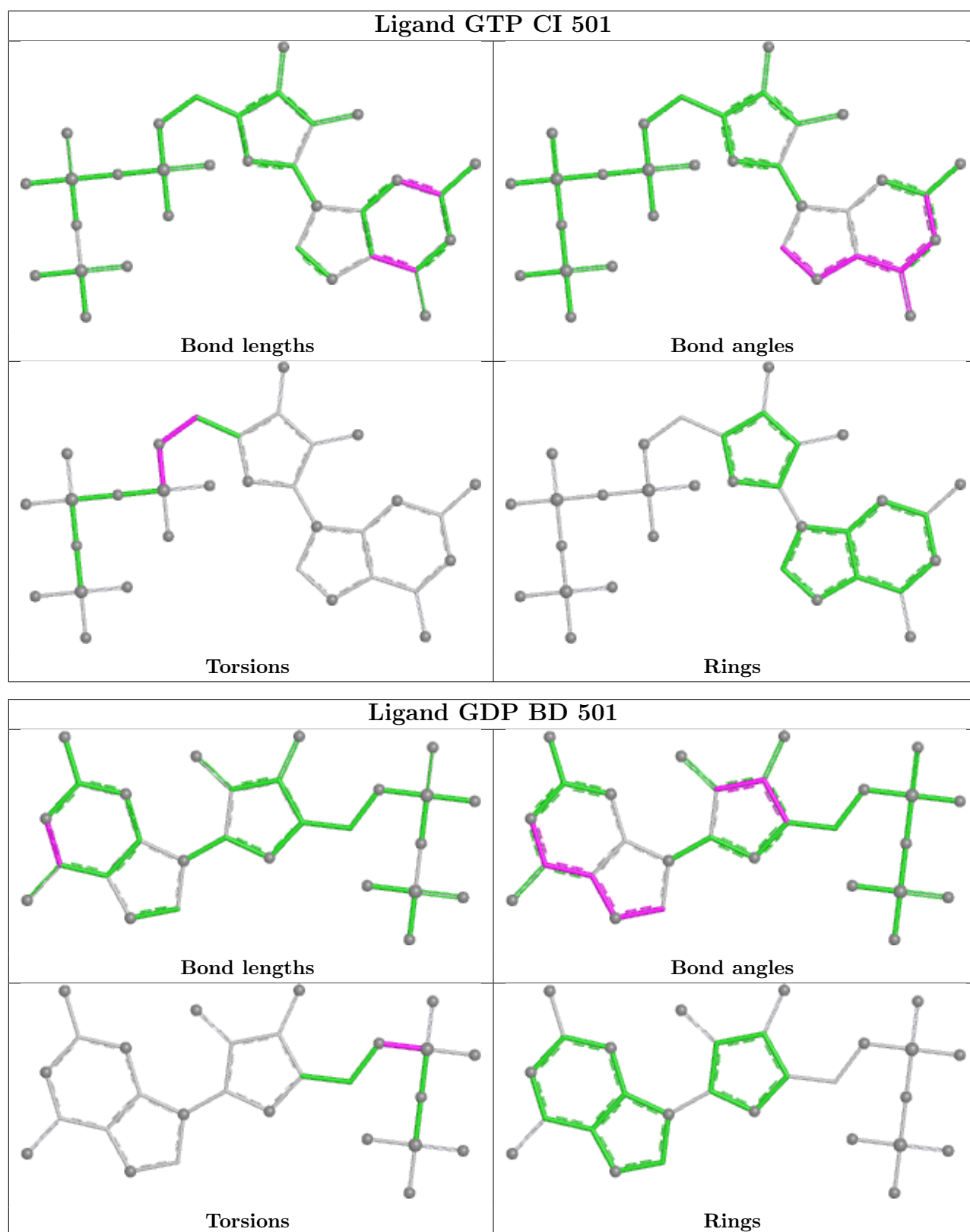


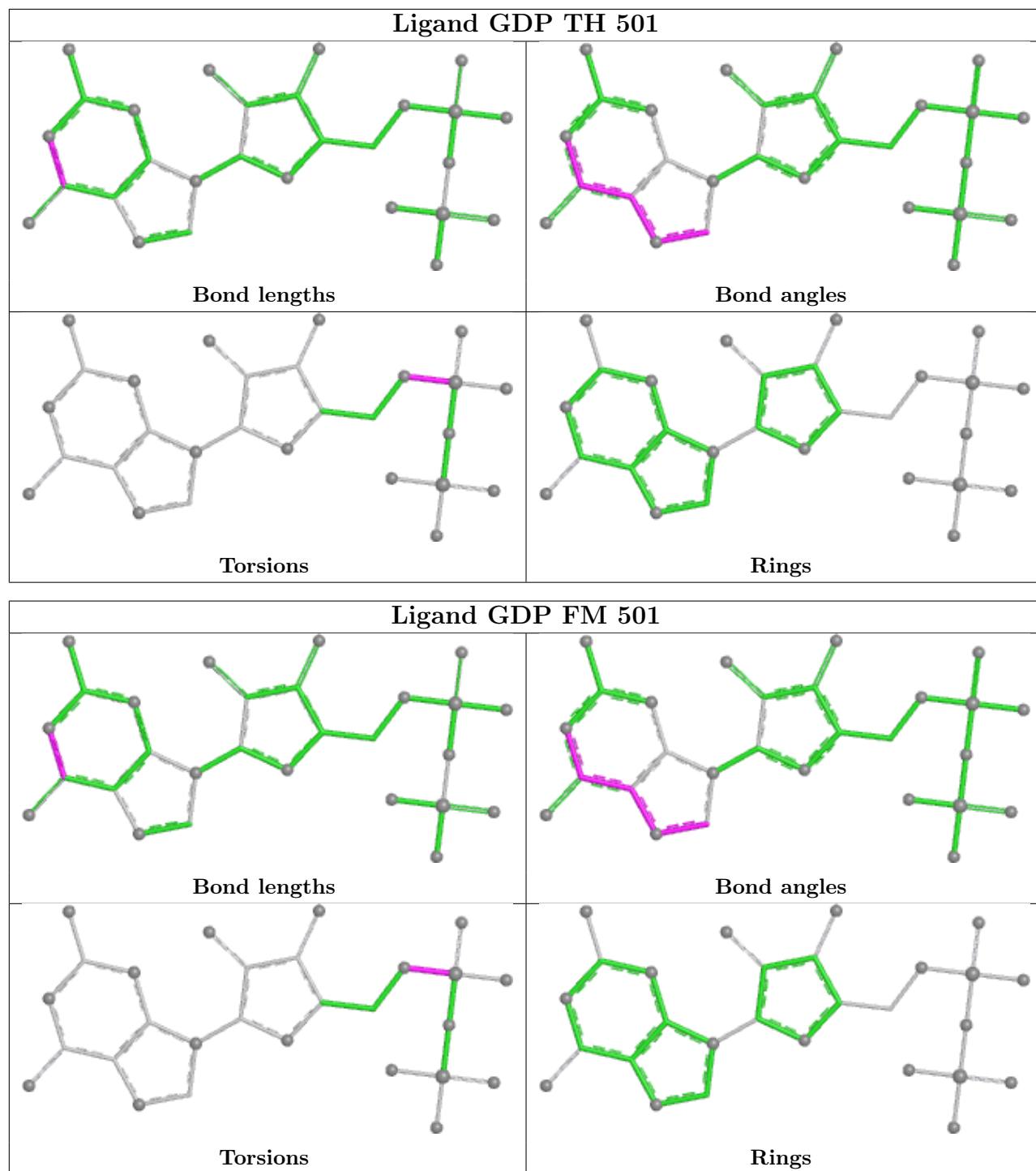


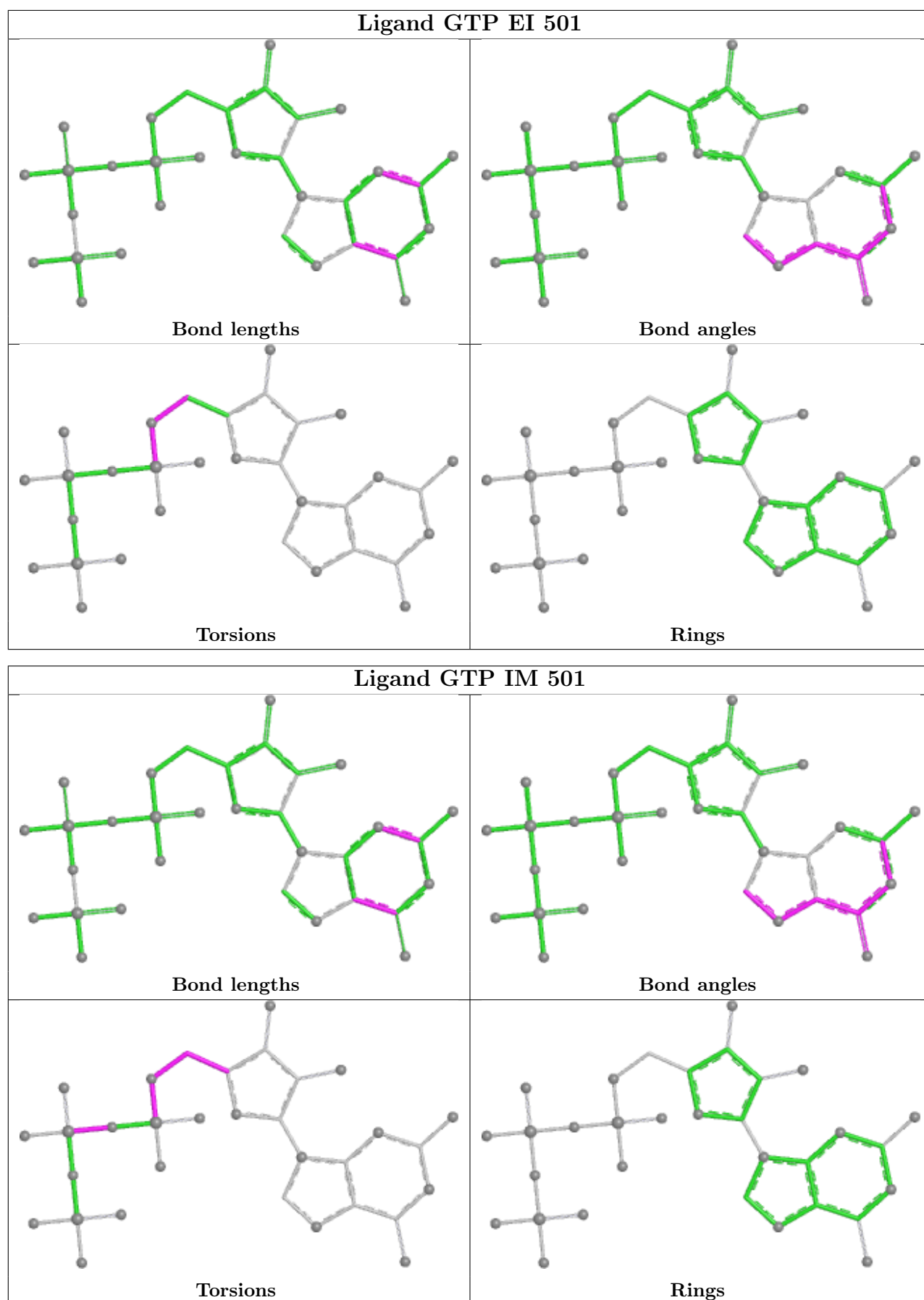


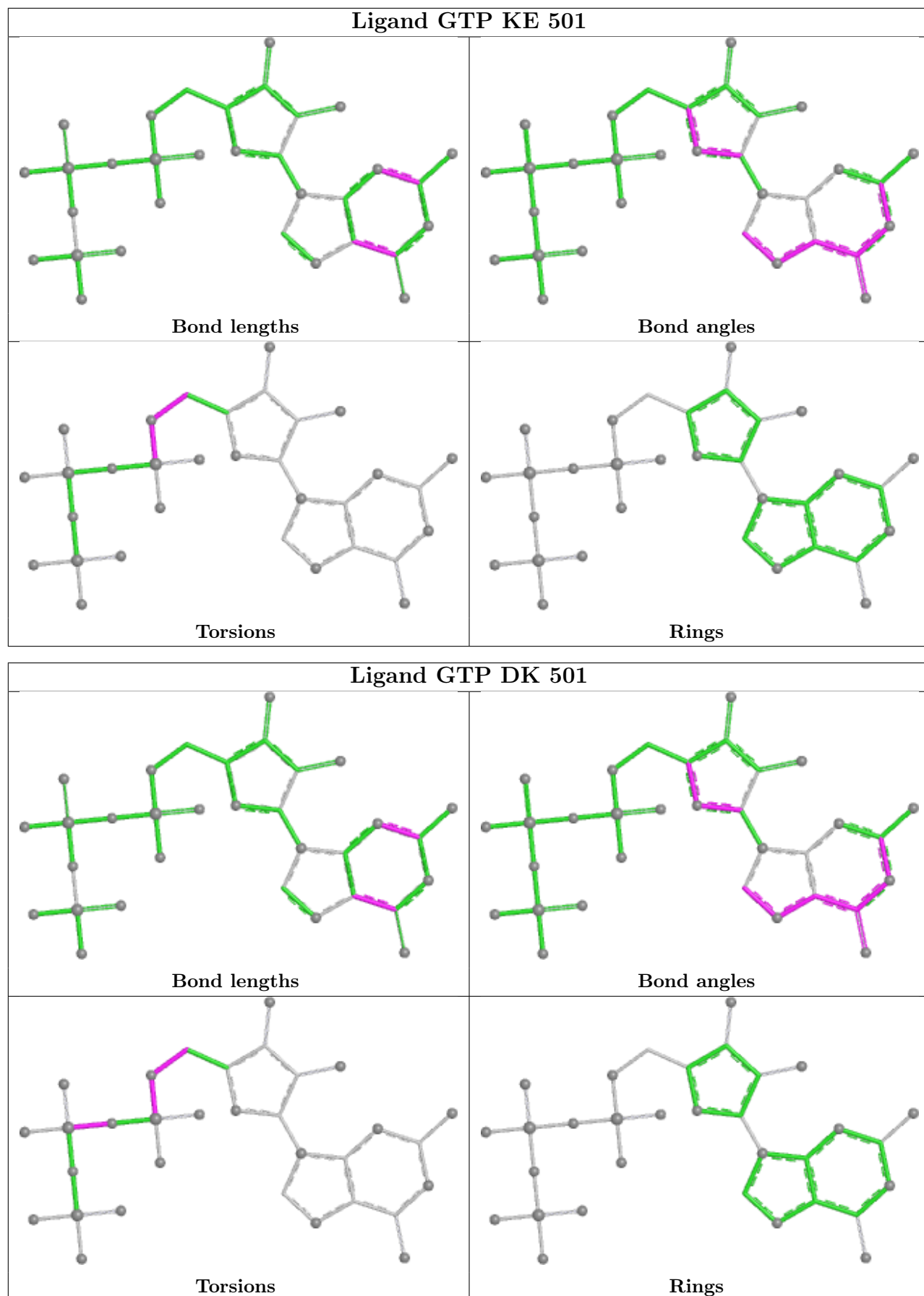


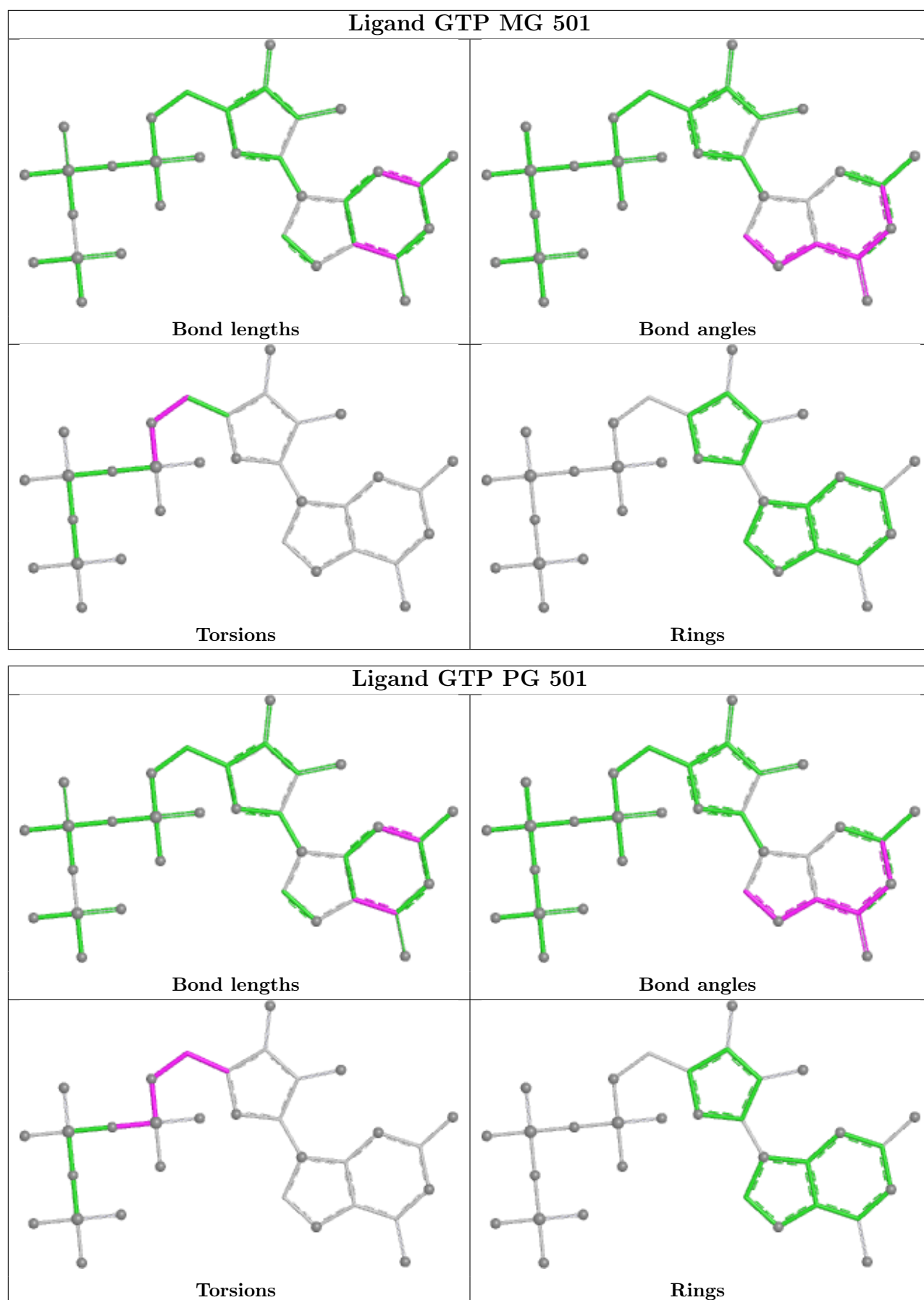


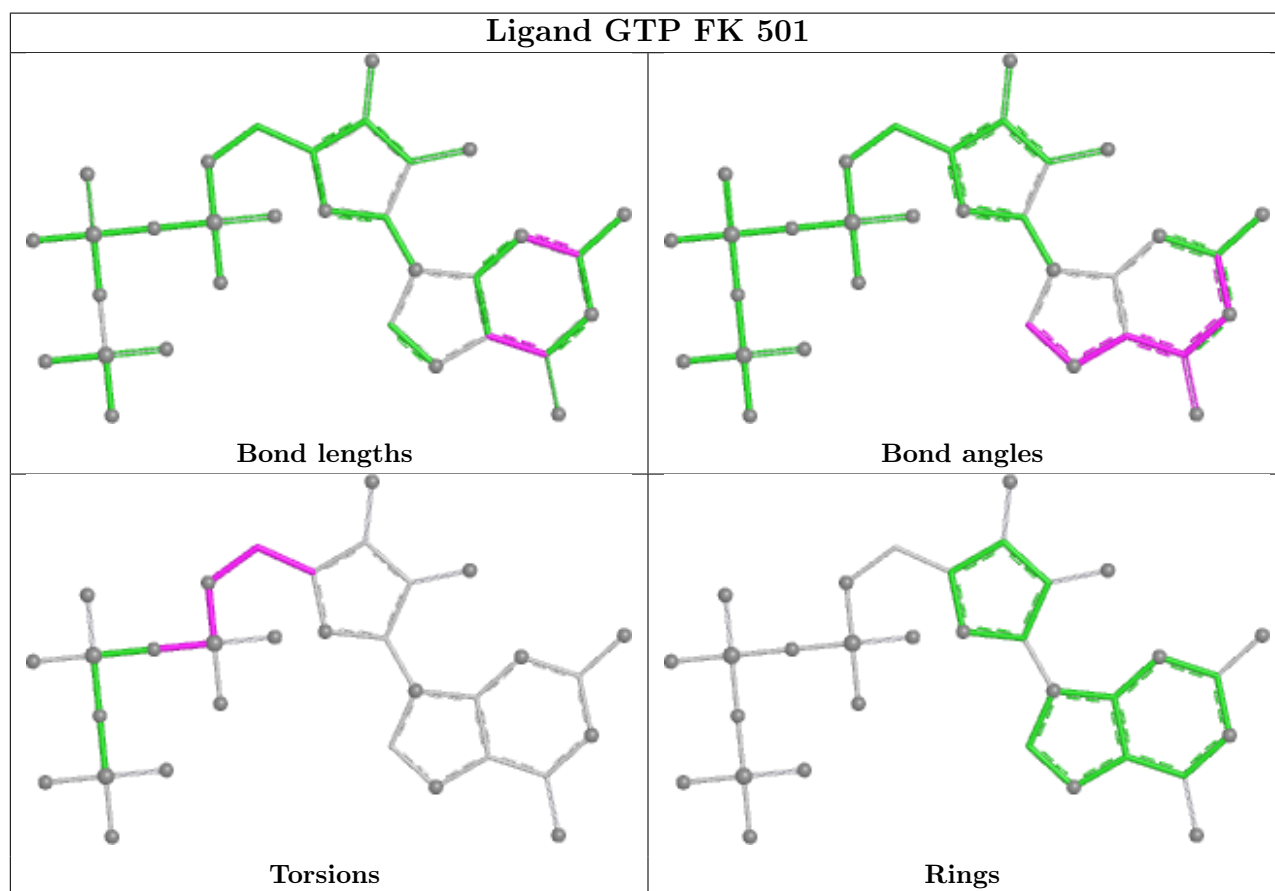
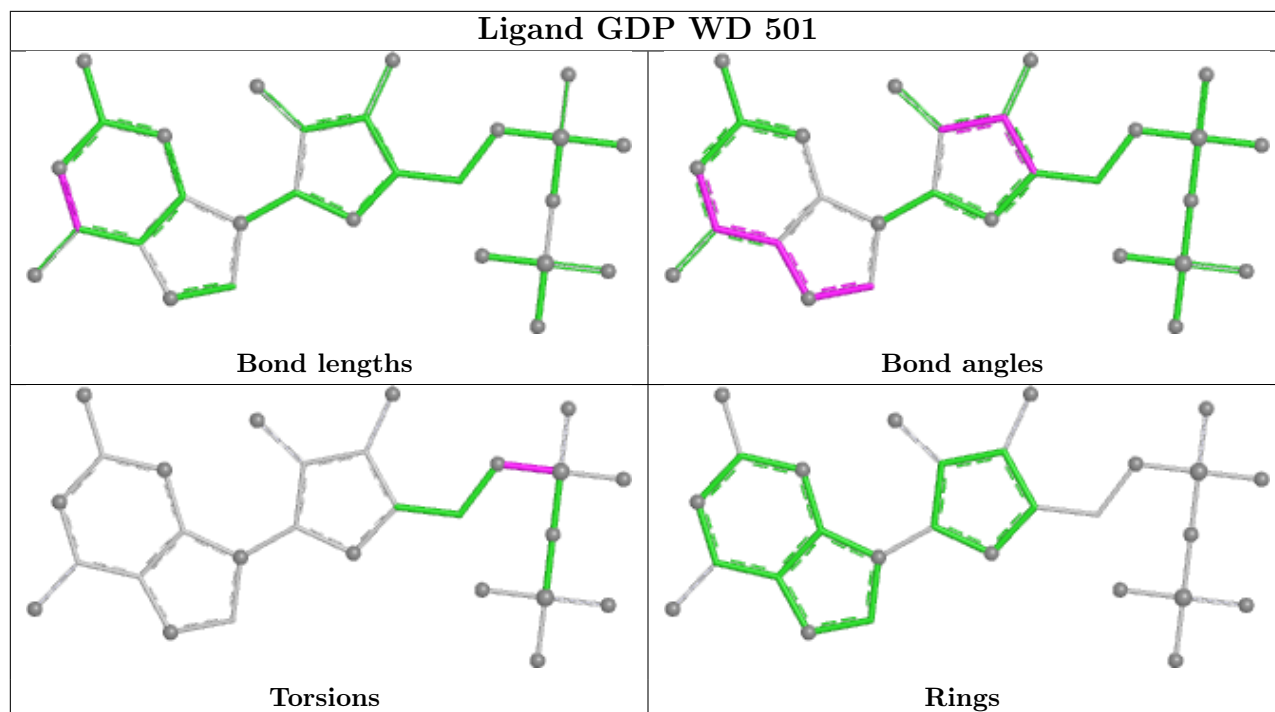


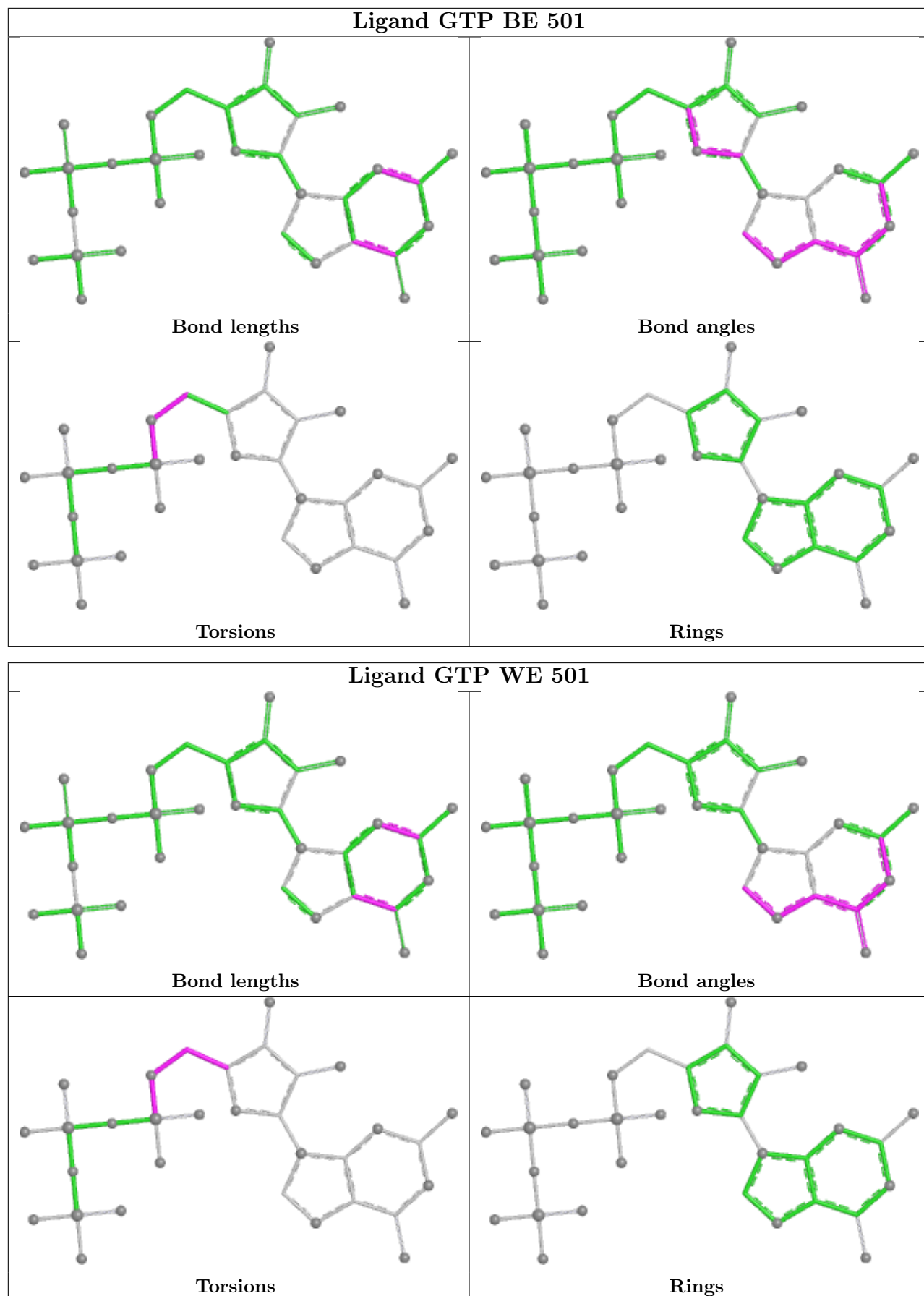


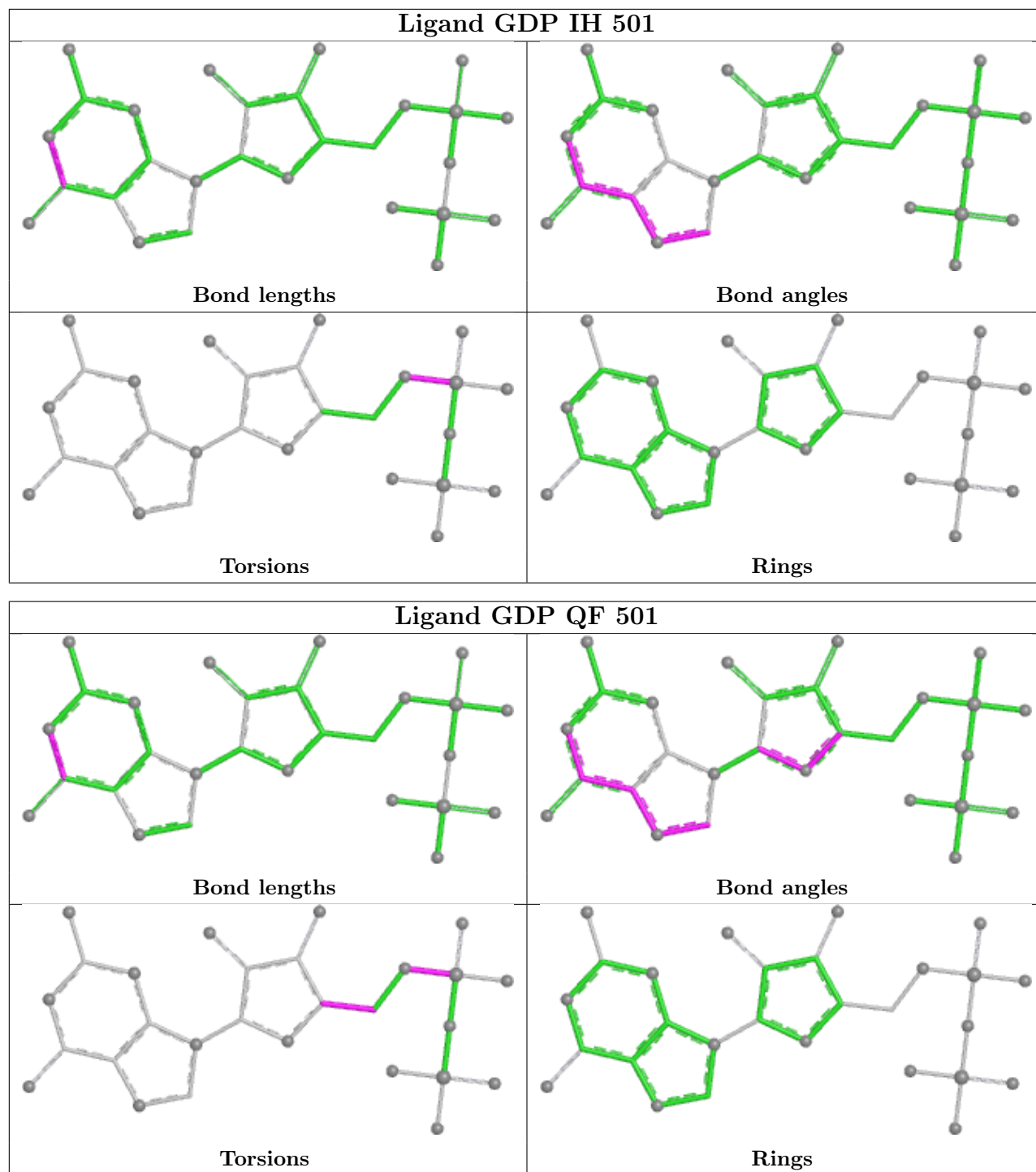


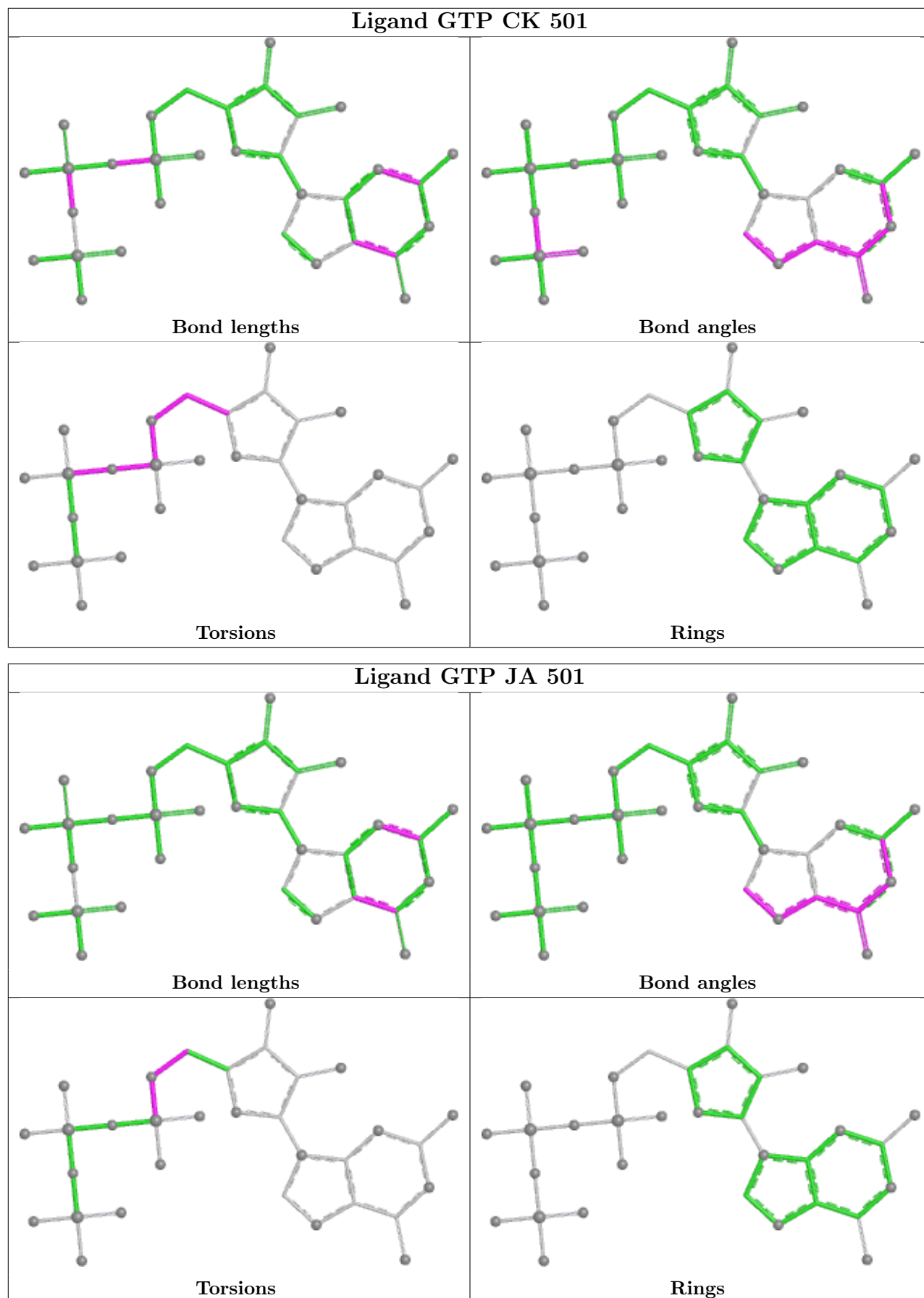


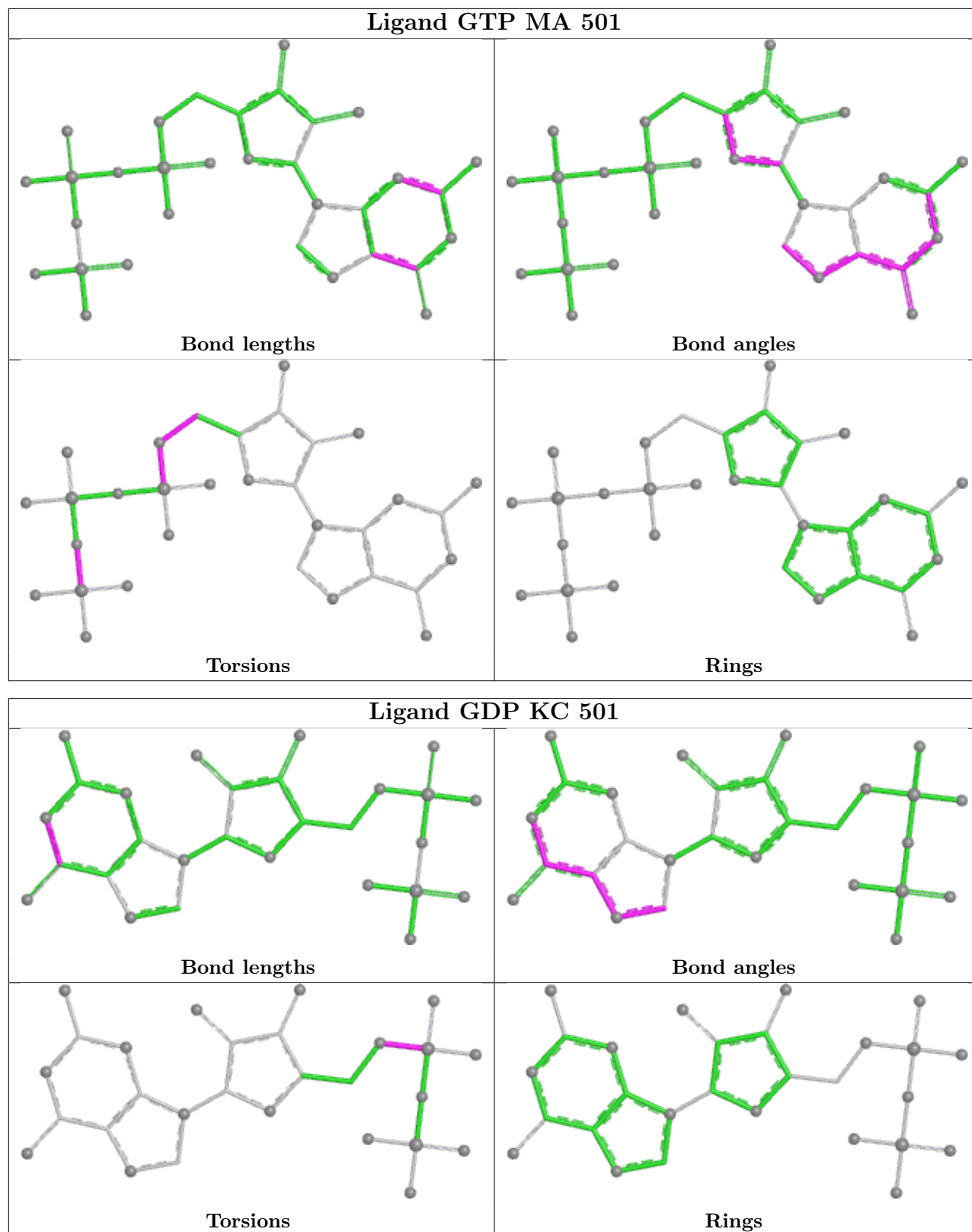


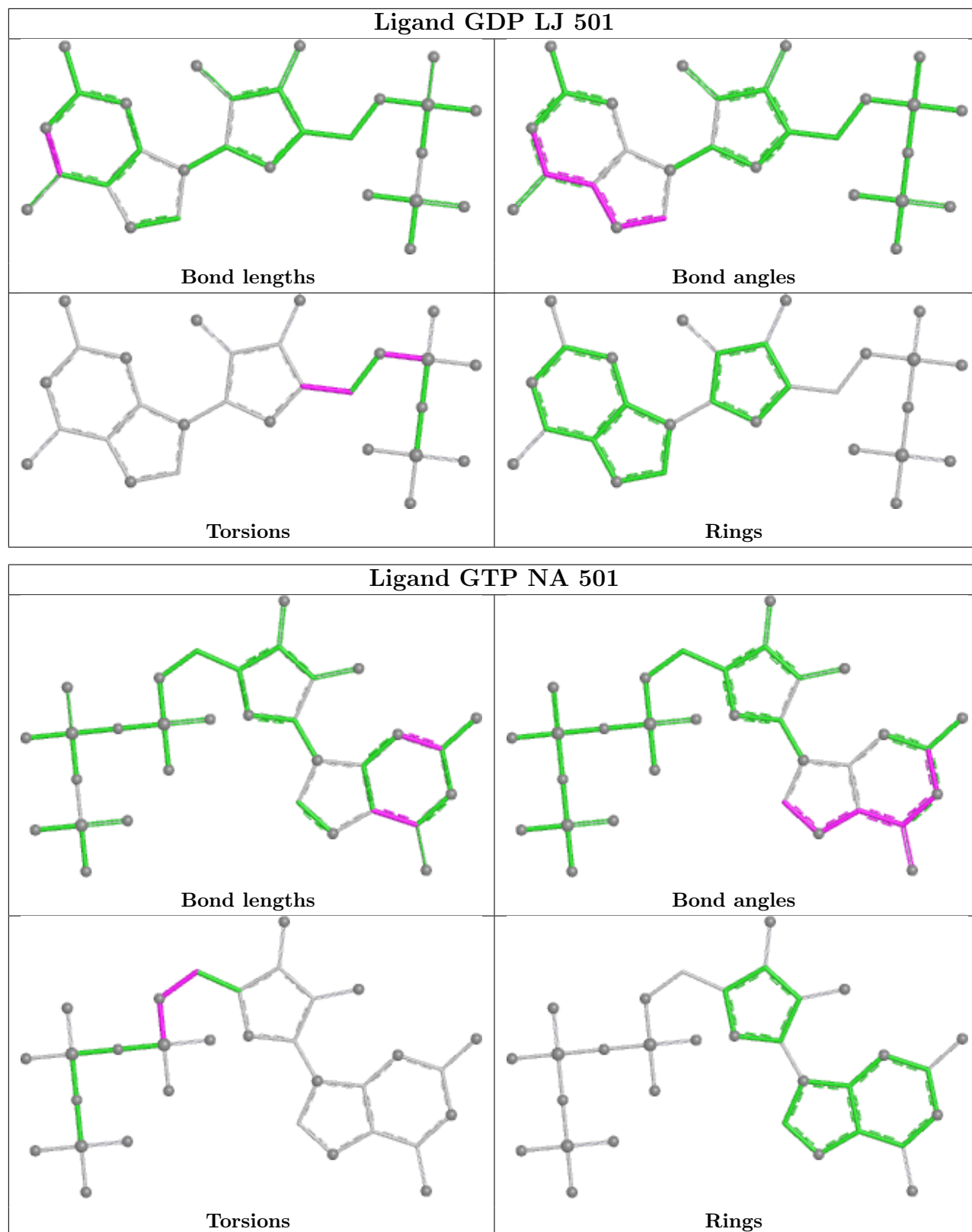


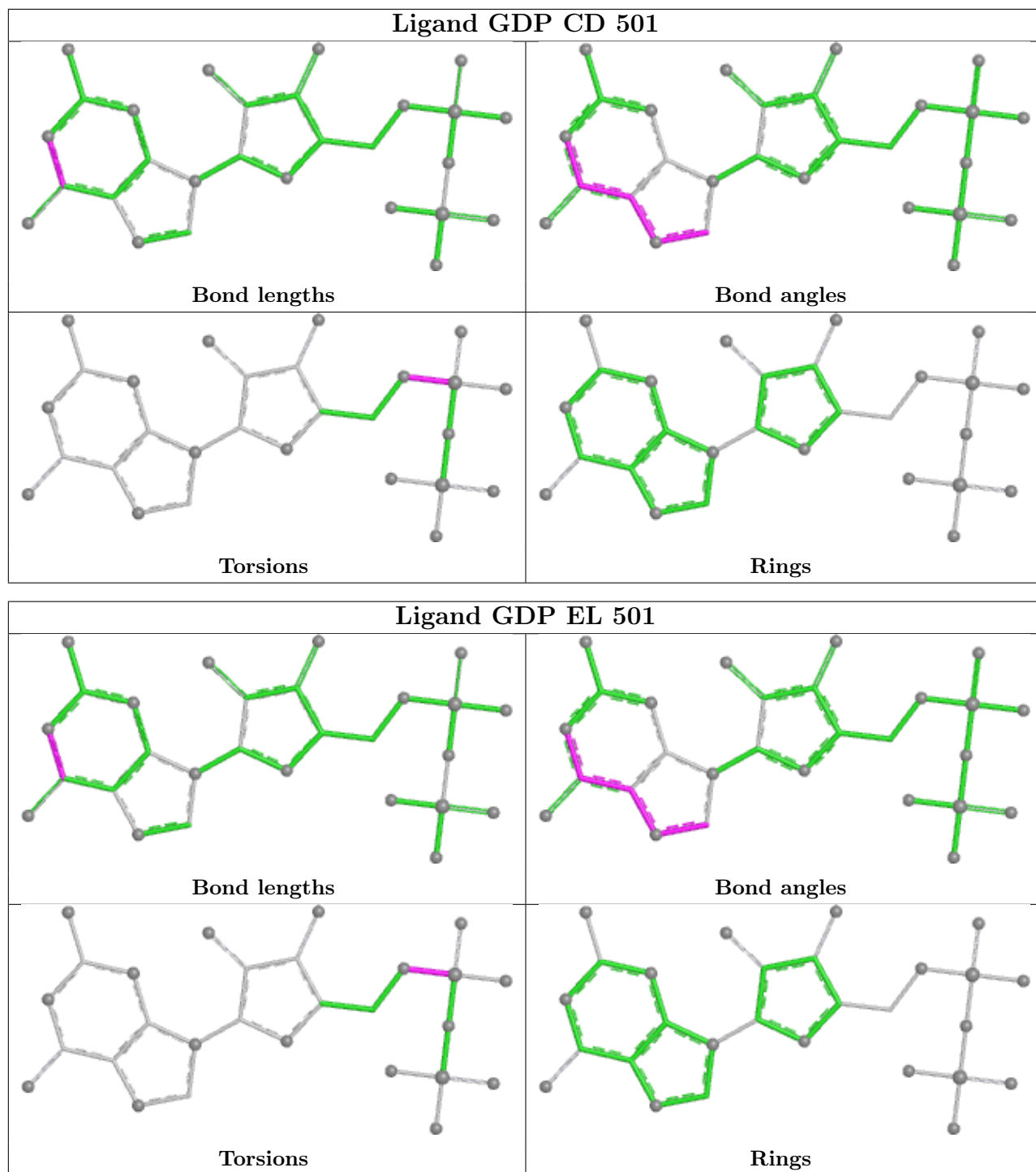


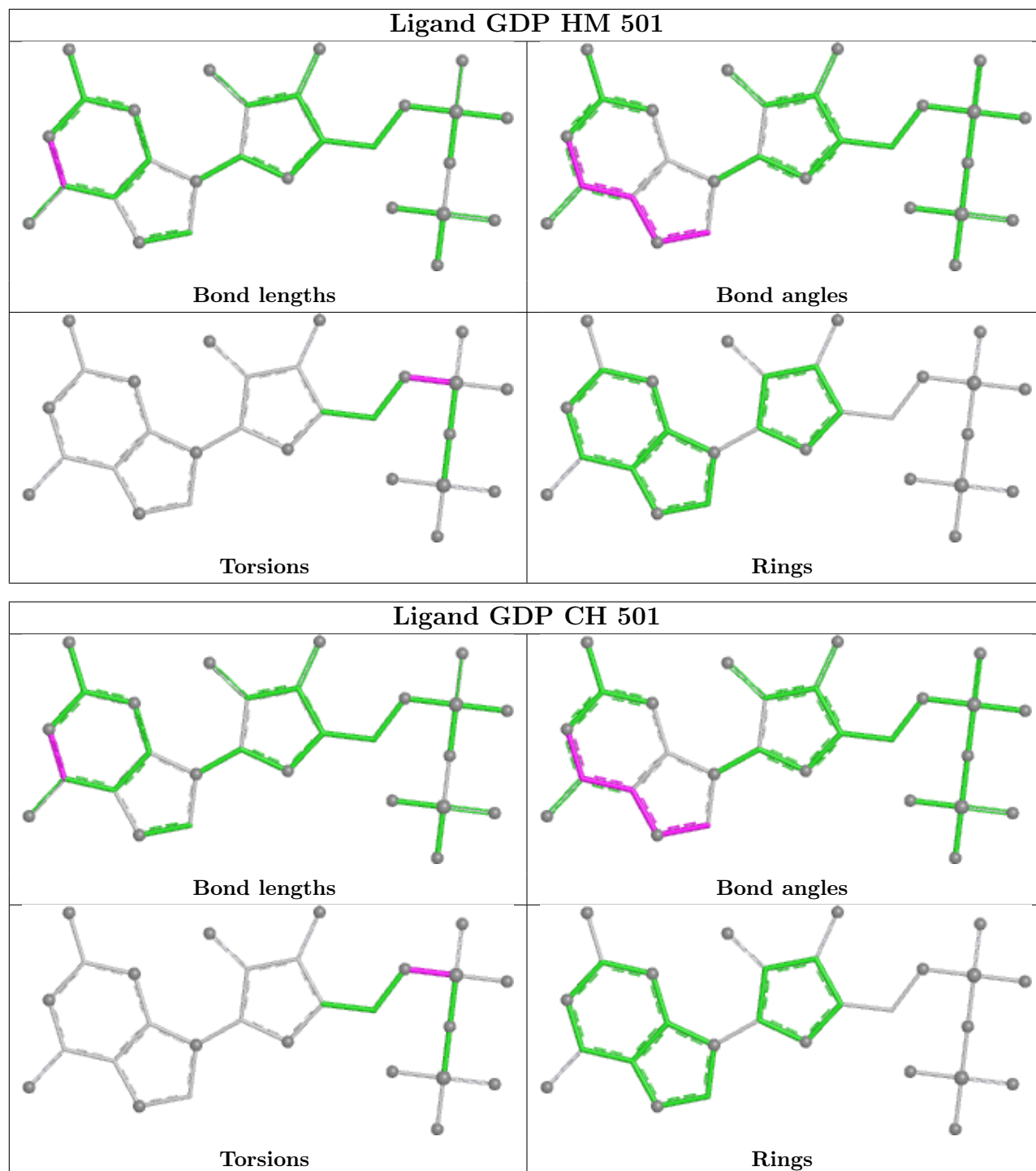


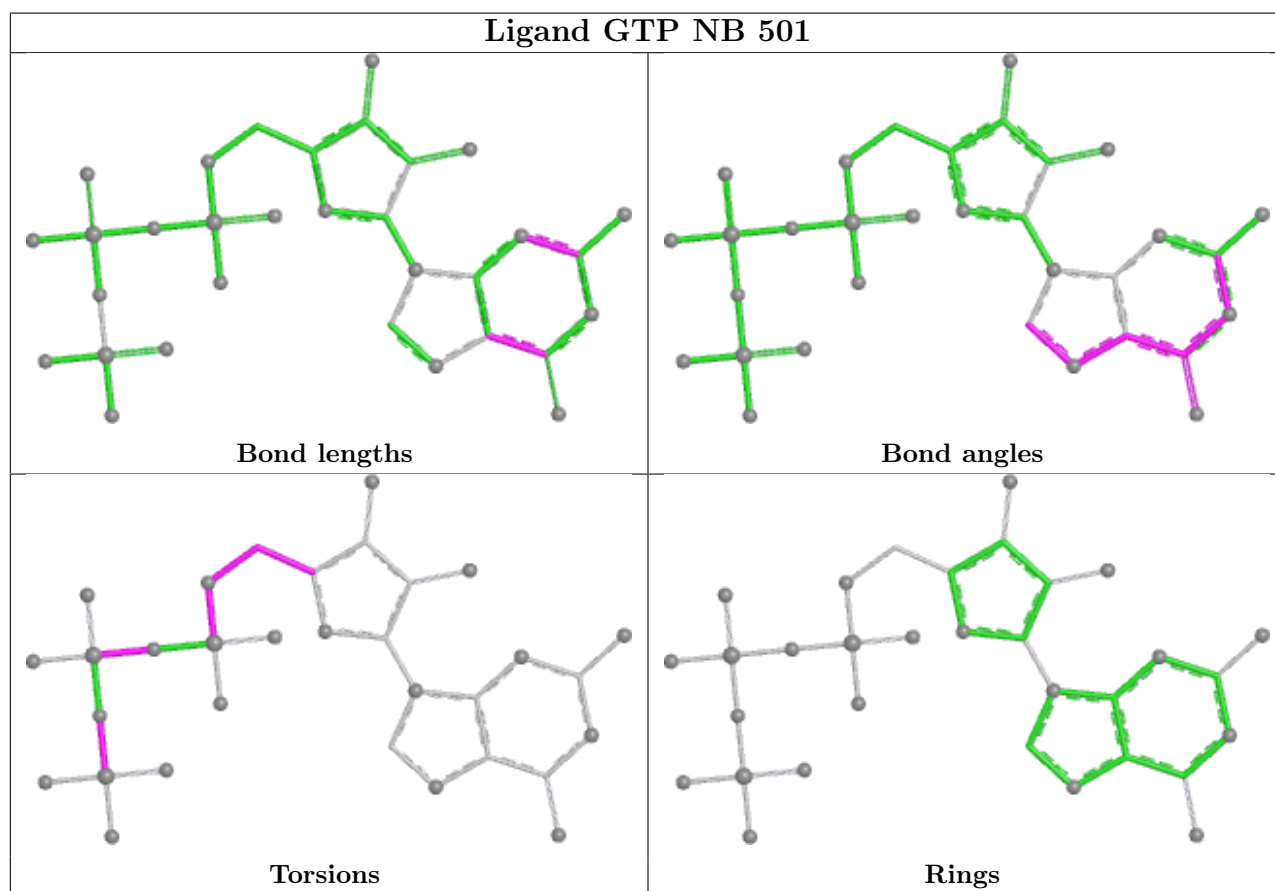
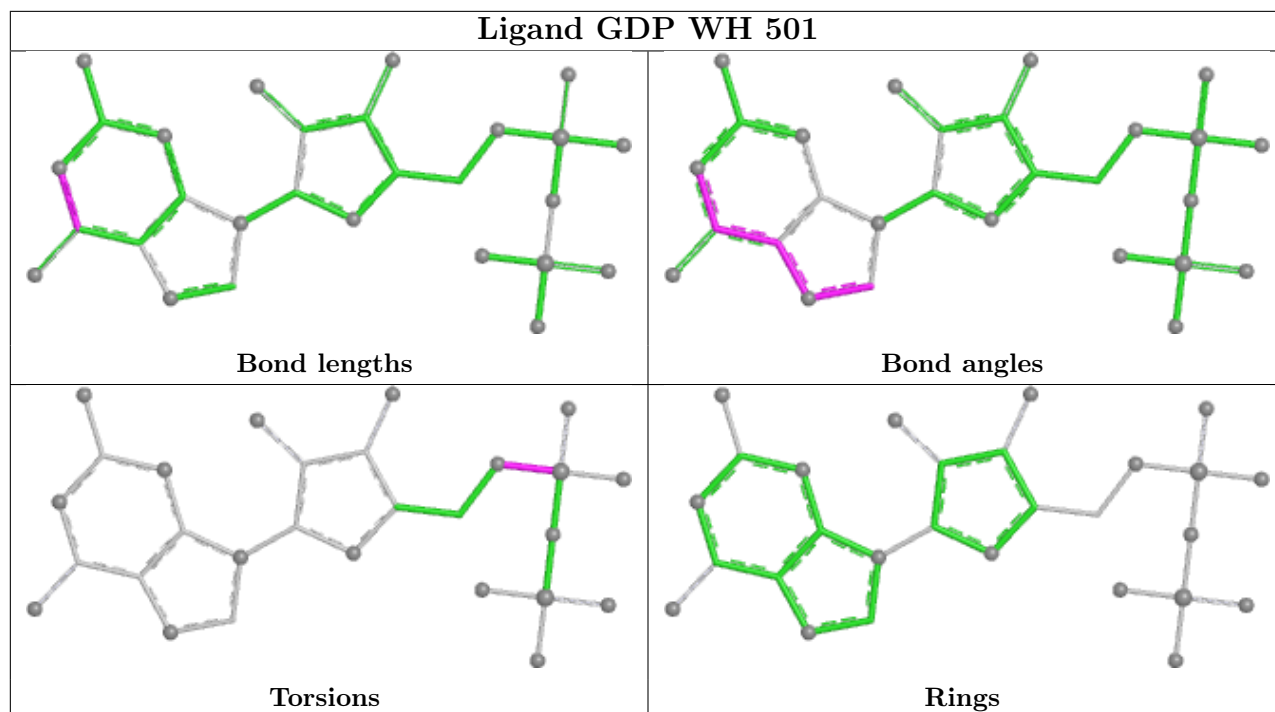


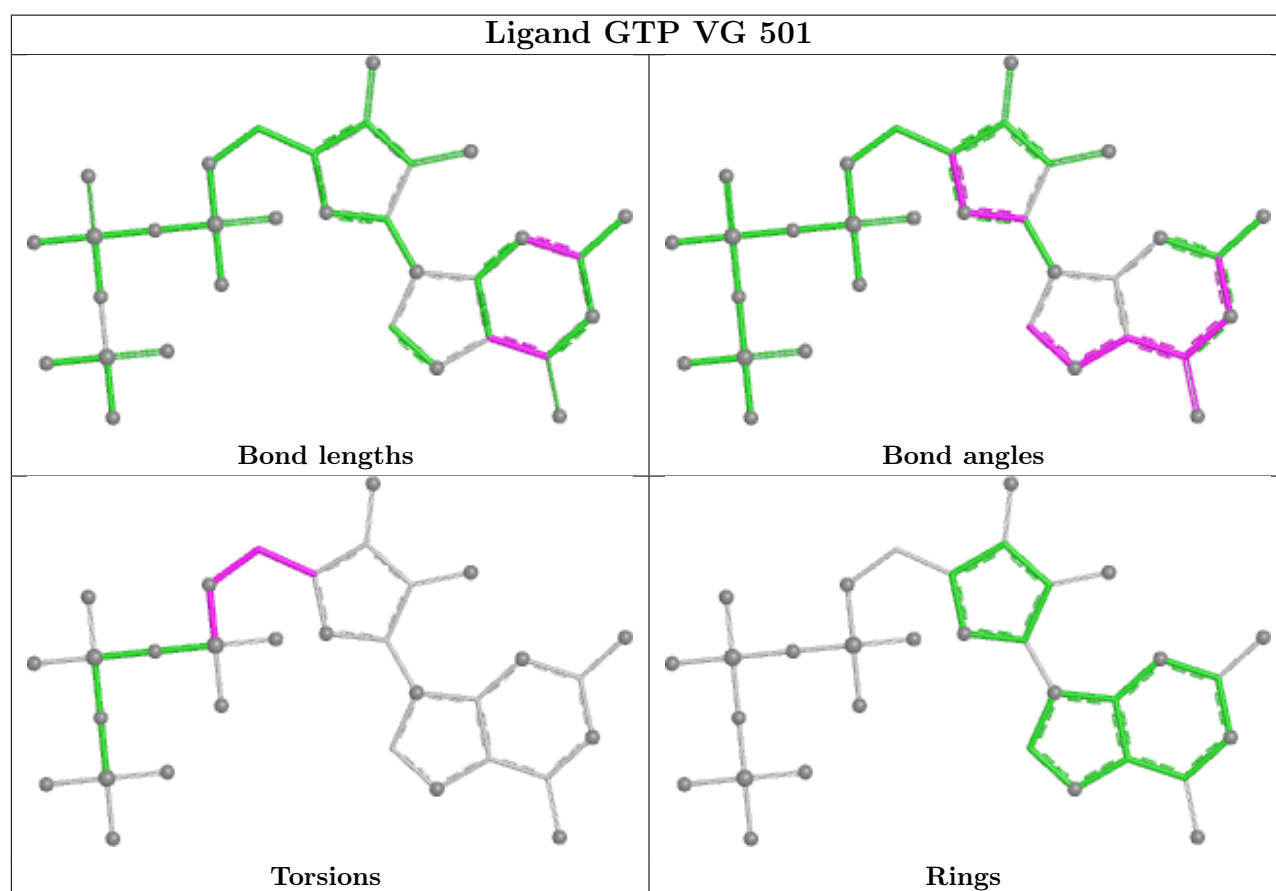
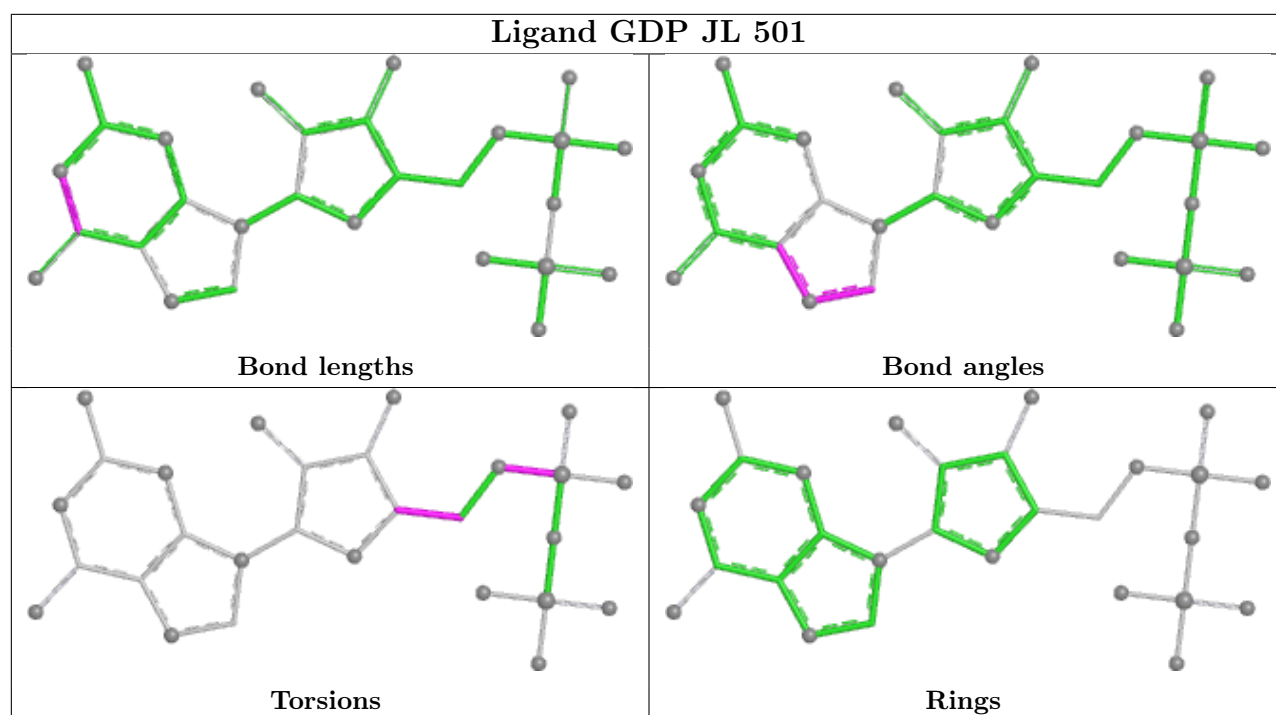


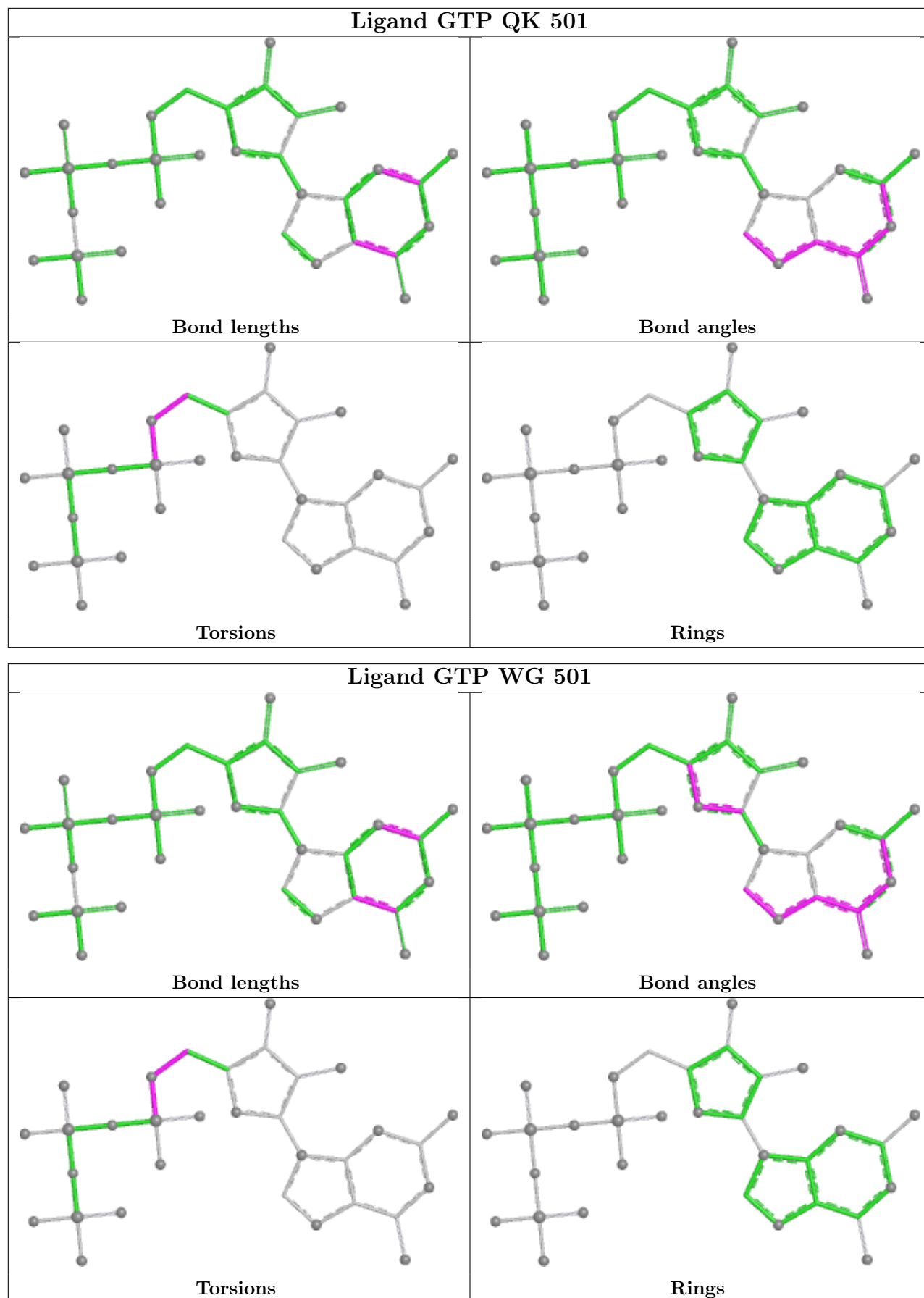


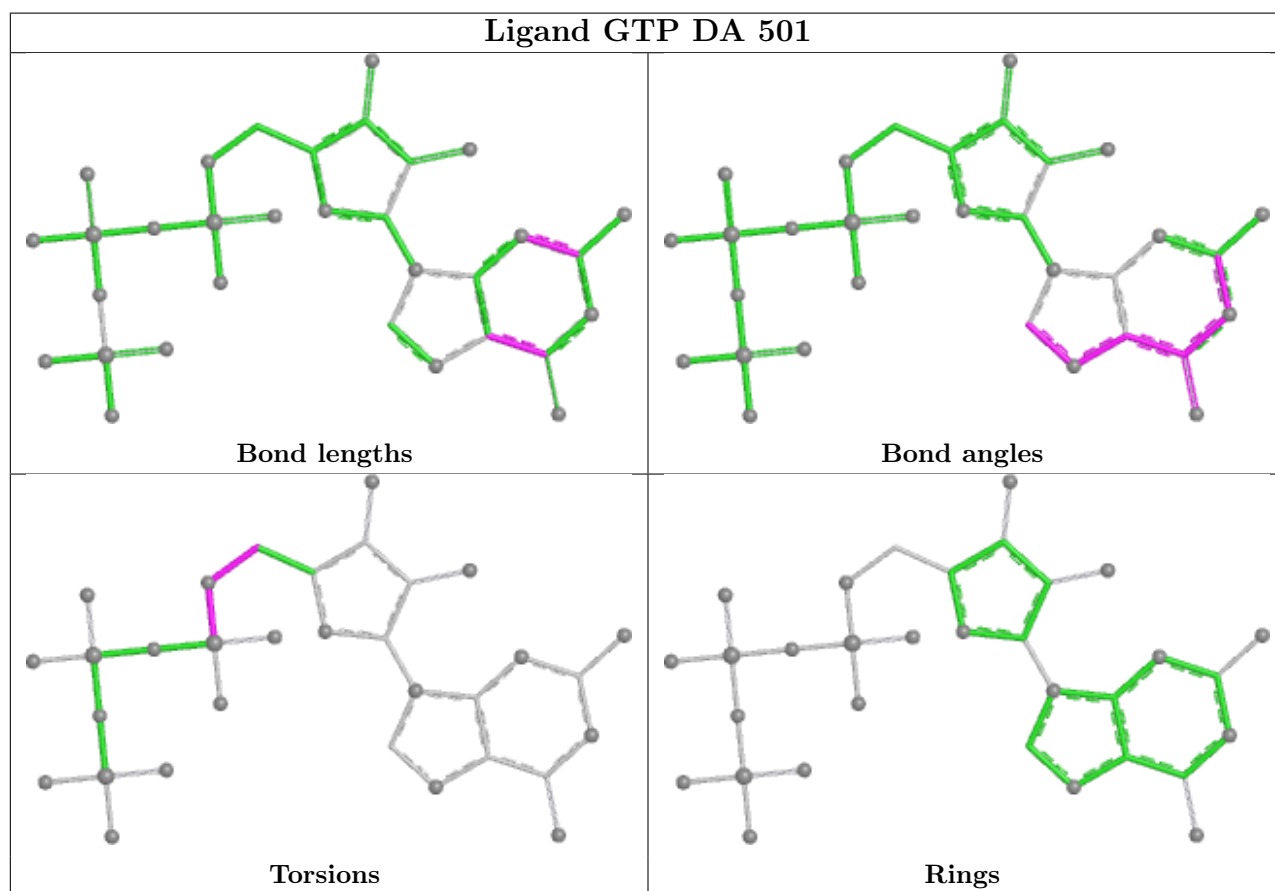
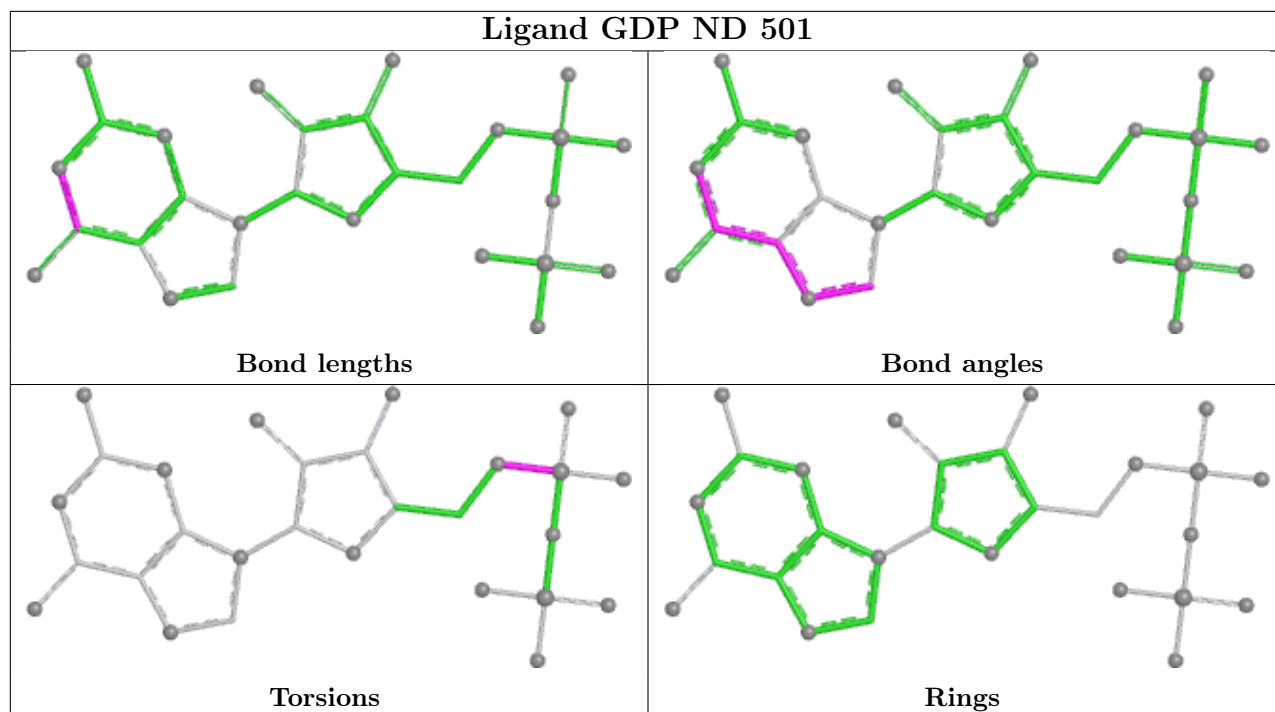


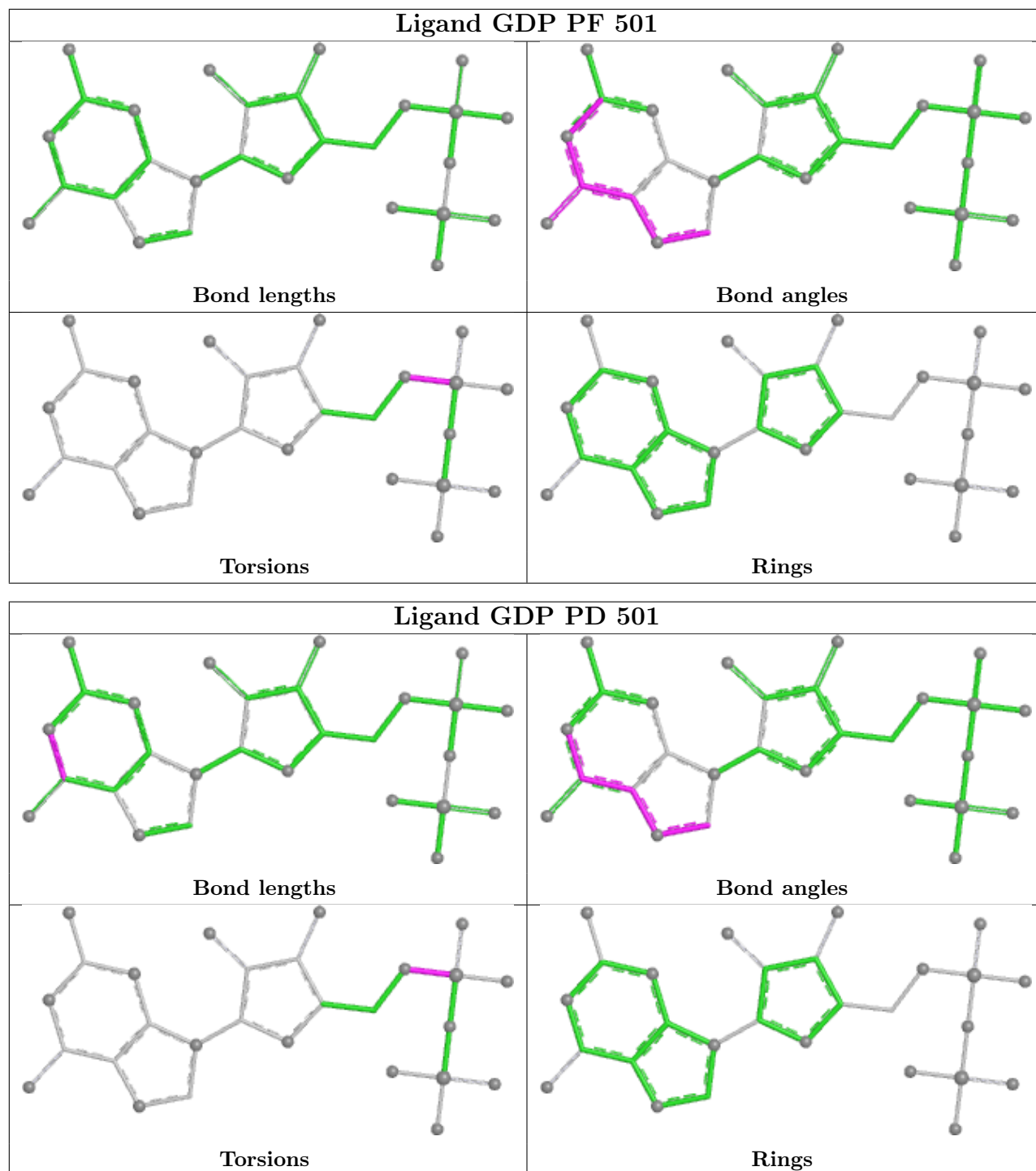


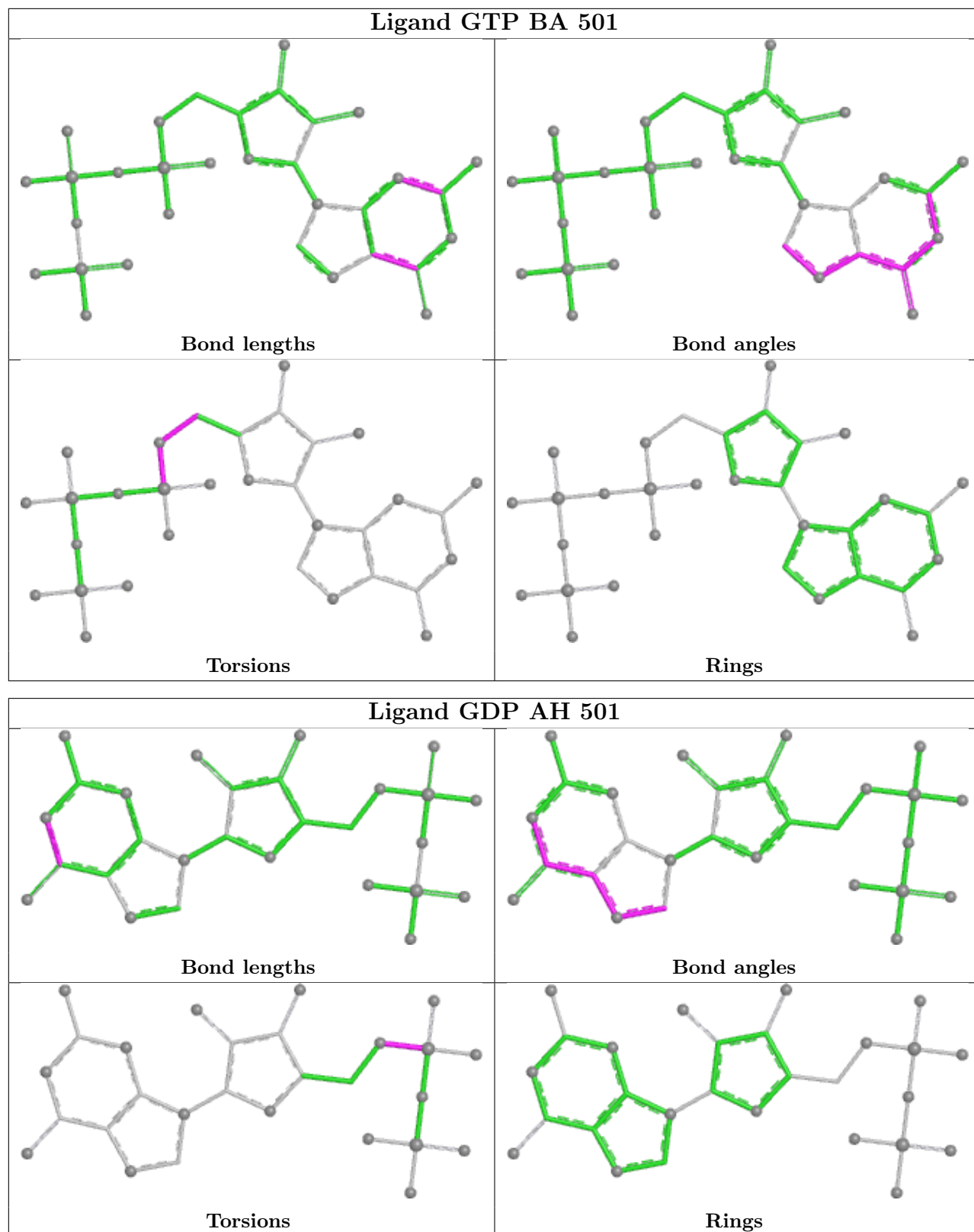


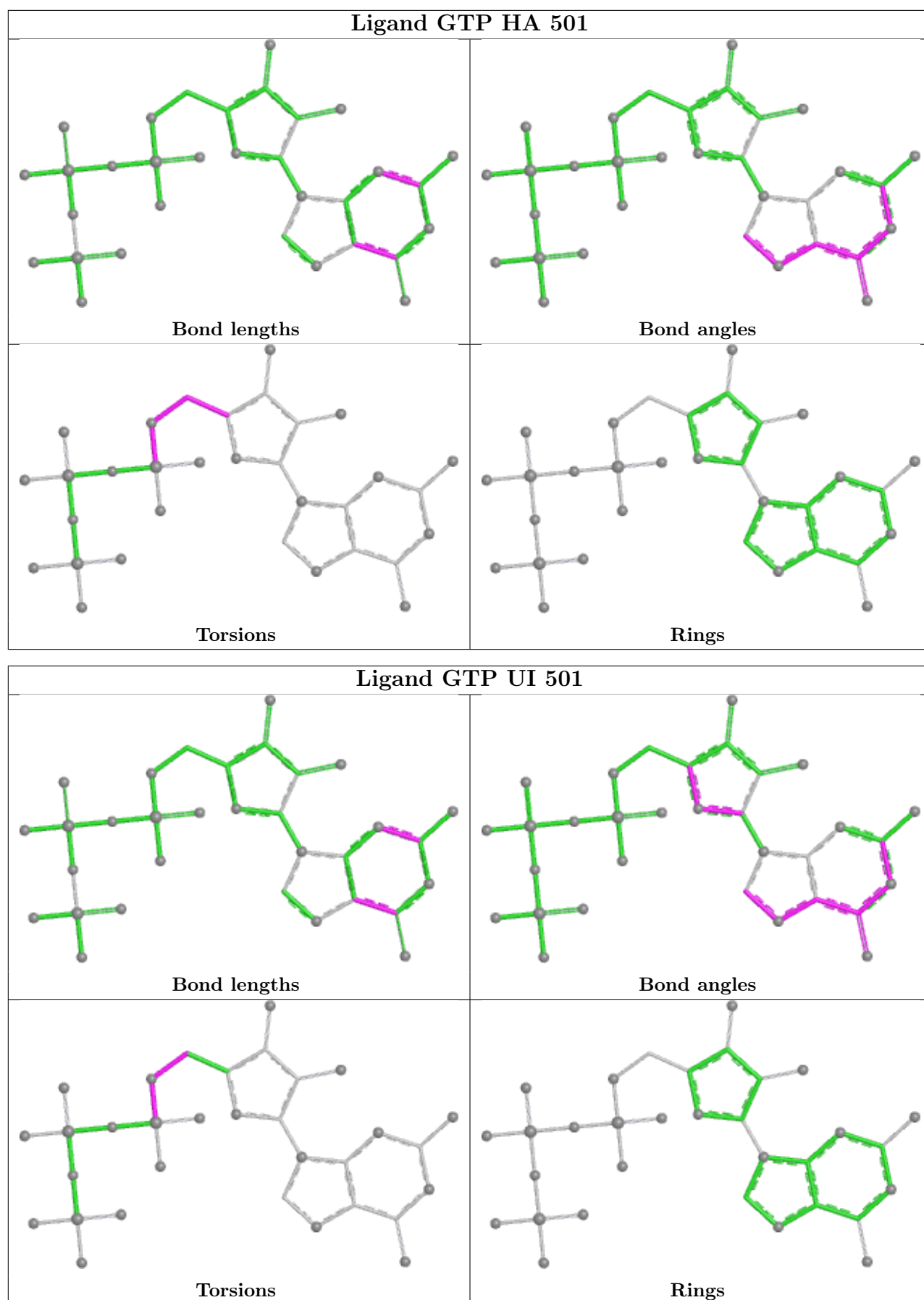


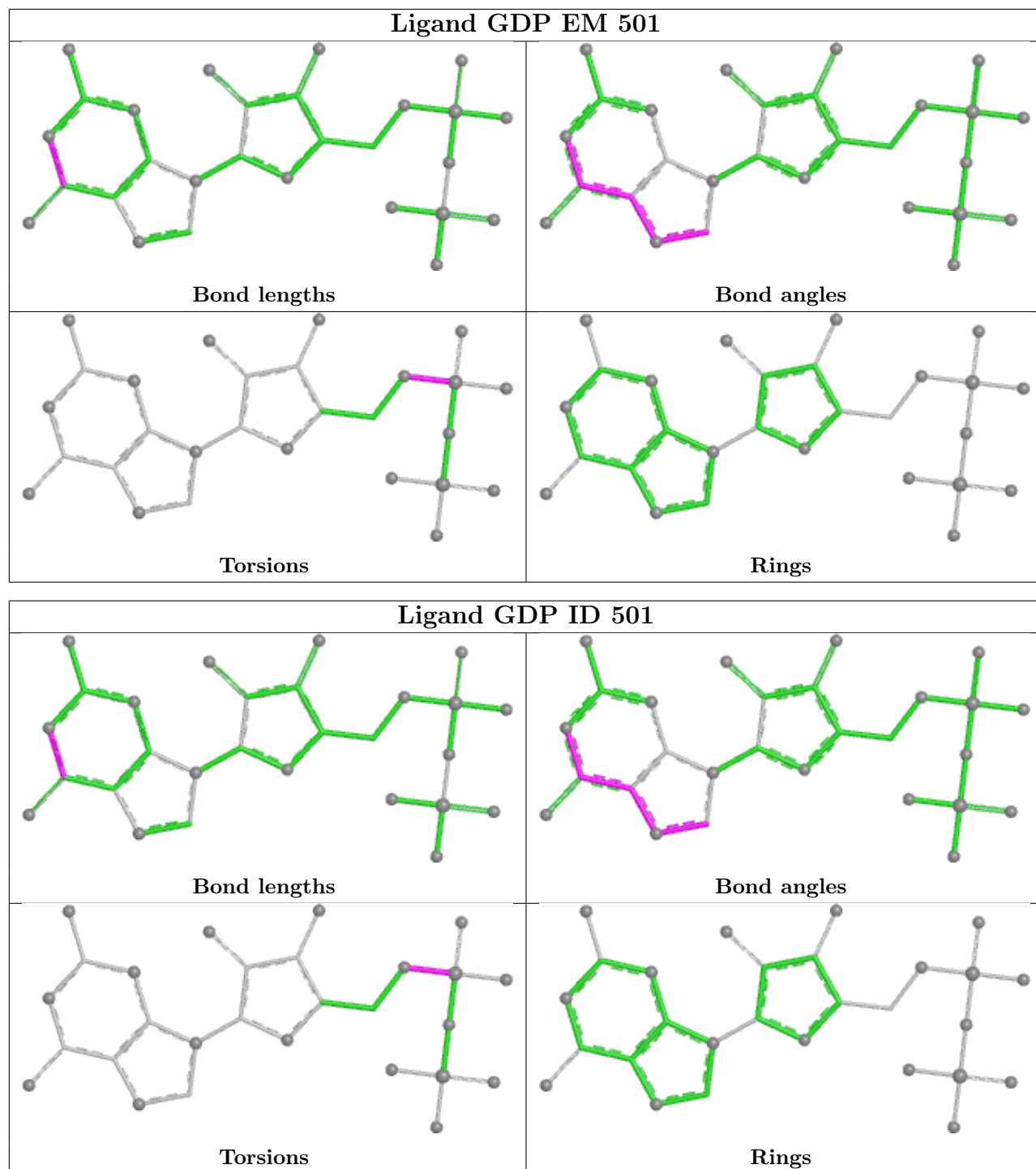


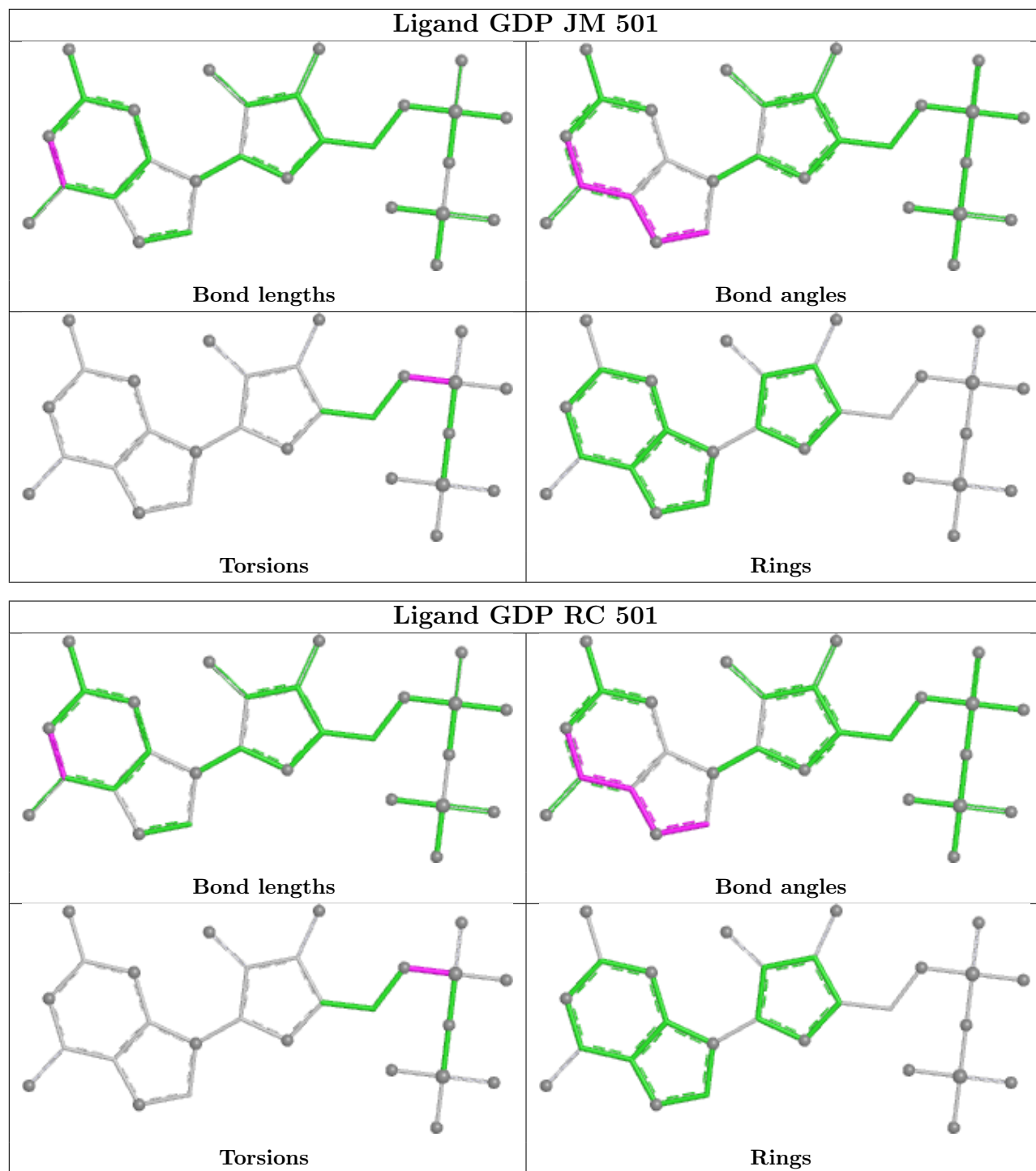


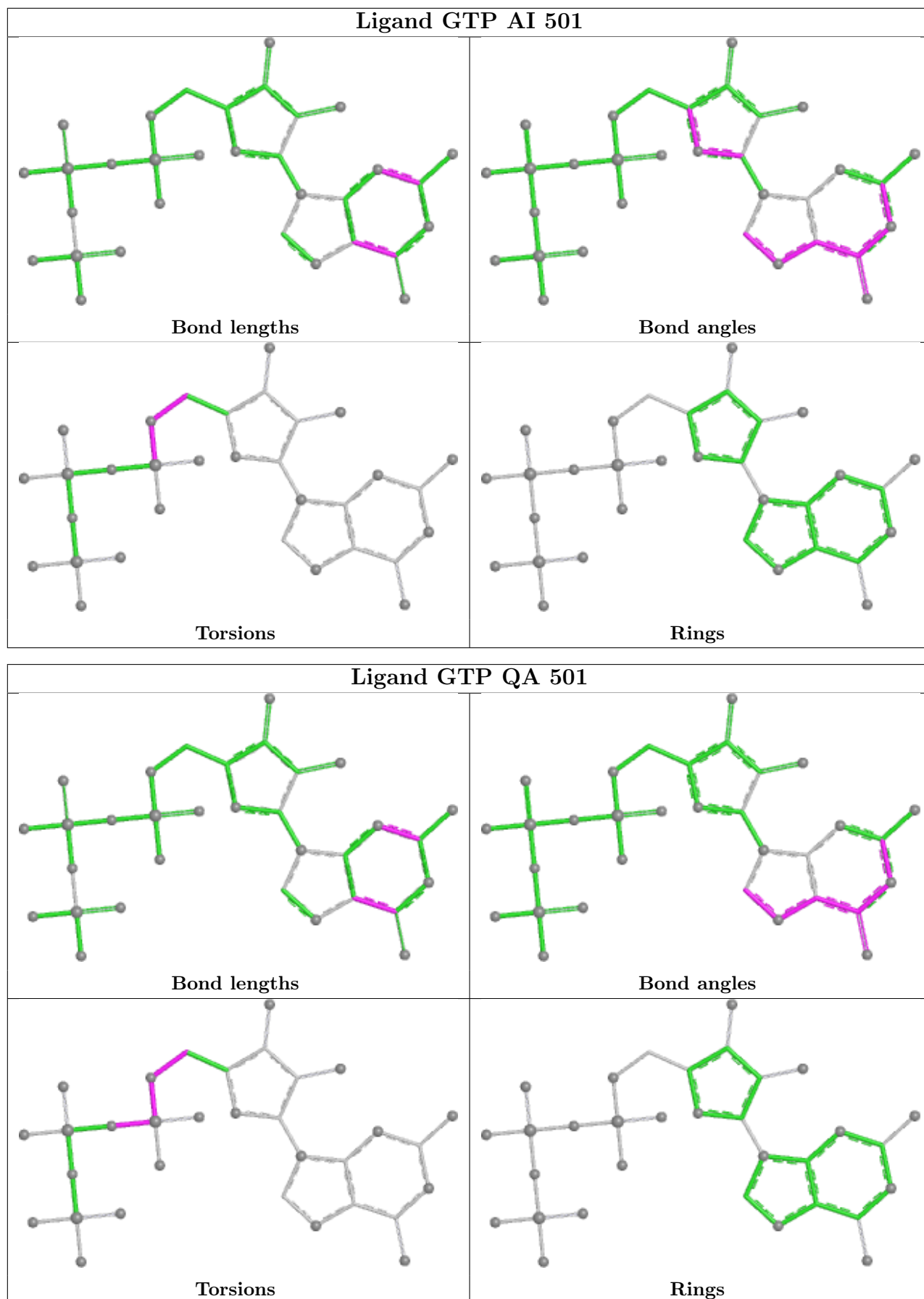


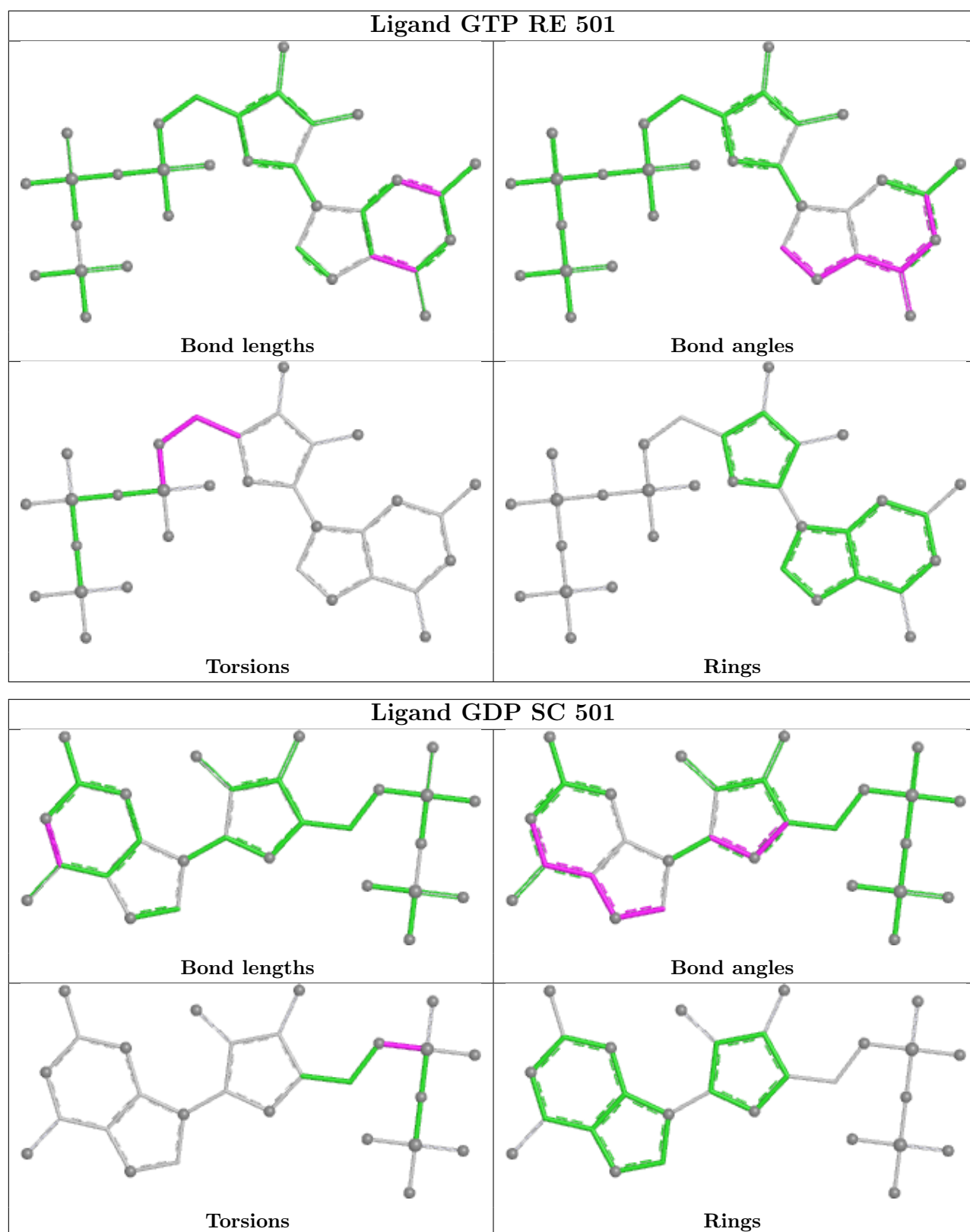


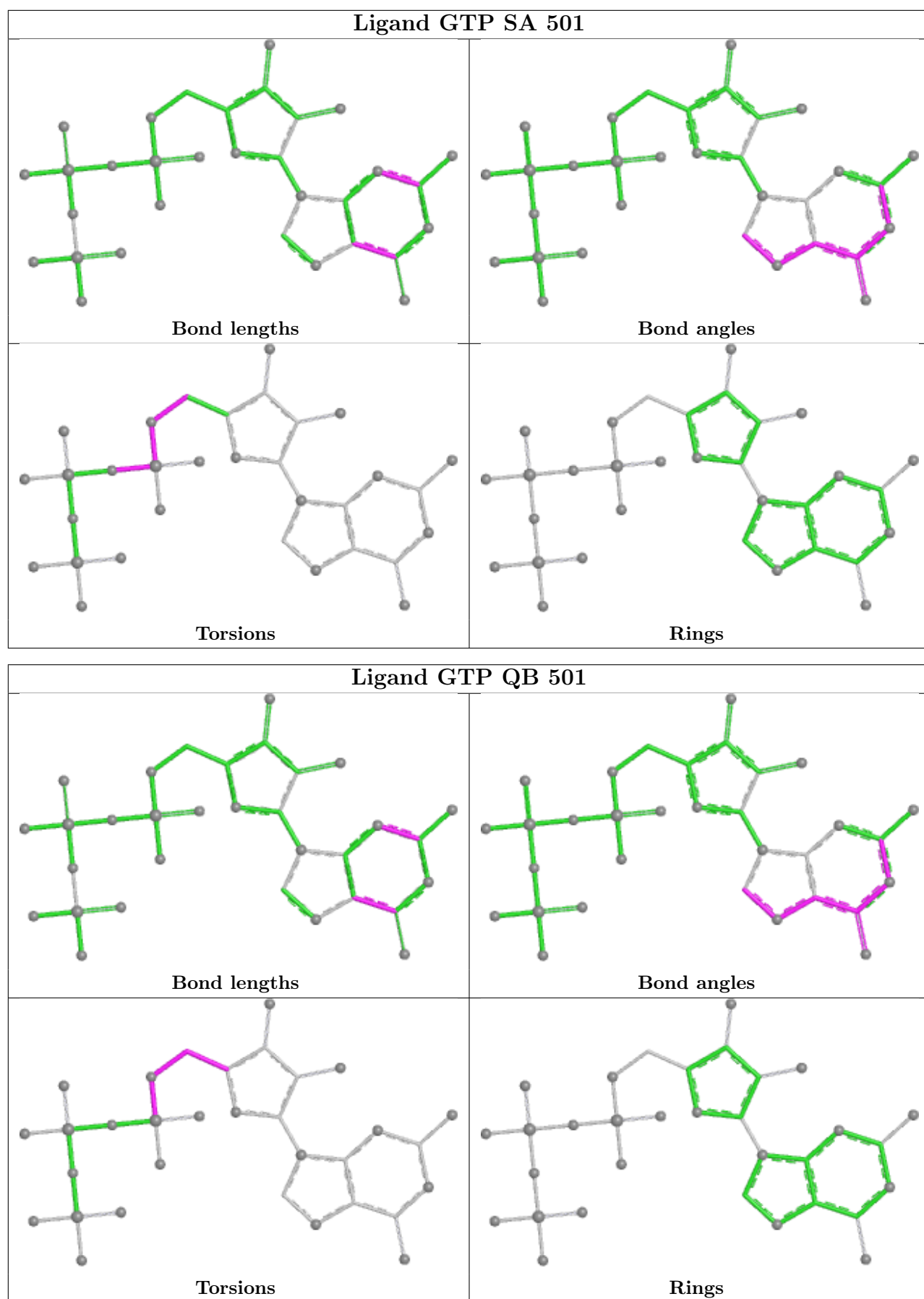


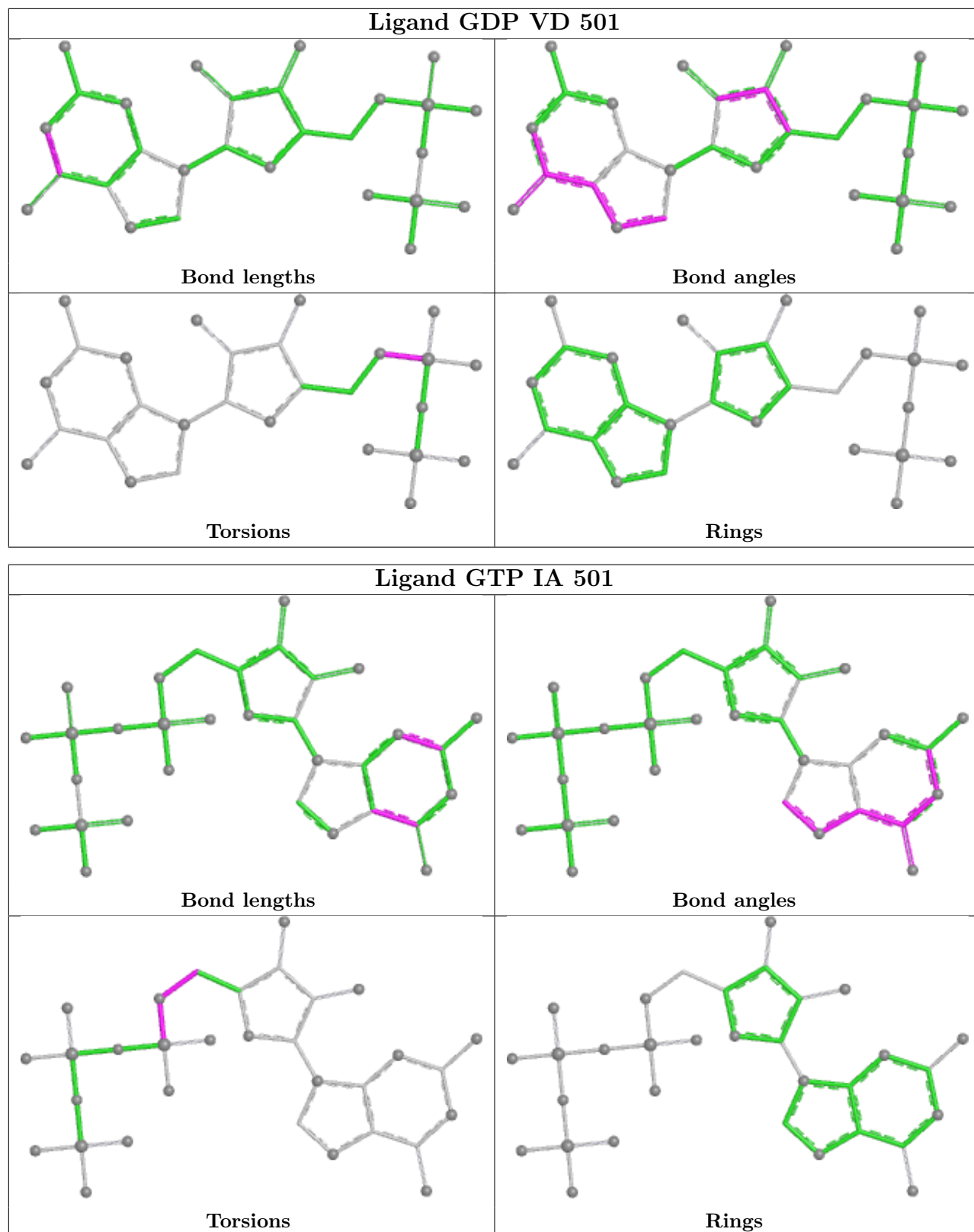


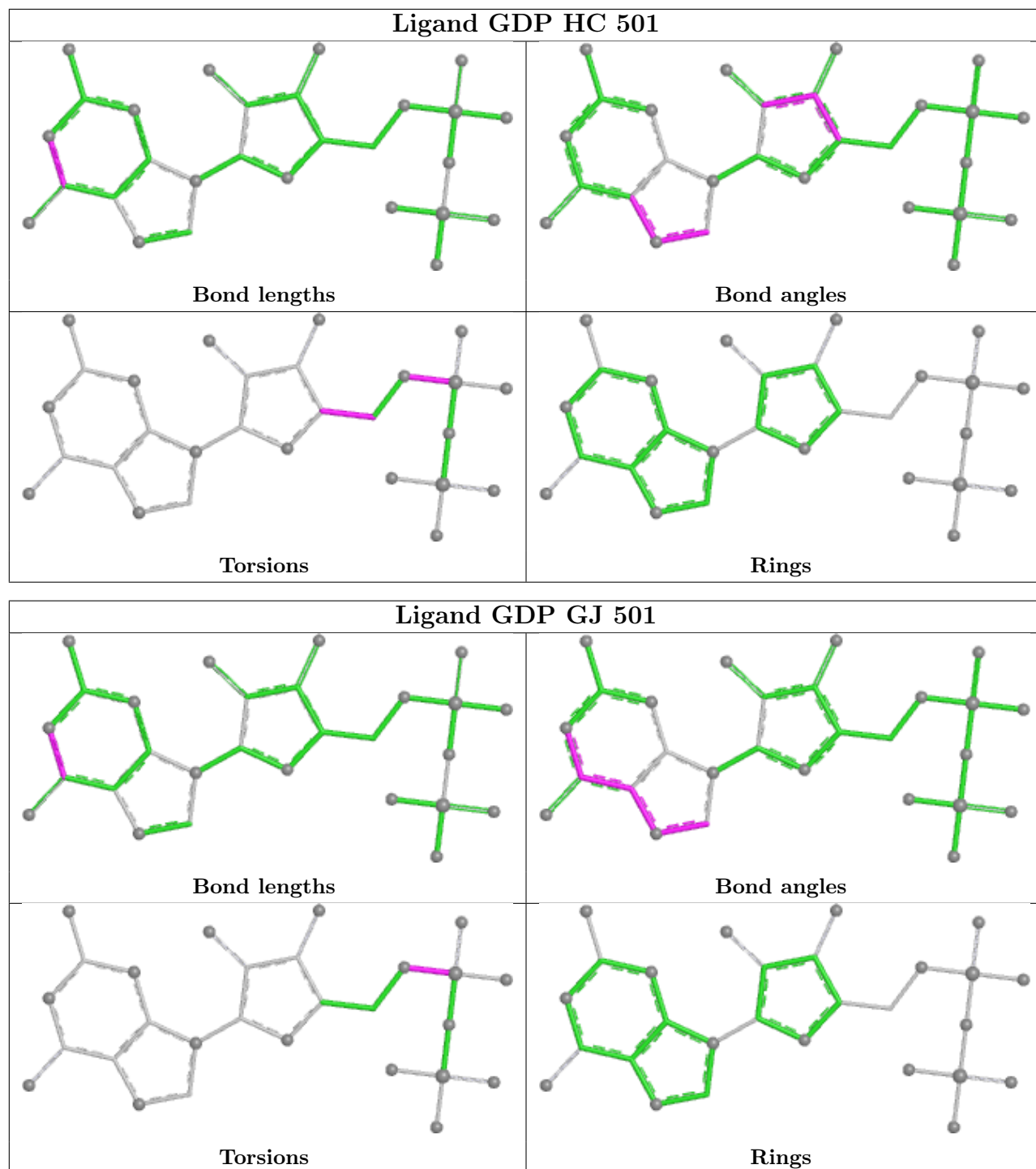


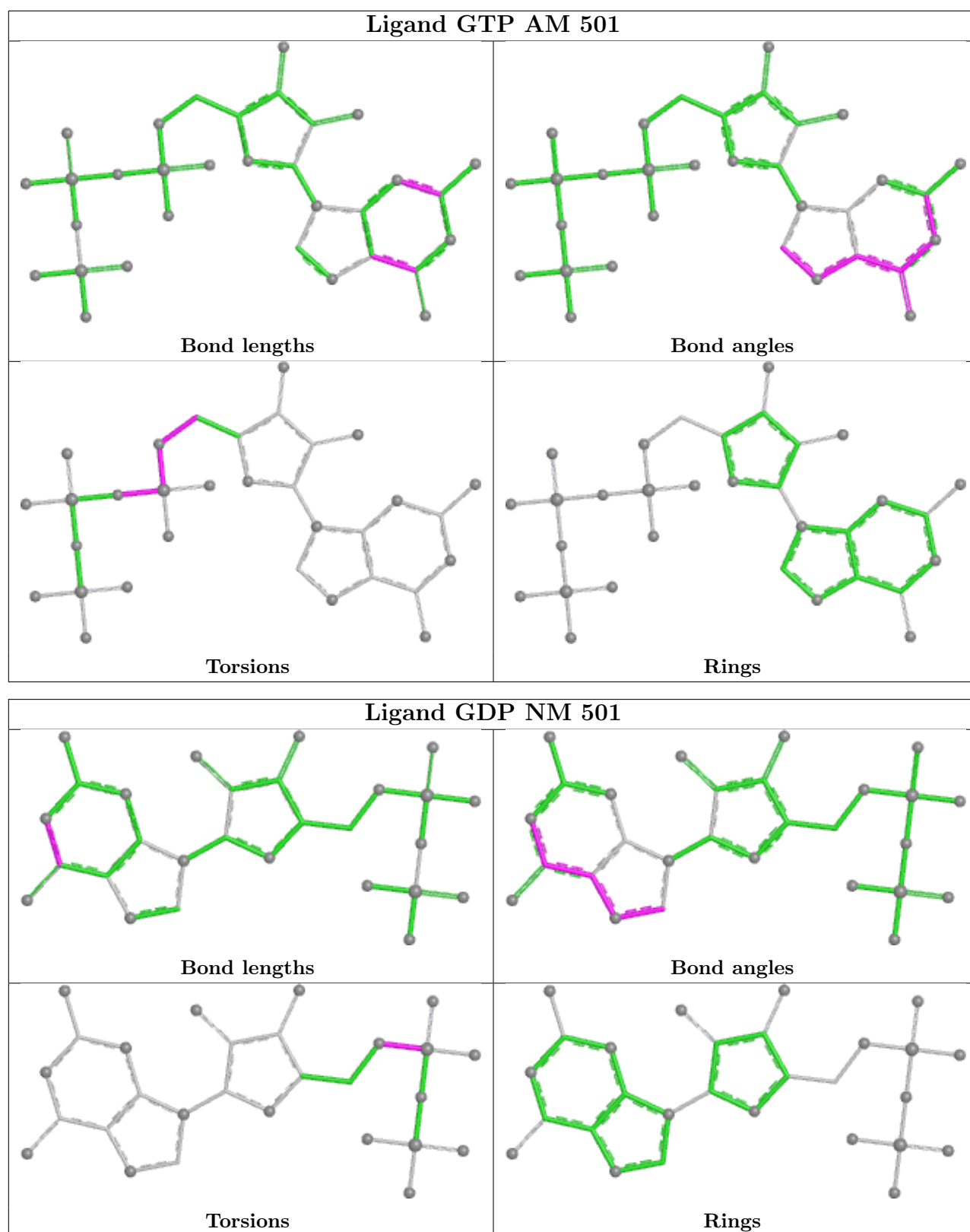


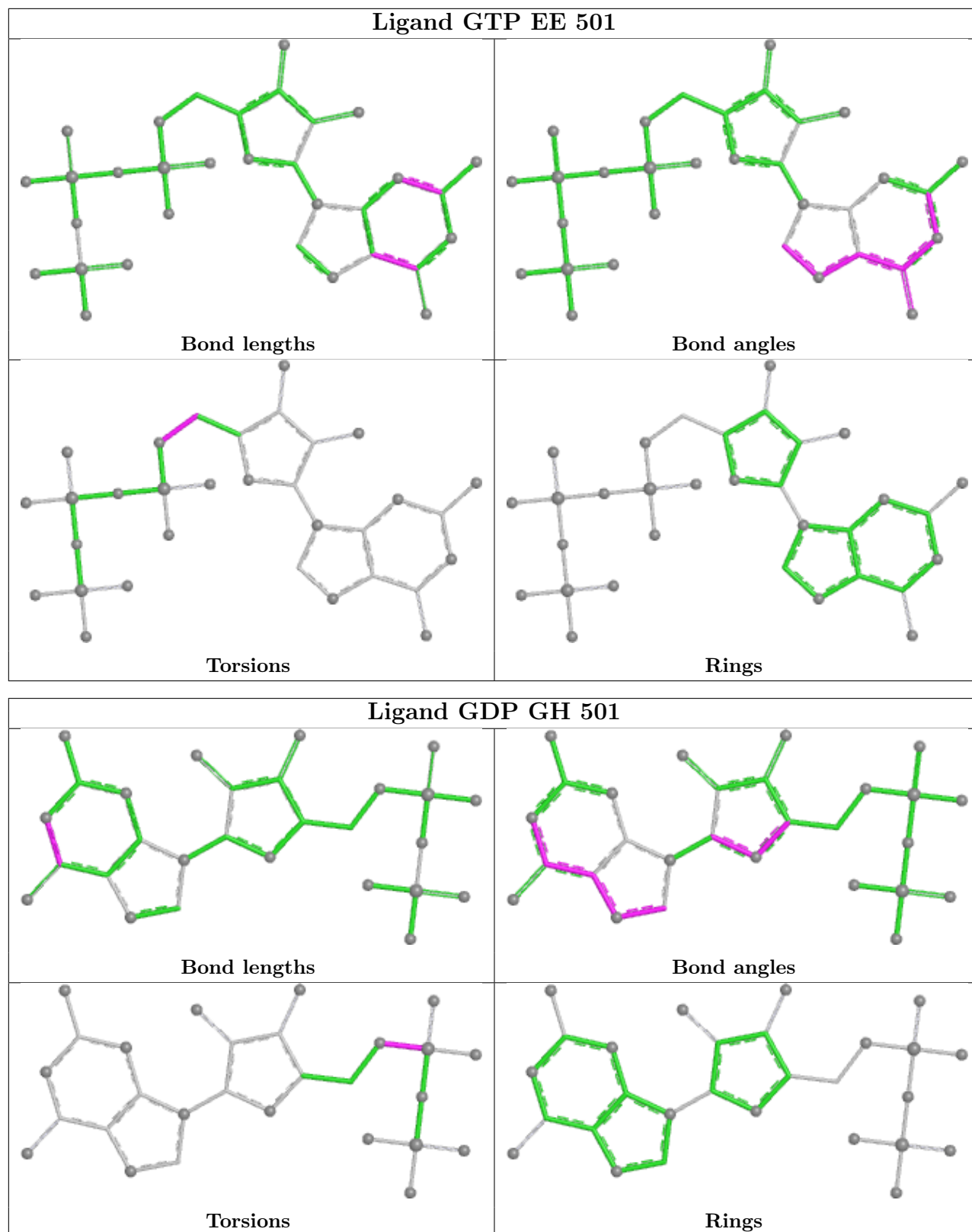


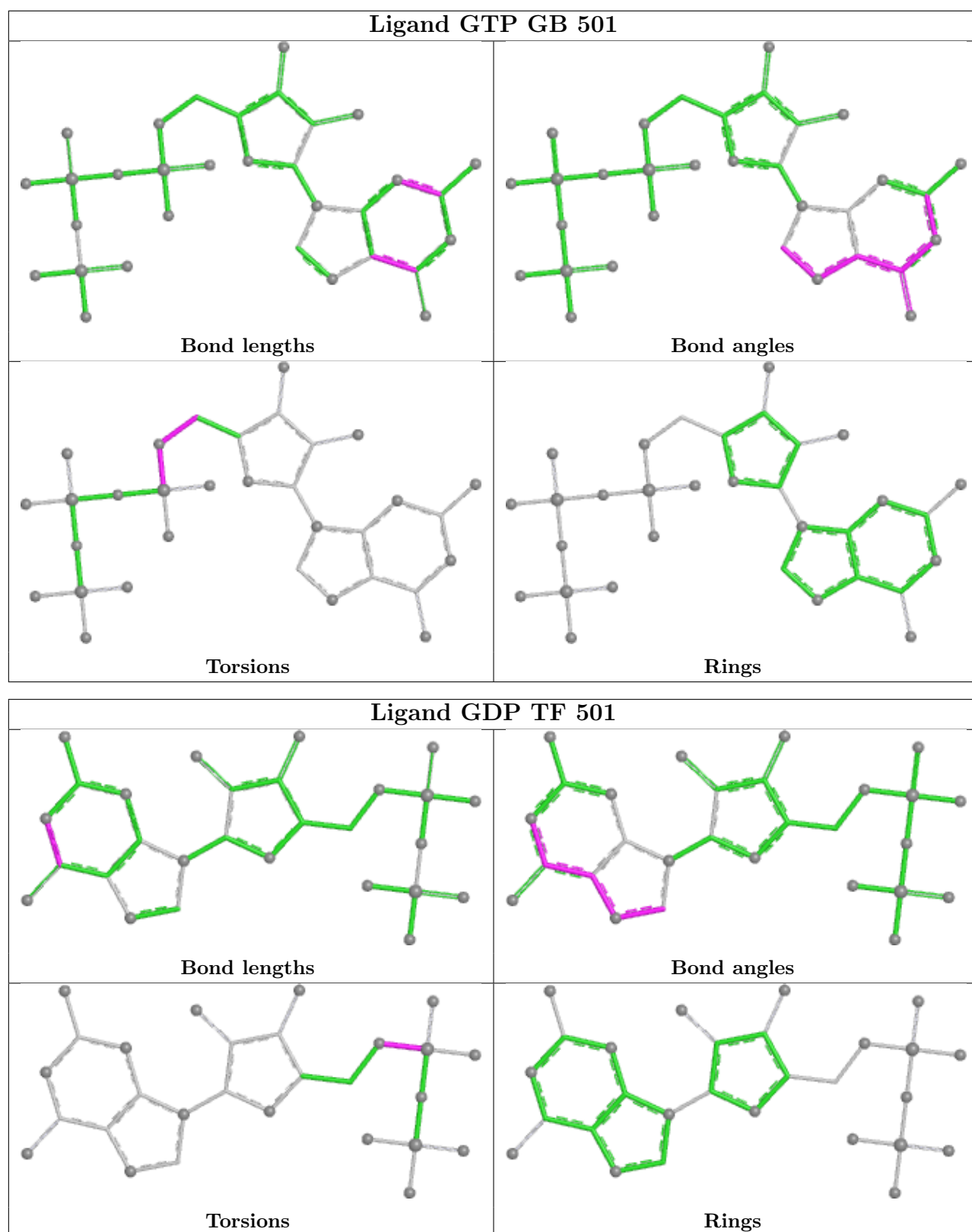


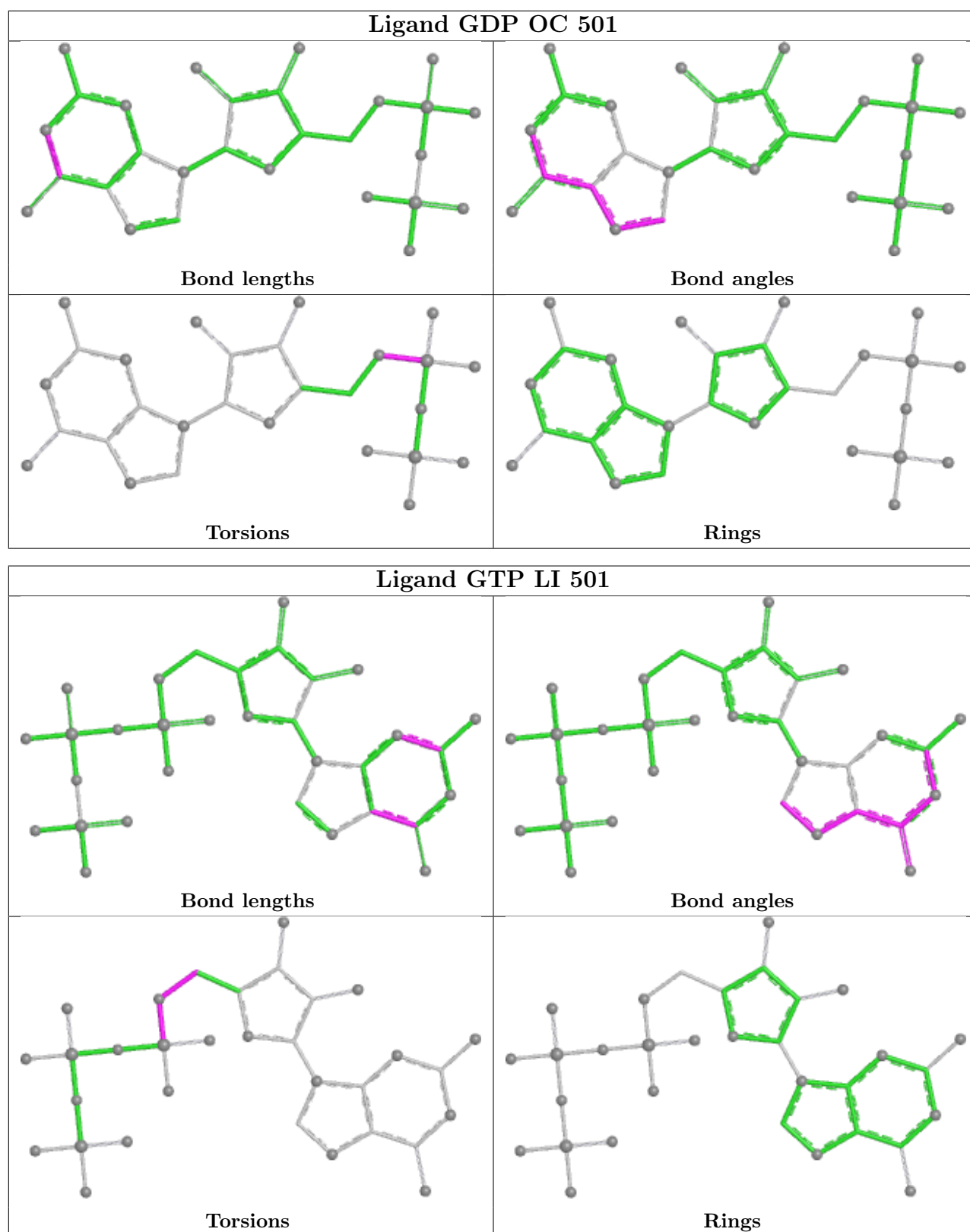












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

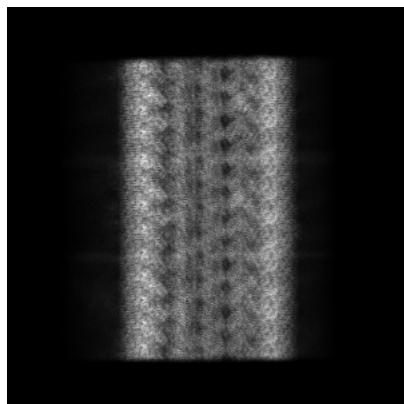
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40619. These allow visual inspection of the internal detail of the map and identification of artifacts.

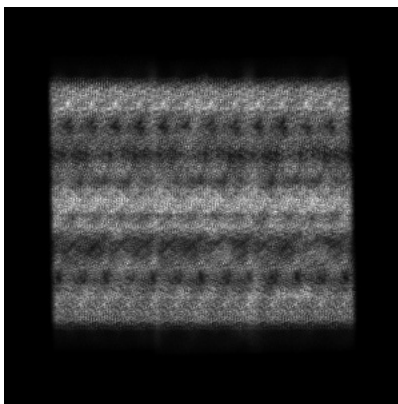
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

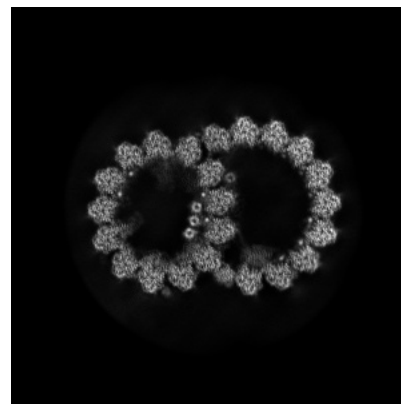
6.1.1 Primary map



X

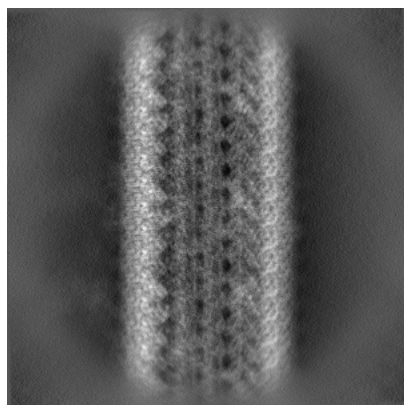


Y

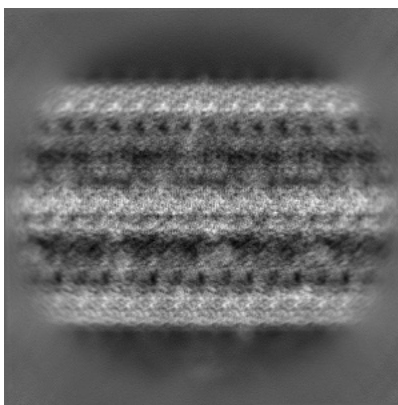


Z

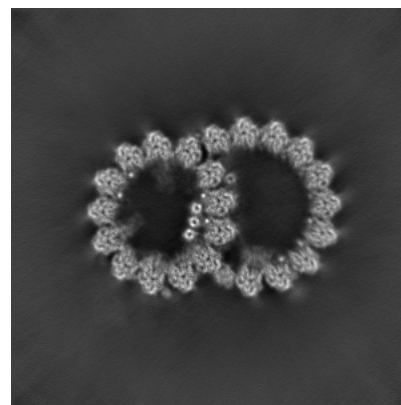
6.1.2 Raw map



X



Y

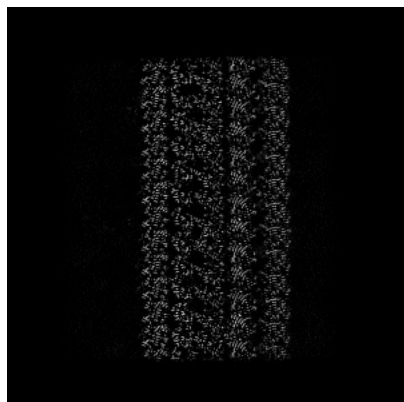


Z

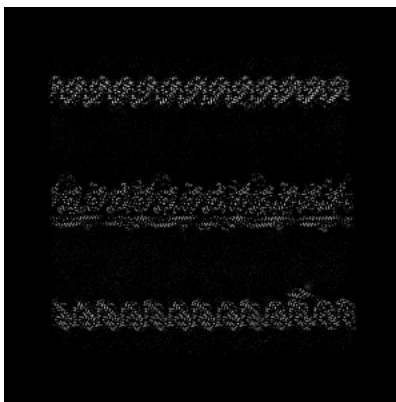
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

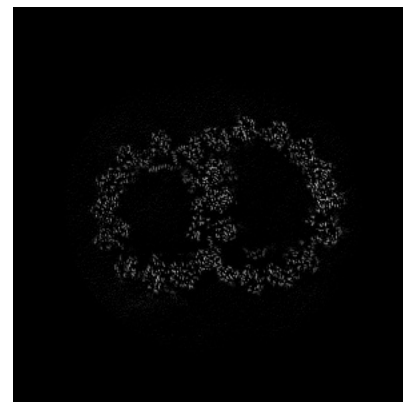
6.2.1 Primary map



X Index: 256

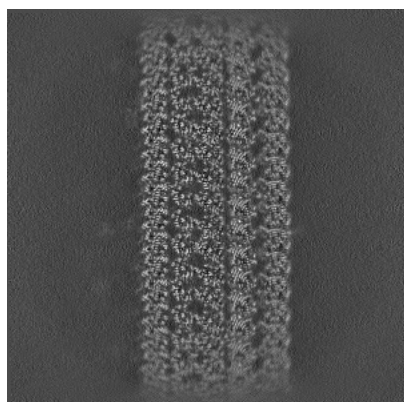


Y Index: 256

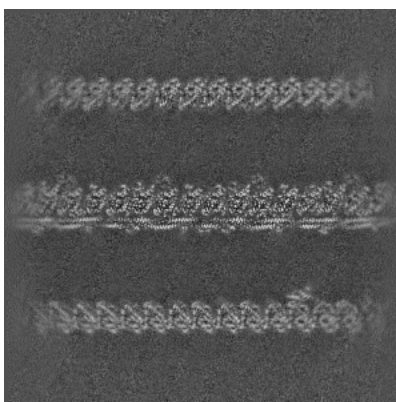


Z Index: 256

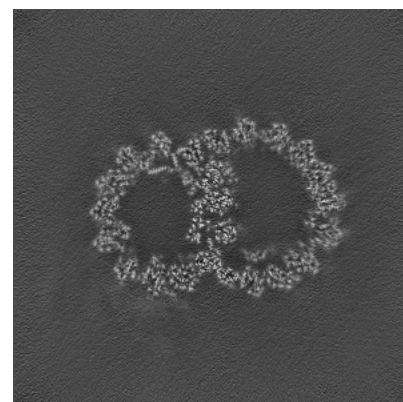
6.2.2 Raw map



X Index: 256



Y Index: 256

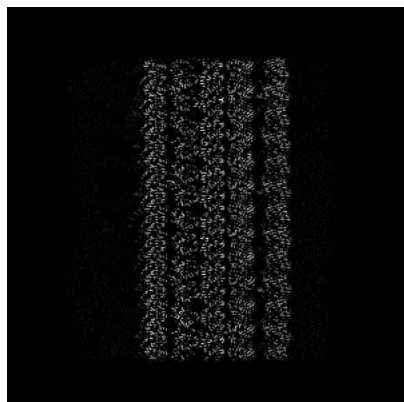


Z Index: 256

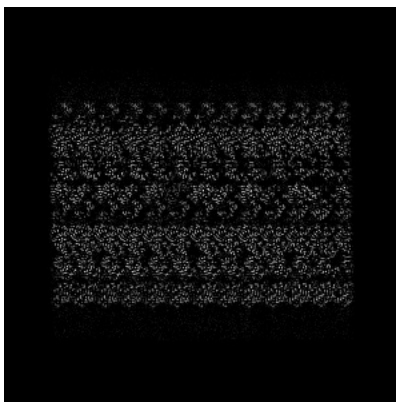
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

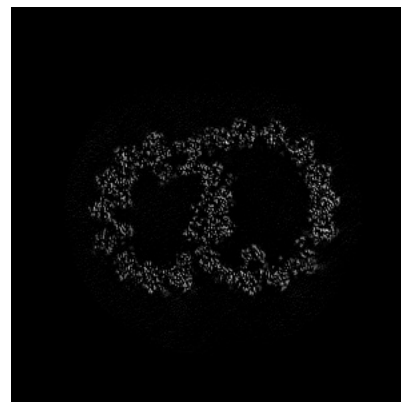
6.3.1 Primary map



X Index: 258

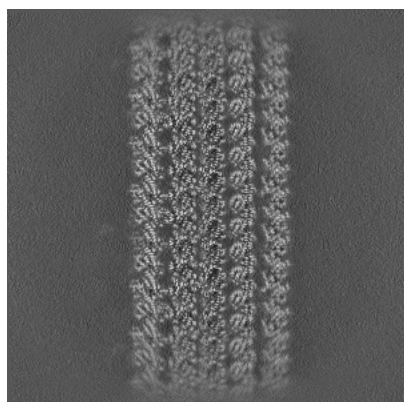


Y Index: 174

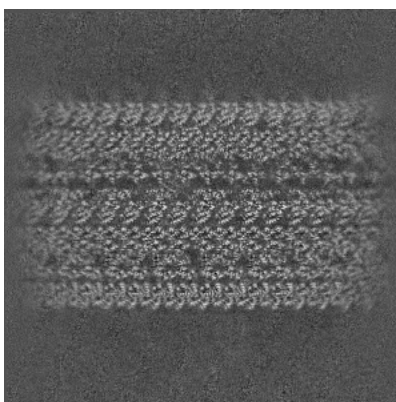


Z Index: 385

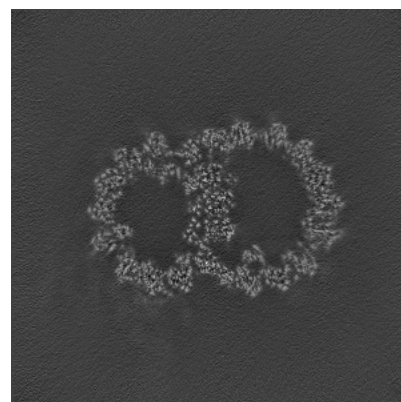
6.3.2 Raw map



X Index: 264



Y Index: 177

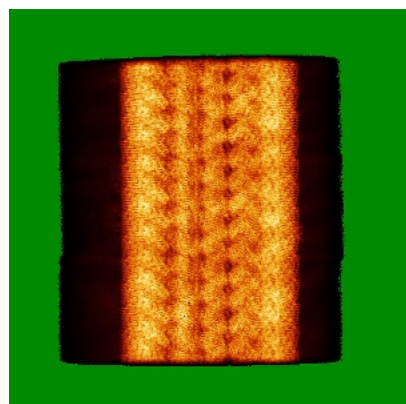


Z Index: 260

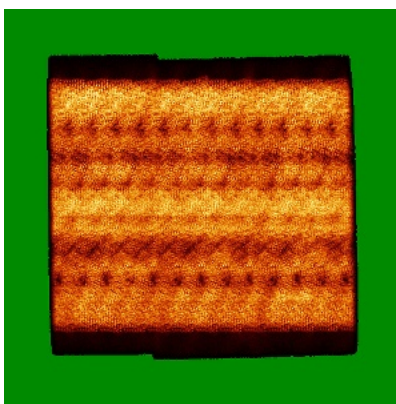
The images above show the largest variance slices of the map in three orthogonal directions.

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

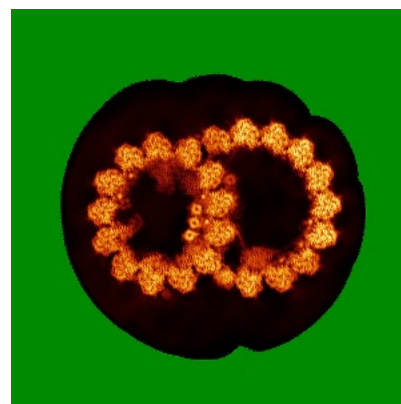
6.4.1 Primary map



X

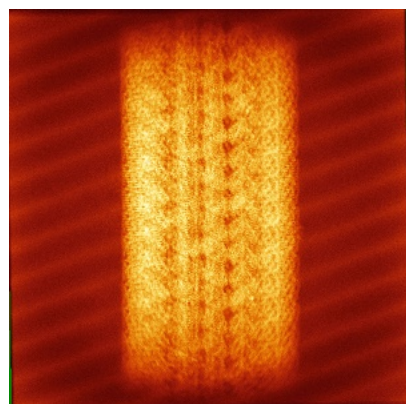


Y

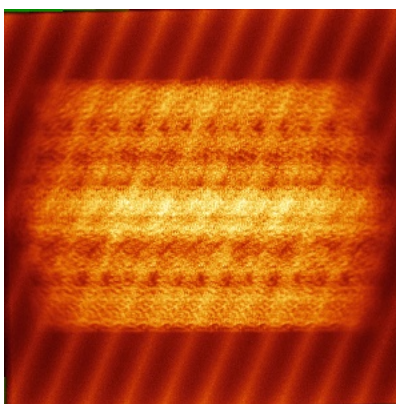


Z

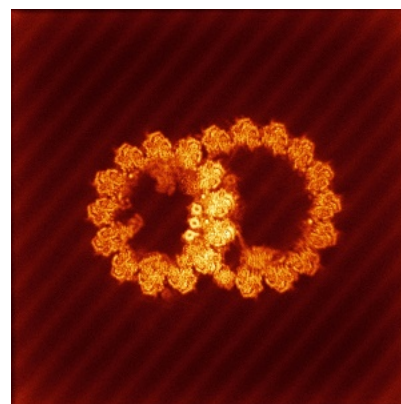
6.4.2 Raw map



X



Y

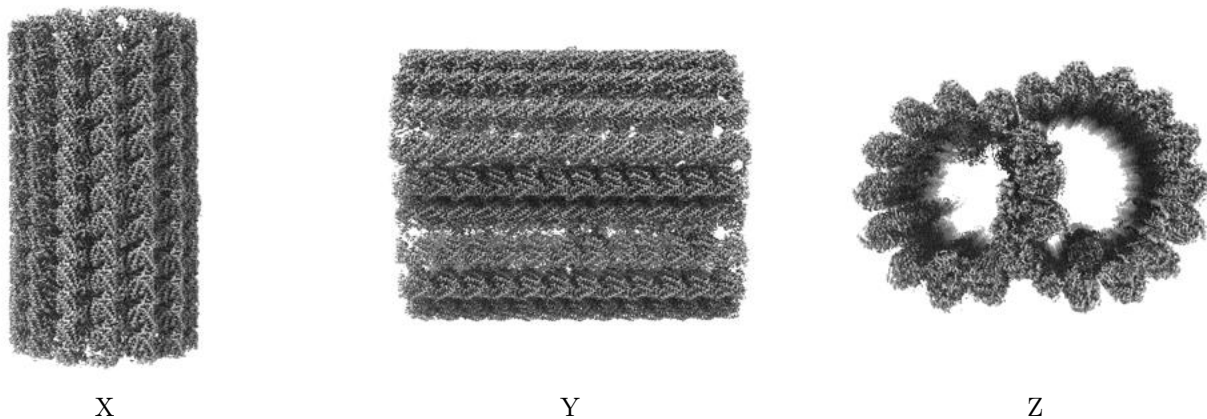


Z

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

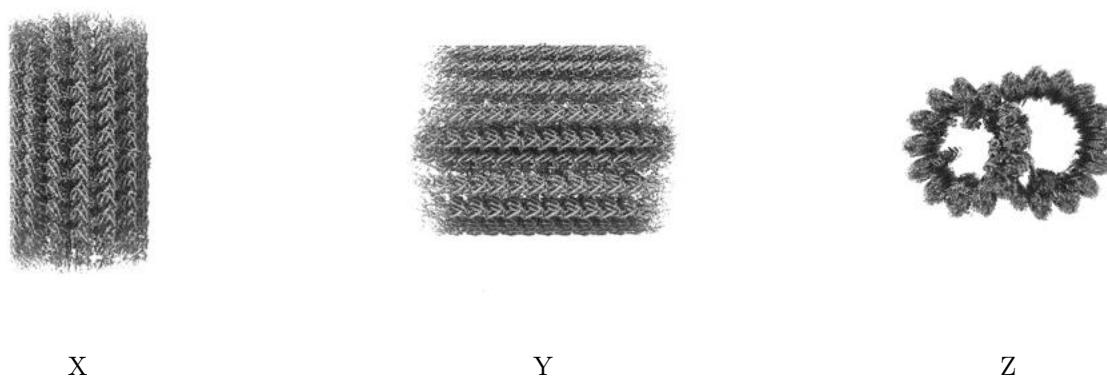
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 6.63. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

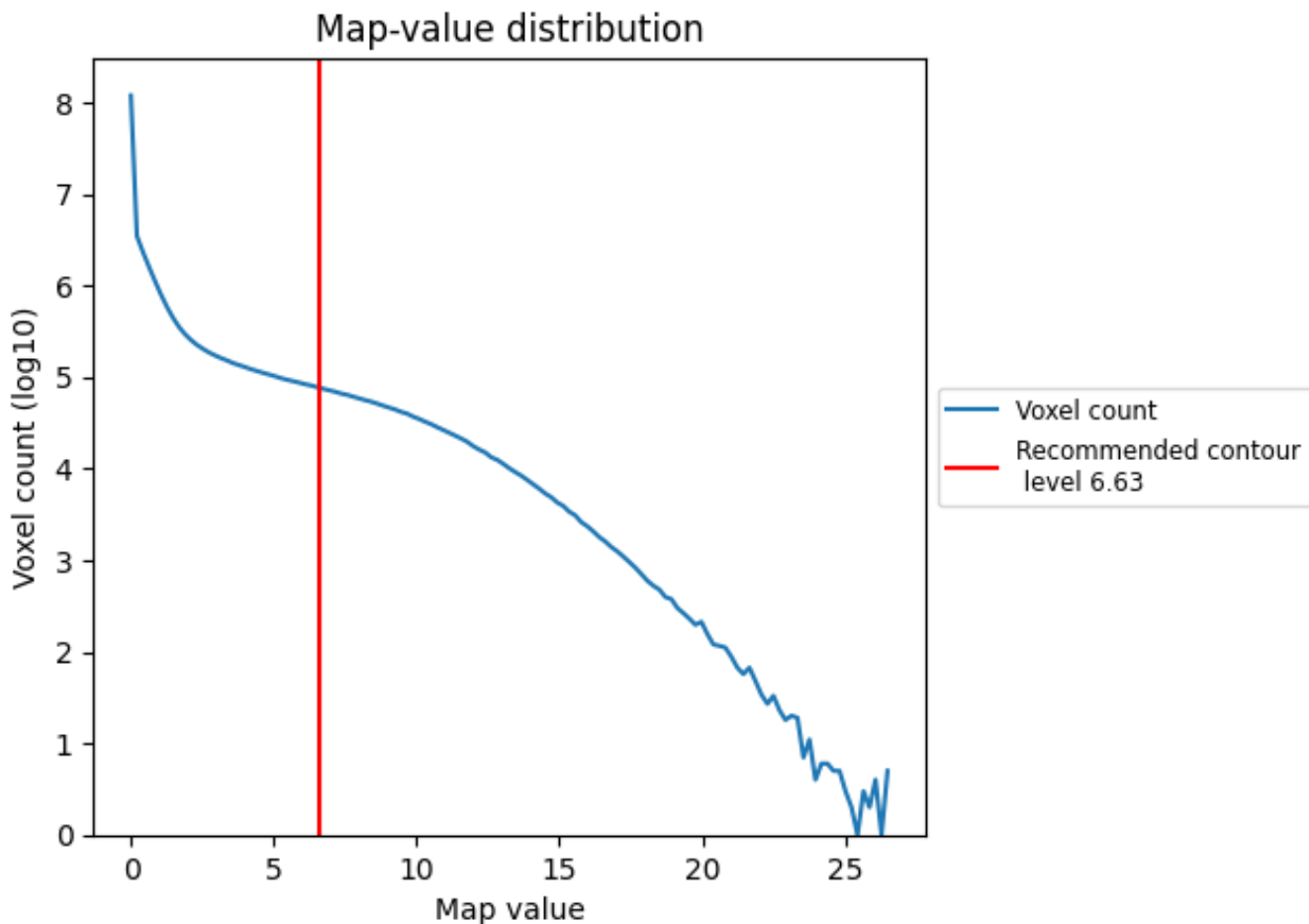
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

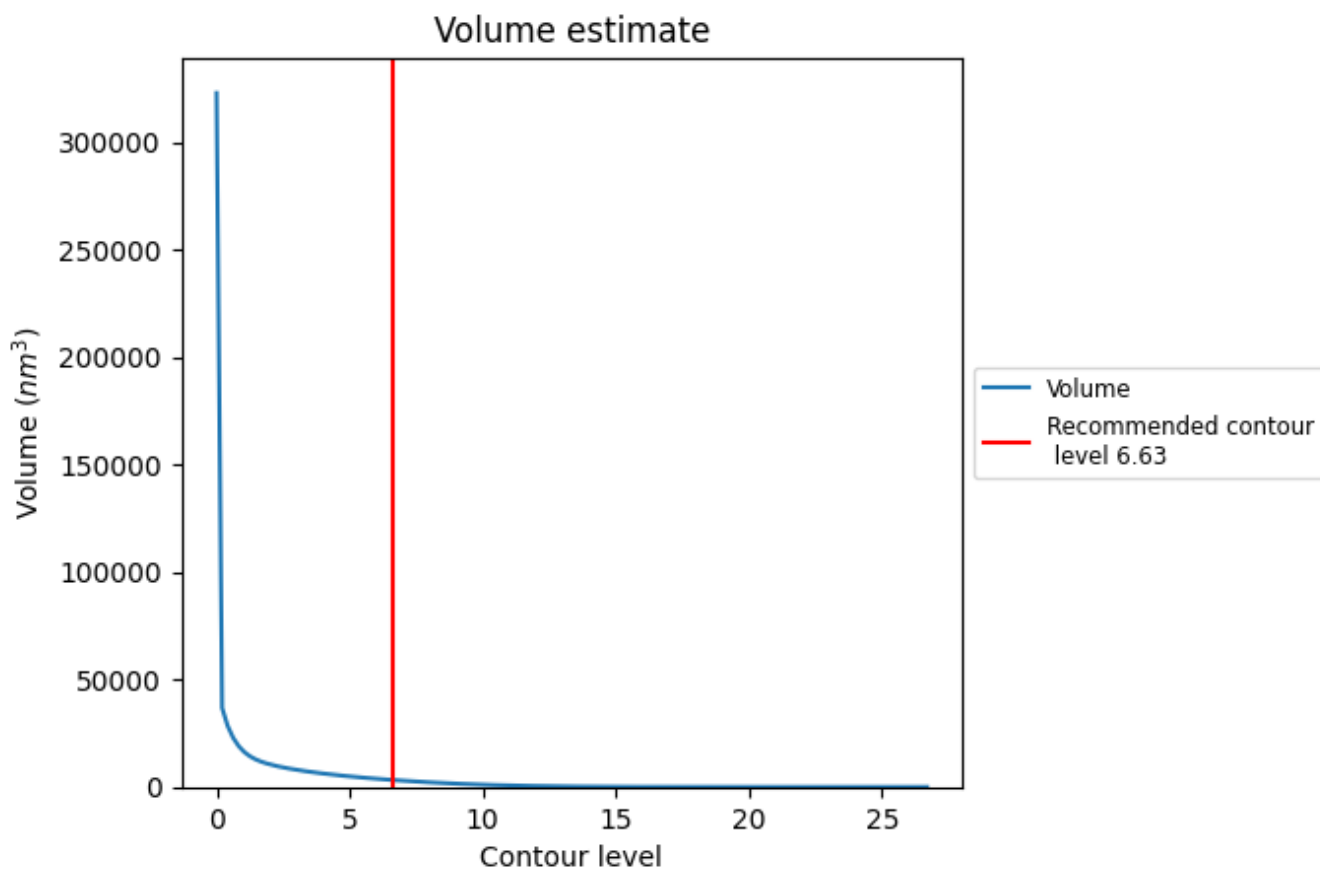
This section contains the results of statistical analysis of the map.

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.

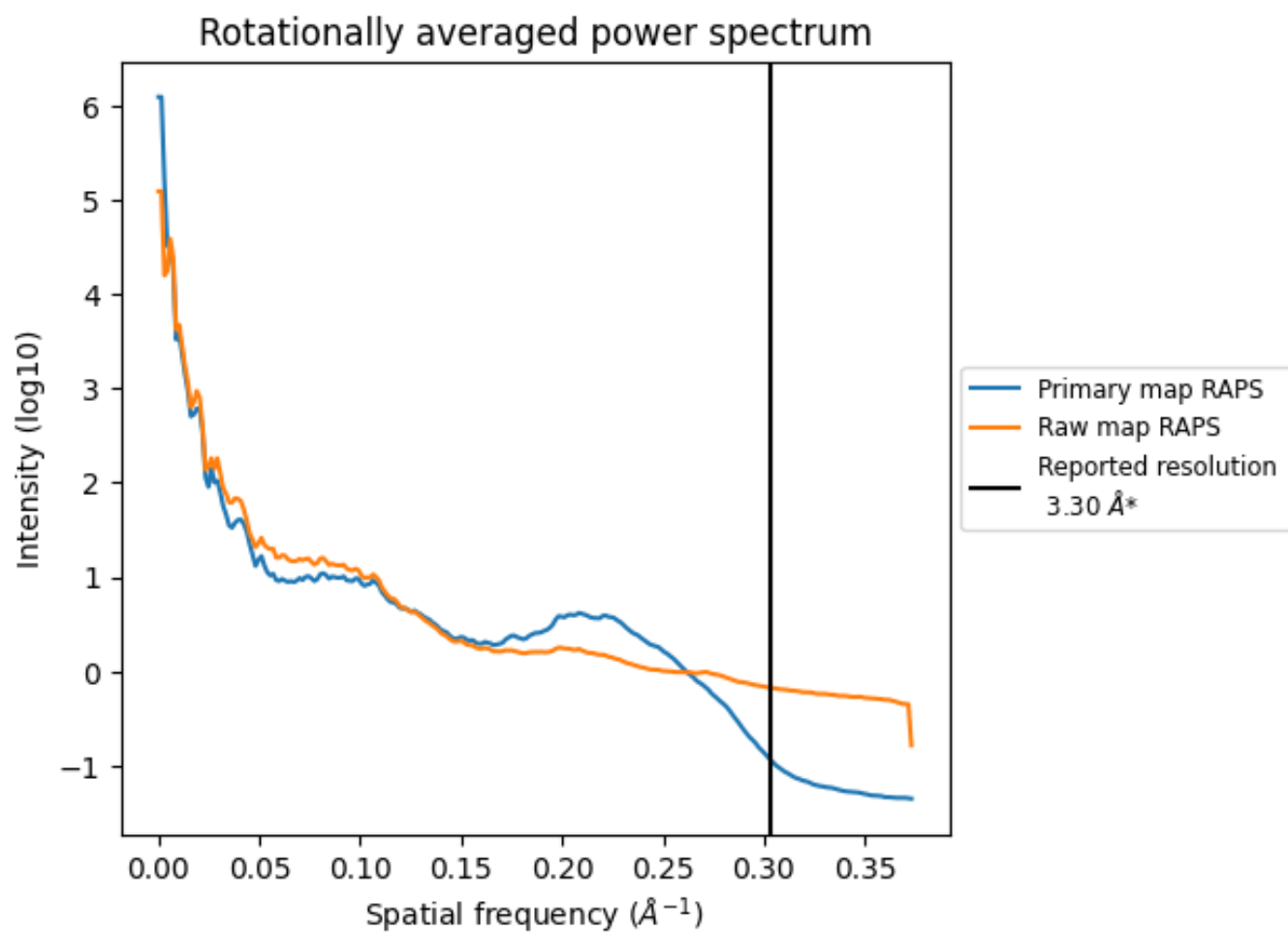
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3228 nm³; this corresponds to an approximate mass of 2916 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 i

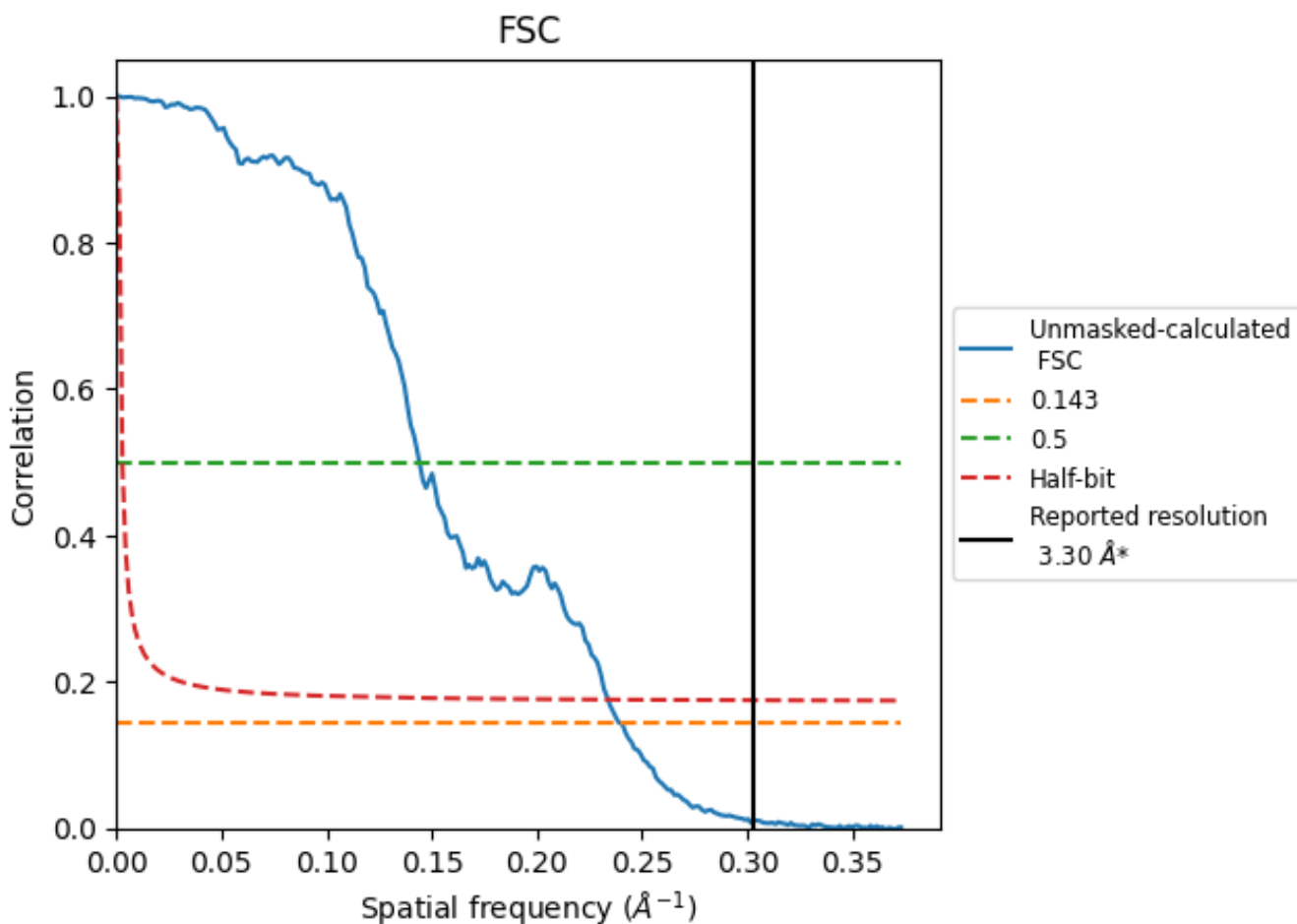


*Reported resolution corresponds to spatial frequency of 0.303 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

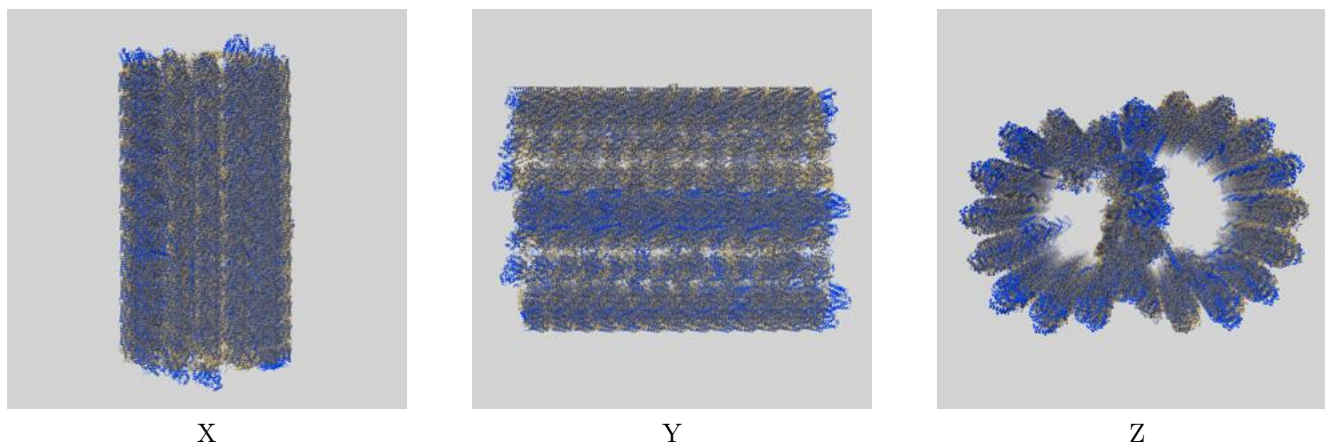
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.18	6.94	4.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.18 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

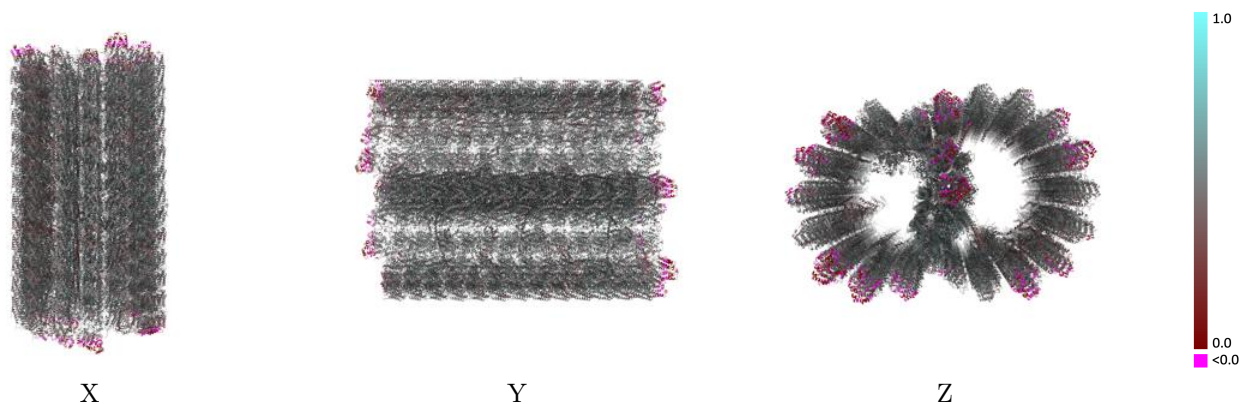
This section contains information regarding the fit between EMDB map EMD-40619 and PDB model 8SNB. Per-residue inclusion information can be found in section 3 on page 71.

9.1 Map-model overlay [i](#)



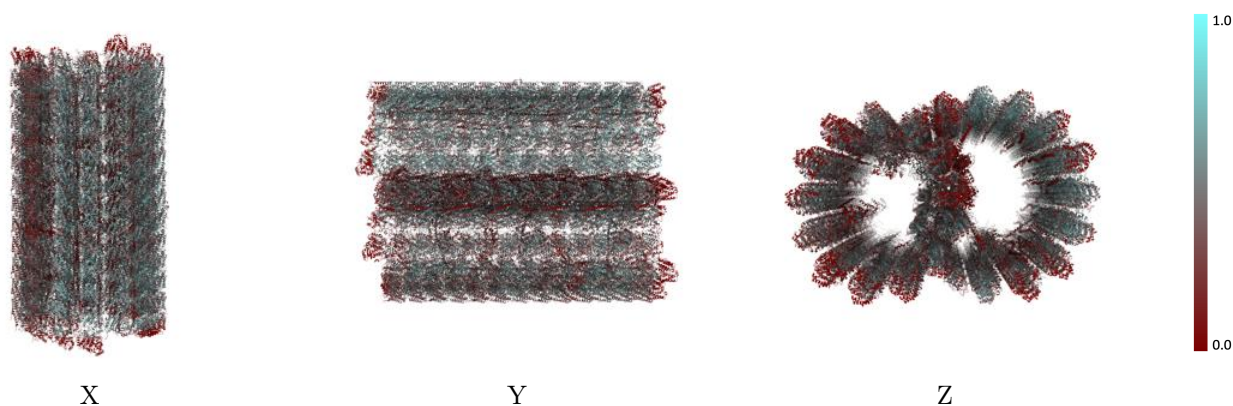
The images above show the 3D surface view of the map at the recommended contour level 6.63 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



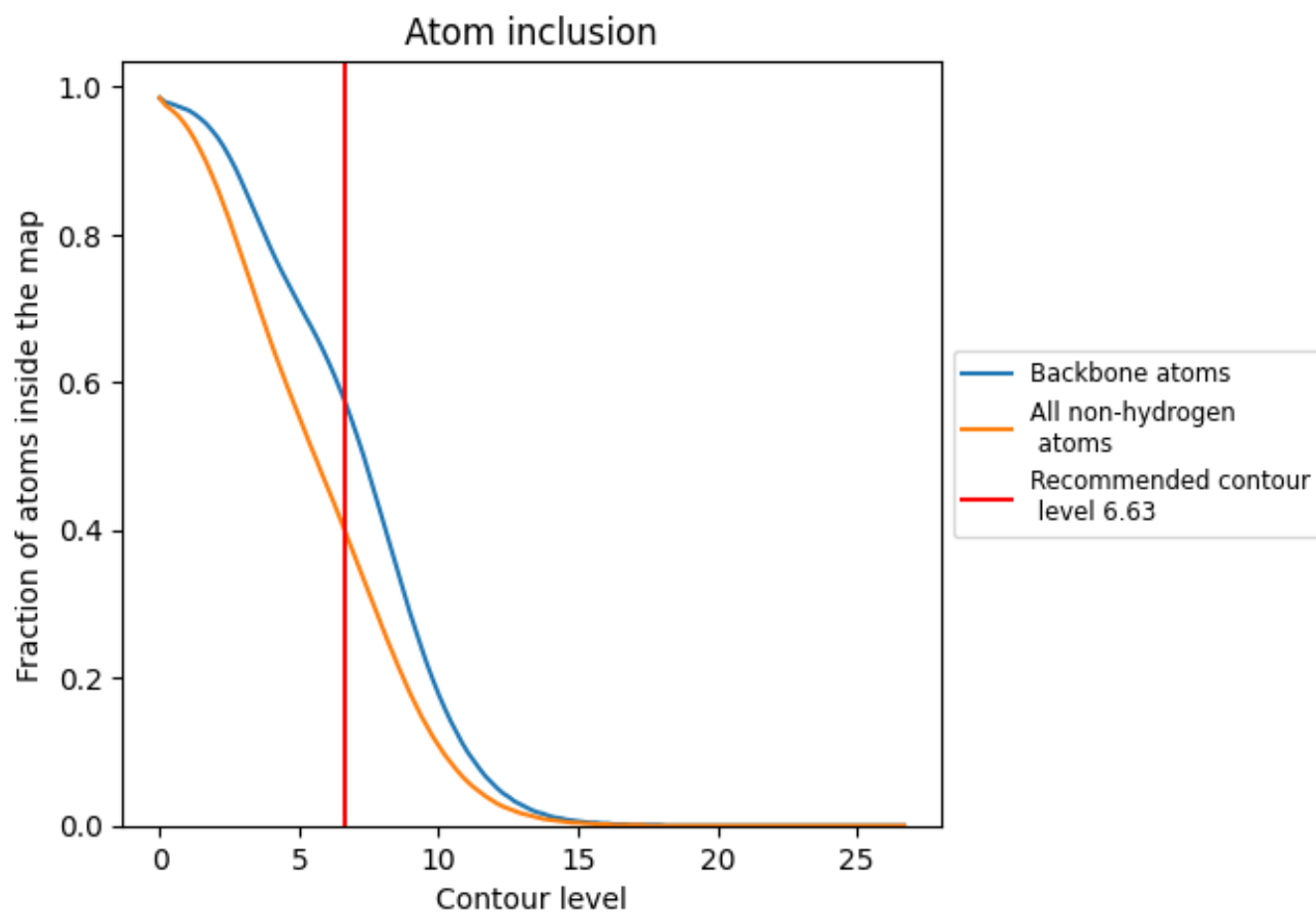
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6.63).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 40% 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 (6.63) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4000	 0.4660
1A	 0.2300	 0.4870
1B	 0.2370	 0.4500
1E	 0.1060	 0.4740
1F	 0.0650	 0.4450
1G	 0.1040	 0.4840
1H	 0.0330	 0.4580
1K	 0.0000	 0.4050
1L	 0.0000	 0.4140
1M	 0.0000	 0.4350
1P	 0.3380	 0.4850
1Q	 0.2620	 0.4250
1T	 0.3330	 0.4780
1U	 0.3860	 0.4800
1V	 0.3120	 0.4780
1W	 0.3130	 0.4720
1Y	 0.1950	 0.4020
1a	 0.1090	 0.4400
1b	 0.0630	 0.4220
1d	 0.0350	 0.4010
1f	 0.3110	 0.3900
1g	 0.2520	 0.3900
1i	 0.2200	 0.4110
1j	 0.2320	 0.4330
1l	 0.0030	 0.3890
1m	 0.0130	 0.3910
1o	 0.2770	 0.4580
1p	 0.3900	 0.4540
1q	 0.3040	 0.4170
1r	 0.3070	 0.4490
1v	 0.0270	 0.4260
1w	 0.0140	 0.3970
1x	 0.0040	 0.3490
1y	 0.0040	 0.3610
1z	 0.0060	 0.3450



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
2A	0.2450	0.4620
2B	0.2510	0.4430
2C	0.2320	0.4520
2D	0.2460	0.4260
2G	0.3030	0.4950
2J	0.0790	0.4560
2K	0.1610	0.4810
2L	0.2380	0.4920
2O	0.2750	0.4660
2R	0.3660	0.4520
2S	0.2590	0.4370
2V	0.3270	0.4920
2W	0.3440	0.4920
2a	0.0140	0.3200
3A	0.4710	0.5070
3B	0.4630	0.4870
3C	0.3300	0.4660
3D	0.3340	0.4640
3E	0.4550	0.5060
3F	0.3670	0.4770
3G	0.4810	0.5060
3J	0.2750	0.4500
3K	0.1310	0.4050
3N	0.3440	0.4080
3O	0.3370	0.4220
3R	0.2060	0.4740
3S	0.2230	0.4720
3T	0.2020	0.4670
3W	0.1430	0.3880
3X	0.2380	0.3920
3Y	0.2550	0.4370
3Z	0.2560	0.4150
4A	0.3310	0.4840
4B	0.3870	0.4830
4C	0.3550	0.4820
4F	0.3350	0.4370
4G	0.3810	0.4700
4J	0.3330	0.4700
4K	0.2700	0.4560
4N	0.2530	0.4710
4O	0.0480	0.4180
4P	0.0730	0.4320

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Chain	Atom inclusion	Q-score
4Q	0.0850	0.4150
4T	0.0030	0.4390
4U	0.0010	0.4270
4V	0.0000	0.3900
4Y	0.3690	0.5020
5A	0.0620	0.4830
5B	0.2180	0.4670
5E	0.2560	0.4580
5F	0.3250	0.4680
5G	0.3060	0.4430
5H	0.3360	0.4390
5I	0.1130	0.3900
5J	0.2820	0.4330
5K	0.3680	0.4210
5L	0.4200	0.4410
5M	0.2700	0.4390
5N	0.3410	0.4330
5O	0.0530	0.4630
6A	0.4290	0.5010
6B	0.0300	0.4660
6C	0.3150	0.4820
6D	0.4400	0.4990
6E	0.4580	0.5100
6F	0.4260	0.4940
6I	0.3260	0.4550
6J	0.2770	0.4490
6M	0.3810	0.5150
6N	0.3090	0.4940
6Q	0.3950	0.4880
6R	0.3190	0.5020
6U	0.3730	0.4970
6V	0.4340	0.5060
6W	0.4200	0.4920
6X	0.4200	0.4900
7A	0.3180	0.4640
7B	0.1530	0.4100
7C	0.3290	0.4680
7D	0.3300	0.4600
7G	0.3840	0.4800
7H	0.3790	0.4780
7I	0.3090	0.4650
7M	0.3950	0.5270

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Chain	Atom inclusion	Q-score
7N	0.3650	0.5030
7Q	0.3120	0.4820
7R	0.1320	0.4600
7U	0.1270	0.4100
7V	0.1810	0.4140
7Y	0.2980	0.4570
7Z	0.1020	0.3970
8A	0.2820	0.4570
8D	0.4450	0.5040
8E	0.3870	0.4870
8F	0.4200	0.5110
8G	0.3990	0.4920
8J	0.4570	0.5040
8K	0.4180	0.5030
8L	0.4290	0.4880
8M	0.4160	0.4860
8N	0.4230	0.5350
8Q	0.4940	0.5320
8R	0.4470	0.4910
8S	0.4310	0.4880
8T	0.4700	0.4910
8U	0.4800	0.4980
8X	0.0360	0.4510
8Y	0.1000	0.4650
8Z	0.0320	0.4450
9A	0.2910	0.4670
9D	0.1900	0.4420
9G	0.3320	0.4640
9J	0.1040	0.4530
9M	0.2020	0.4350
9N	0.2620	0.4730
9O	0.0270	0.2600
9R	0.4140	0.5090
9T	0.2940	0.4910
9V	0.0060	0.3600
9W	0.0020	0.4150
9Y	0.0430	0.4620
9Z	0.0200	0.4280
AA	0.4710	0.5110
AB	0.4640	0.5090
AC	0.4480	0.5000
AD	0.4700	0.4990

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Chain	Atom inclusion	Q-score
AE	█ 0.4800	█ 0.5100
AF	█ 0.4620	█ 0.4970
AG	█ 0.4400	█ 0.5010
AH	█ 0.4930	█ 0.5080
AI	█ 0.5090	█ 0.5180
AJ	█ 0.5120	█ 0.5120
AK	█ 0.3500	█ 0.4750
AL	█ 0.4950	█ 0.5140
AM	█ 0.2850	█ 0.3990
BA	█ 0.4360	█ 0.4940
BB	█ 0.4030	█ 0.4790
BC	█ 0.4320	█ 0.4850
BD	█ 0.4270	█ 0.4780
BE	█ 0.4230	█ 0.4810
BF	█ 0.3750	█ 0.4640
BG	█ 0.3610	█ 0.4660
BH	█ 0.4300	█ 0.4770
BI	█ 0.4120	█ 0.4790
BJ	█ 0.4150	█ 0.4750
BK	█ 0.2310	█ 0.3620
BL	█ 0.4190	█ 0.4900
BM	█ 0.3650	█ 0.4560
CA	█ 0.4850	█ 0.4970
CB	█ 0.4500	█ 0.4900
CC	█ 0.4620	█ 0.4880
CD	█ 0.4690	█ 0.4910
CE	█ 0.4820	█ 0.4920
CF	█ 0.4280	█ 0.4780
CG	█ 0.3650	█ 0.4730
CH	█ 0.4710	█ 0.4880
CI	█ 0.4630	█ 0.4870
CJ	█ 0.4080	█ 0.4710
CK	█ 0.1490	█ 0.2580
CL	█ 0.4520	█ 0.4870
CM	█ 0.3900	█ 0.4770
DA	█ 0.4060	█ 0.4820
DB	█ 0.3530	█ 0.4740
DC	█ 0.4220	█ 0.4880
DD	█ 0.3950	█ 0.4800
DE	█ 0.4260	█ 0.4800
DF	█ 0.3760	█ 0.4750
DG	█ 0.3250	█ 0.4640

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Chain	Atom inclusion	Q-score
DH	0.3500	0.4720
DI	0.3740	0.4750
DJ	0.3870	0.4770
DK	0.0420	0.1280
DL	0.3750	0.4760
DM	0.3640	0.4740
EA	0.3920	0.4700
EB	0.3970	0.4730
EC	0.3680	0.4790
ED	0.3540	0.4680
EE	0.3790	0.4840
EF	0.3870	0.4720
EG	0.3450	0.4720
EH	0.3180	0.4590
EI	0.3410	0.4660
EJ	0.4210	0.4790
EK	0.3900	0.4810
EL	0.1180	0.2590
EM	0.3060	0.4670
FA	0.4480	0.4700
FB	0.4290	0.4770
FC	0.4600	0.4820
FD	0.3720	0.4530
FE	0.4310	0.4680
FF	0.4560	0.4760
FG	0.4200	0.4720
FH	0.3260	0.4480
FI	0.4010	0.4620
FJ	0.4490	0.4750
FK	0.4270	0.4740
FL	0.2420	0.3820
FM	0.3010	0.4200
GA	0.4280	0.4790
GB	0.4800	0.4920
GC	0.4690	0.4840
GD	0.3460	0.4480
GE	0.4050	0.4670
GF	0.4630	0.4790
GG	0.4460	0.4760
GH	0.3470	0.4600
GI	0.4150	0.4700
GJ	0.4230	0.4860

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Chain	Atom inclusion	Q-score
GK	█ 0.4470	█ 0.4830
GL	█ 0.3110	█ 0.4540
GM	█ 0.2270	█ 0.3320
HA	█ 0.4190	█ 0.4800
HB	█ 0.4890	█ 0.4930
HC	█ 0.4590	█ 0.4830
HD	█ 0.3390	█ 0.4560
HE	█ 0.3940	█ 0.4760
HF	█ 0.4700	█ 0.4900
HG	█ 0.4680	█ 0.4860
HH	█ 0.3890	█ 0.4720
HI	█ 0.4460	█ 0.4800
HJ	█ 0.4790	█ 0.4940
HK	█ 0.5190	█ 0.4990
HL	█ 0.3460	█ 0.4700
HM	█ 0.1070	█ 0.2130
IA	█ 0.3780	█ 0.4810
IB	█ 0.4680	█ 0.5000
IC	█ 0.4230	█ 0.4890
ID	█ 0.4020	█ 0.4810
IE	█ 0.3060	█ 0.4640
IF	█ 0.4610	█ 0.4990
IG	█ 0.4440	█ 0.4970
IH	█ 0.3460	█ 0.4750
II	█ 0.4200	█ 0.4940
IJ	█ 0.4330	█ 0.4920
IK	█ 0.4500	█ 0.4950
IL	█ 0.3010	█ 0.4750
IM	█ 0.0910	█ 0.2470
JA	█ 0.4540	█ 0.5000
JB	█ 0.4600	█ 0.5000
JC	█ 0.4920	█ 0.5010
JD	█ 0.3820	█ 0.4920
JE	█ 0.4320	█ 0.4950
JF	█ 0.4410	█ 0.5030
JG	█ 0.3920	█ 0.4940
JH	█ 0.4660	█ 0.5000
JI	█ 0.4120	█ 0.4940
JJ	█ 0.4820	█ 0.5080
JK	█ 0.4260	█ 0.5000
JL	█ 0.2230	█ 0.3830
JM	█ 0.3500	█ 0.4610

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Chain	Atom inclusion	Q-score
KA	█ 0.4680	█ 0.5060
KB	█ 0.4850	█ 0.5020
KC	█ 0.4670	█ 0.5020
KD	█ 0.4420	█ 0.4950
KE	█ 0.4500	█ 0.5030
KF	█ 0.4780	█ 0.5060
KG	█ 0.4720	█ 0.5040
KH	█ 0.4630	█ 0.5020
KI	█ 0.4190	█ 0.5120
KJ	█ 0.4190	█ 0.5080
KK	█ 0.4810	█ 0.5110
KL	█ 0.3550	█ 0.4840
KM	█ 0.2640	█ 0.3640
LA	█ 0.4810	█ 0.5140
LB	█ 0.4700	█ 0.5120
LC	█ 0.4440	█ 0.5070
LD	█ 0.4740	█ 0.5150
LE	█ 0.4480	█ 0.5130
LF	█ 0.4690	█ 0.5120
LG	█ 0.4610	█ 0.5190
LH	█ 0.4940	█ 0.5280
LI	█ 0.4850	█ 0.5250
LJ	█ 0.4970	█ 0.5270
LK	█ 0.4710	█ 0.5140
LL	█ 0.4710	█ 0.5180
LM	█ 0.1310	█ 0.2360
MA	█ 0.4690	█ 0.5140
MB	█ 0.4590	█ 0.5060
MC	█ 0.4390	█ 0.5080
MD	█ 0.4740	█ 0.5140
ME	█ 0.4700	█ 0.5120
MF	█ 0.4690	█ 0.5130
MG	█ 0.4620	█ 0.5210
MH	█ 0.5050	█ 0.5330
MI	█ 0.5460	█ 0.5330
MJ	█ 0.4740	█ 0.5200
MK	█ 0.1520	█ 0.2610
ML	█ 0.4450	█ 0.5090
MM	█ 0.4610	█ 0.5140
NA	█ 0.4130	█ 0.4870
NB	█ 0.3610	█ 0.4700
NC	█ 0.3490	█ 0.4630

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Chain	Atom inclusion	Q-score
ND	0.3990	0.4810
NE	0.3950	0.4830
NF	0.4040	0.4840
NG	0.2760	0.4680
NH	0.3810	0.4770
NI	0.3540	0.4740
NJ	0.2800	0.4600
NK	0.1300	0.2640
NL	0.3850	0.4740
NM	0.3970	0.4710
OA	0.5550	0.4990
OB	0.4890	0.4820
OC	0.4970	0.4780
OD	0.5200	0.4870
OE	0.5470	0.4960
OF	0.5540	0.4930
OG	0.4940	0.4720
OH	0.5670	0.4880
OI	0.5420	0.4820
OJ	0.4680	0.4590
OK	0.1240	0.1660
OL	0.5340	0.4840
OM	0.5140	0.4830
PA	0.5550	0.4900
PB	0.4630	0.4690
PC	0.4740	0.4640
PD	0.5420	0.4880
PE	0.5530	0.4970
PF	0.5330	0.4870
PG	0.4690	0.4640
PH	0.5100	0.4720
PI	0.5150	0.4750
PJ	0.4370	0.4520
PK	0.2450	0.3020
PL	0.4430	0.4630
PM	0.5200	0.4790
QA	0.5610	0.4840
QB	0.4710	0.4620
QC	0.5120	0.4750
QD	0.5360	0.4970
QE	0.5360	0.4940
QF	0.5200	0.4930





















































































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Chain	Atom inclusion	Q-score
QG	0.5070	0.4660
QH	0.5130	0.4530
QI	0.5720	0.4680
QJ	0.5360	0.4650
QK	0.4440	0.4230
QL	0.3330	0.3730
QM	0.5630	0.4820
RA	0.5430	0.4770
RB	0.4930	0.4590
RC	0.5310	0.4730
RD	0.5190	0.4880
RE	0.5470	0.4960
RF	0.5410	0.4890
RG	0.5090	0.4730
RH	0.5100	0.4550
RI	0.5250	0.4650
RJ	0.5600	0.4730
RK	0.4960	0.4590
RL	0.1930	0.2530
RM	0.5290	0.4710
SA	0.5380	0.4760
SB	0.5090	0.4660
SC	0.5360	0.4770
SD	0.5440	0.4870
SE	0.5670	0.4930
SF	0.5430	0.4880
SG	0.5280	0.4810
SH	0.5080	0.4590
SI	0.5700	0.4820
SJ	0.5600	0.4840
SK	0.5570	0.4820
SL	0.1120	0.1610
SM	0.4960	0.4630
TA	0.5300	0.4670
TB	0.5290	0.4730
TC	0.5400	0.4750
TD	0.5310	0.4680
TE	0.5420	0.4800
TF	0.5600	0.4820
TG	0.5200	0.4760
TH	0.4940	0.4550
TI	0.5370	0.4740

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Chain	Atom inclusion	Q-score
TJ	 0.5920	 0.4850
TK	 0.5710	 0.4830
TL	 0.2170	 0.2830
TM	 0.4470	 0.4510
UA	 0.3960	 0.4450
UB	 0.4010	 0.4550
UC	 0.3840	 0.4500
UD	 0.3490	 0.4330
UE	 0.3570	 0.4470
UF	 0.3640	 0.4440
UG	 0.3500	 0.4510
UH	 0.2920	 0.4110
UI	 0.3790	 0.4580
UJ	 0.3850	 0.4590
UK	 0.4470	 0.4610
UL	 0.2150	 0.3800
UM	 0.2520	 0.3640
VA	 0.3930	 0.4560
VB	 0.4350	 0.4730
VC	 0.4350	 0.4660
VD	 0.4020	 0.4600
VE	 0.3960	 0.4680
VF	 0.4160	 0.4740
VG	 0.4140	 0.4710
VH	 0.3290	 0.4460
VI	 0.3720	 0.4680
VJ	 0.3670	 0.4710
VK	 0.4080	 0.4780
VL	 0.3370	 0.4640
VM	 0.2240	 0.2990
WA	 0.4190	 0.4750
WB	 0.4720	 0.4820
WC	 0.4770	 0.4900
WD	 0.4330	 0.4760
WE	 0.3980	 0.4730
WF	 0.4640	 0.4840
WG	 0.4550	 0.4770
WH	 0.3940	 0.4770
WI	 0.4590	 0.4940
WJ	 0.4870	 0.4900
WK	 0.4690	 0.4920
WL	 0.4600	 0.4890