



## Full wwPDB EM Validation Report ⓘ

Jun 22, 2023 – 08:07 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

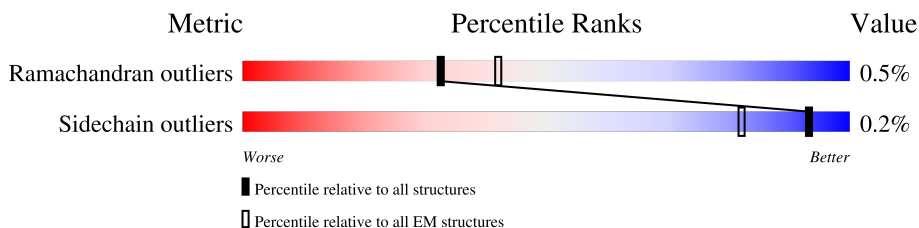
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.33

# 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	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	30% 29% 70%
3	1w	696	12% 12% 88%
3	1x	696	36% 35% 64%
3	1y	696	28% 28% 72%
3	1z	696	12% 12% 88%
3	2a	696	8% 7% 92%
4	1P	204	57% 100%
4	1Q	204	49% 67% 32%
5	1T	429	31% 52% 47%
5	1U	429	12% 26% 74%
5	1V	429	33% 52% 47%
5	1W	429	15% 24% 75%
6	1Y	139	74% 85% 14%
7	1a	251	50% 52% 47%
7	1b	251	48% 46% 51%
7	5E	251	44% 61% 39%
7	5F	251	25% 43% 55%
7	5G	251	35% 55% 43%
7	5H	251	27% 45% 53%
7	5I	251	10% 10% 89%
7	5J	251	63% 91% 7%
7	5K	251	27% 51% 47%
7	5L	251	22% 48% 50%
7	5M	251	5% 94%
7	5N	251	57% 96%

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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% 81% 16%
20	3K	592	11% 11% 88%
21	3N	560	26% 45% 54%
21	3O	560	32% 49% 50%
22	3R	172	80% 92%
22	3S	172	61% 71% 26%
22	3T	172	79% 94%
23	3W	541	66% 70% 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%

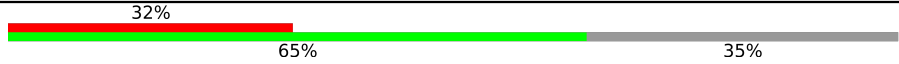



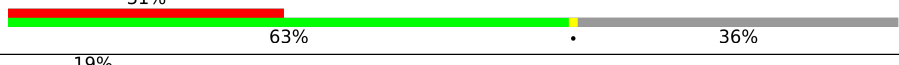

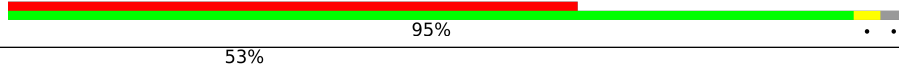


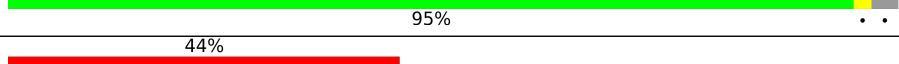


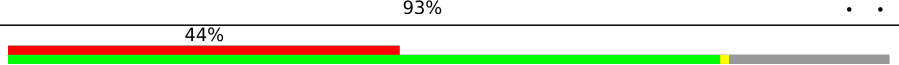

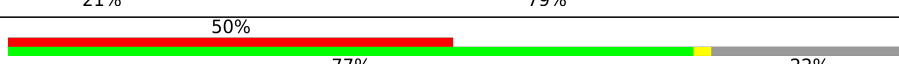

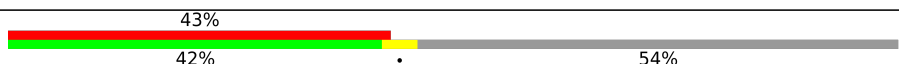
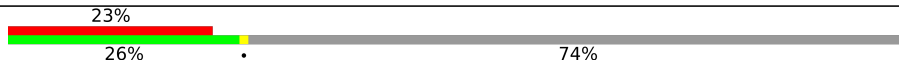
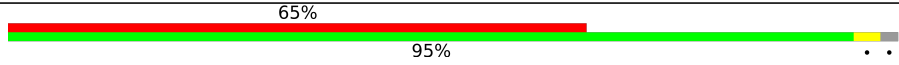


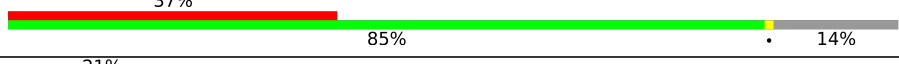



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Mol	Chain	Length	Quality of chain
25	4G	516	25% 39% 60%
26	4J	380	61% 97%
26	4K	380	73% 98%
27	4N	243	49% 60% 38%
27	4O	243	44% 44% 56%
27	4P	243	59% 61% 38%
27	4Q	243	37% 37% 62%
28	4T	231	62% 60% 38%
28	4U	231	62% 61% 38%
28	4V	231	6% 6% 94%
29	4Y	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	53% 96%
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	41% 96%
54	FB	451	42% 96%
54	FE	451	44% 95%
54	FG	451	43% 96%
54	FI	451	51% 95%
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 1270878 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 CFAP21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	3J	495	Total	C	N	O	S	0	0
			3931	2458	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
			2125	1306	406	404	9		
21	3O	278	Total	C	N	O	S	0	0
			2325	1427	444	448	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
			3220	1969	600	639	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	2983	1874	520	566	23	0	0
26	4K	376	2972	1868	518	563	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 A1.

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 B1.

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 C1.

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

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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	3414	2164	581	647	22	0	0
54	LG	437	3414	2164	581	647	22	0	0
54	LI	437	3414	2164	581	647	22	0	0
54	LK	437	3414	2164	581	647	22	0	0
54	MA	437	3414	2164	581	647	22	0	0
54	MB	437	3414	2164	581	647	22	0	0
54	ME	437	3414	2164	581	647	22	0	0
54	MG	437	3414	2164	581	647	22	0	0
54	MI	437	3414	2164	581	647	22	0	0
54	MK	437	3414	2164	581	647	22	0	0
54	ML	437	3414	2164	581	647	22	0	0
54	NA	435	3406	2160	579	645	22	0	0
54	NB	437	3414	2164	581	647	22	0	0
54	NE	437	3414	2164	581	647	22	0	0
54	NG	437	3414	2164	581	647	22	0	0
54	NI	434	3398	2154	578	644	22	0	0
54	NL	433	3391	2150	577	642	22	0	0
54	OA	437	3414	2164	581	647	22	0	0
54	OB	434	3398	2154	578	644	22	0	0
54	OE	437	3414	2164	581	647	22	0	0
54	OG	437	3414	2164	581	647	22	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	OI	437	3414	2164	581	647	22	0	0
54	OK	437	3414	2164	581	647	22	0	0
54	OL	437	3414	2164	581	647	22	0	0
54	PA	437	3414	2164	581	647	22	0	0
54	PB	437	3414	2164	581	647	22	0	0
54	PE	437	3414	2164	581	647	22	0	0
54	PG	437	3414	2164	581	647	22	0	0
54	PI	437	3414	2164	581	647	22	0	0
54	PK	437	3414	2164	581	647	22	0	0
54	PL	437	3414	2164	581	647	22	0	0
54	QA	437	3414	2164	581	647	22	0	0
54	QB	437	3414	2164	581	647	22	0	0
54	QE	437	3414	2164	581	647	22	0	0
54	QG	437	3414	2164	581	647	22	0	0
54	QI	437	3414	2164	581	647	22	0	0
54	QK	433	3391	2150	577	642	22	0	0
54	QL	436	3410	2162	580	646	22	0	0
54	RA	437	3414	2164	581	647	22	0	0
54	RB	437	3414	2164	581	647	22	0	0
54	RE	437	3414	2164	581	647	22	0	0
54	RG	437	3414	2164	581	647	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
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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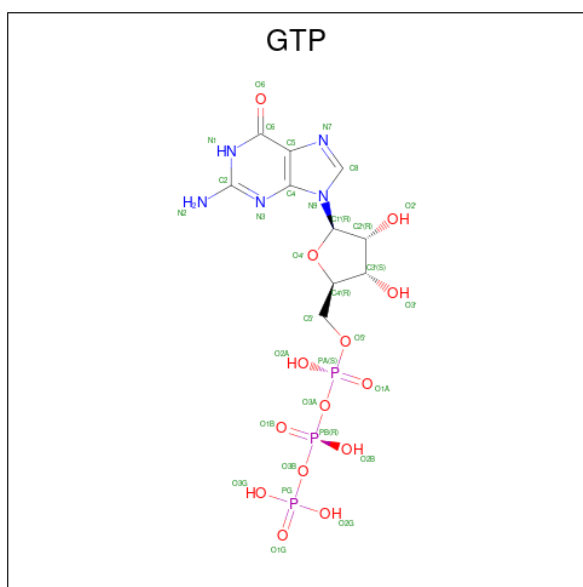
Mol	Chain	Residues	Atoms					AltConf	Trace
55	RF	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	RH	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	RJ	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	RM	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SC	431	Total 3383	C 2124	N 579	O 653	S 27	0	0
55	SD	431	Total 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	C	N	O	P	0
			32	10	5	14	3	
56	AB	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AE	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AG	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AI	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AK	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	AM	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BA	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BB	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BE	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BG	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BI	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BK	1	Total	C	N	O	P	0
			32	10	5	14	3	
56	BM	1	Total	C	N	O	P	0
			32	10	5	14	3	

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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	FB	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	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	FM	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	AF	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	BF	1	1	1	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
57	BI	1	Total 1	Mg 1	0
57	BJ	1	Total 1	Mg 1	0
57	BK	1	Total 1	Mg 1	0
57	CA	1	Total 1	Mg 1	0
57	CB	1	Total 1	Mg 1	0
57	CE	1	Total 1	Mg 1	0
57	CG	1	Total 1	Mg 1	0
57	CI	1	Total 1	Mg 1	0
57	CK	1	Total 1	Mg 1	0
57	CM	1	Total 1	Mg 1	0
57	DA	1	Total 1	Mg 1	0
57	DB	1	Total 1	Mg 1	0
57	DE	1	Total 1	Mg 1	0
57	DG	1	Total 1	Mg 1	0
57	DI	1	Total 1	Mg 1	0
57	DK	1	Total 1	Mg 1	0
57	DM	1	Total 1	Mg 1	0
57	EA	1	Total 1	Mg 1	0
57	EC	1	Total 1	Mg 1	0
57	ED	1	Total 1	Mg 1	0
57	EG	1	Total 1	Mg 1	0

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

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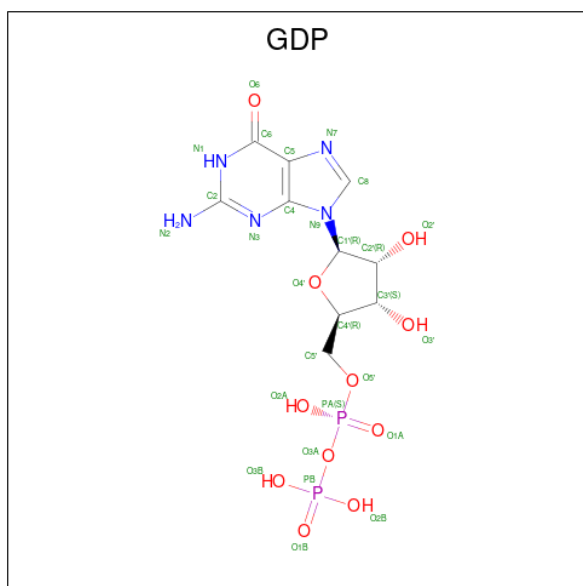
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	RK	1	1	1	0
57	RL	1	1	1	0
57	SA	1	1	1	0
57	SB	1	1	1	0
57	SE	1	1	1	0
57	SG	1	1	1	0
57	SI	1	1	1	0
57	SK	1	1	1	0
57	TA	1	1	1	0
57	TB	1	1	1	0
57	TE	1	1	1	0
57	TG	1	1	1	0
57	TI	1	1	1	0
57	TJ	1	1	1	0
57	UA	1	1	1	0
57	UB	1	1	1	0
57	UD	1	1	1	0
57	UG	1	1	1	0
57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

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Mol	Chain	Residues	Atoms	AltConf
57	VB	1	Total Mg 1 1	0
57	VE	1	Total Mg 1 1	0
57	VG	1	Total Mg 1 1	0
57	VI	1	Total Mg 1 1	0
57	VK	1	Total Mg 1 1	0
57	WA	1	Total Mg 1 1	0
57	WB	1	Total Mg 1 1	0
57	WE	1	Total Mg 1 1	0
57	WG	1	Total Mg 1 1	0
57	WI	1	Total Mg 1 1	0
57	WK	1	Total Mg 1 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	Total 28	C 10	N 5	O 11	P 2	0
58	ND	1	Total 28	C 10	N 5	O 11	P 2	0
58	NF	1	Total 28	C 10	N 5	O 11	P 2	0
58	NH	1	Total 28	C 10	N 5	O 11	P 2	0
58	NJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	NK	1	Total 28	C 10	N 5	O 11	P 2	0
58	NM	1	Total 28	C 10	N 5	O 11	P 2	0
58	OC	1	Total 28	C 10	N 5	O 11	P 2	0
58	OD	1	Total 28	C 10	N 5	O 11	P 2	0
58	OF	1	Total 28	C 10	N 5	O 11	P 2	0
58	OH	1	Total 28	C 10	N 5	O 11	P 2	0
58	OJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	OM	1	Total 28	C 10	N 5	O 11	P 2	0
58	PC	1	Total 28	C 10	N 5	O 11	P 2	0
58	PD	1	Total 28	C 10	N 5	O 11	P 2	0
58	PF	1	Total 28	C 10	N 5	O 11	P 2	0
58	PH	1	Total 28	C 10	N 5	O 11	P 2	0
58	PJ	1	Total 28	C 10	N 5	O 11	P 2	0
58	PM	1	Total 28	C 10	N 5	O 11	P 2	0
58	QC	1	Total 28	C 10	N 5	O 11	P 2	0
58	QD	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	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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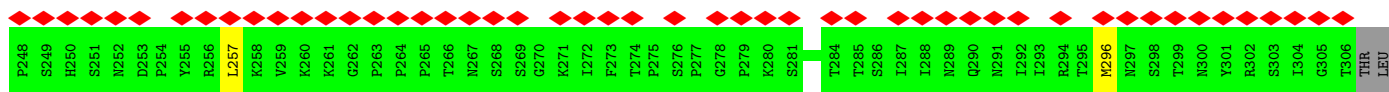
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	TJ	1	28	10	5	11	2	0
58	TL	1	28	10	5	11	2	0
58	TM	1	28	10	5	11	2	0
58	UC	1	28	10	5	11	2	0
58	UD	1	28	10	5	11	2	0
58	UF	1	28	10	5	11	2	0
58	UH	1	28	10	5	11	2	0
58	UJ	1	28	10	5	11	2	0
58	UL	1	28	10	5	11	2	0
58	UM	1	28	10	5	11	2	0
58	VC	1	28	10	5	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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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



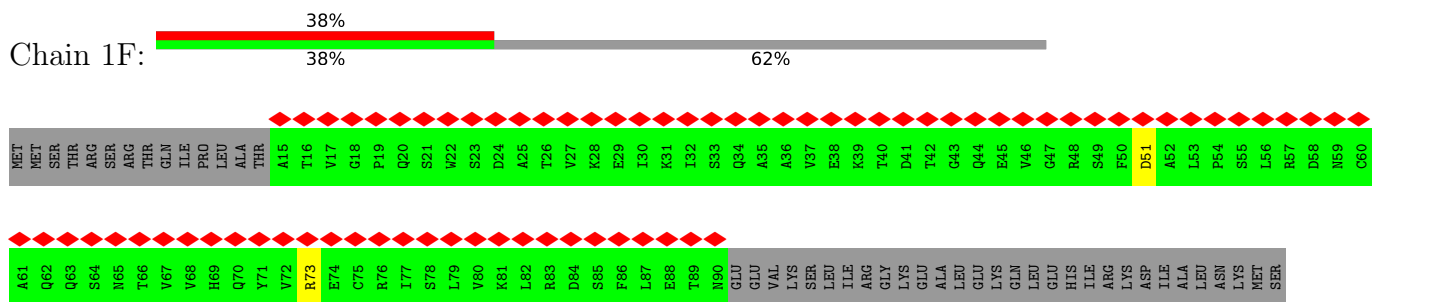


ALA

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



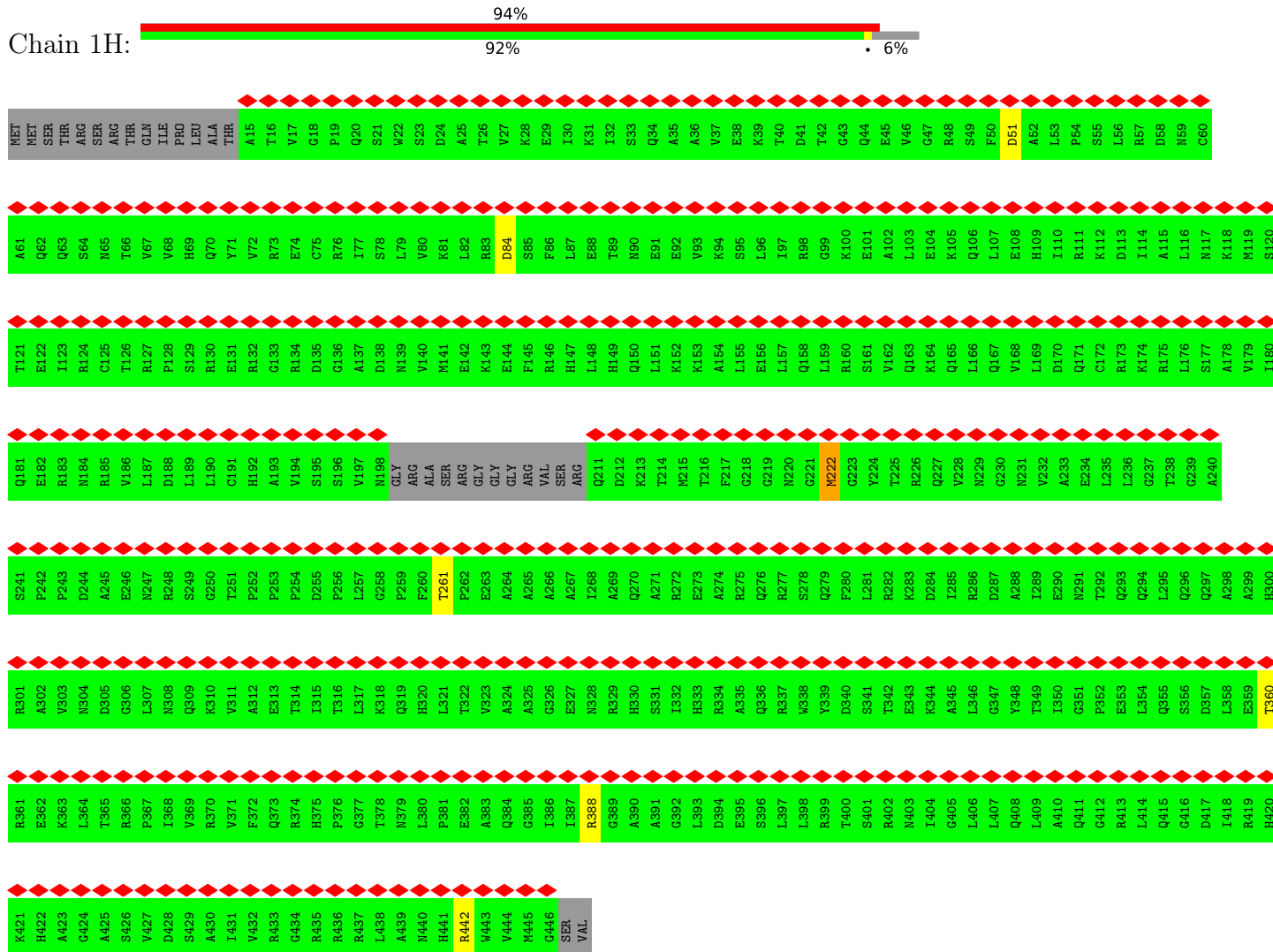
• Molecule 2: Coiled-coil domain-containing protein 105



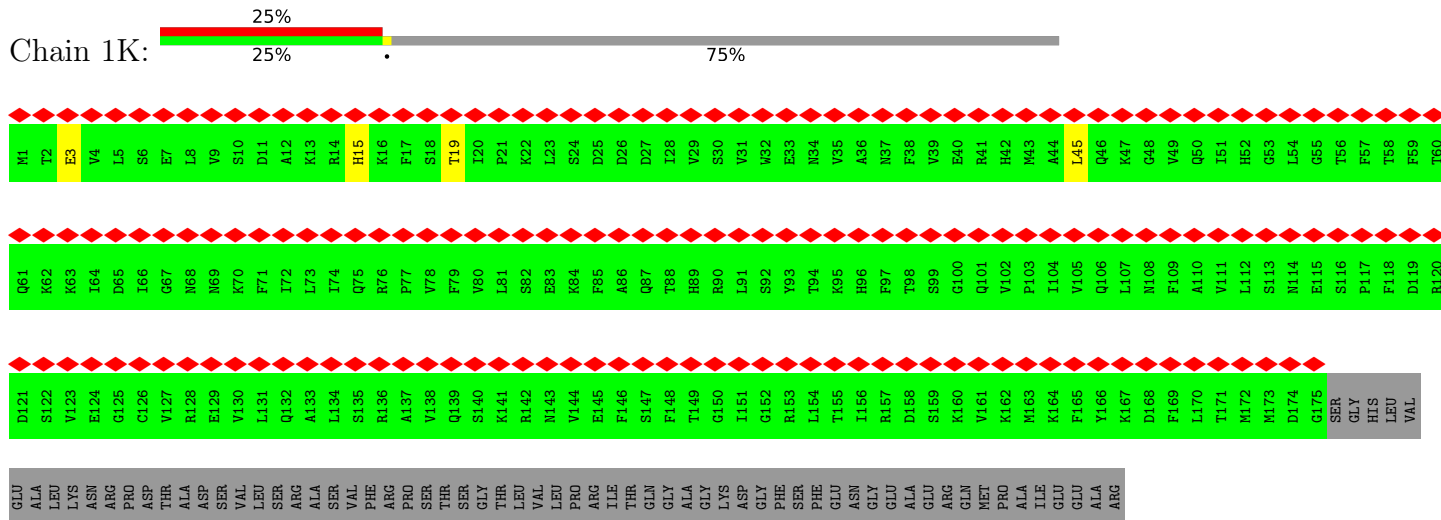




• Molecule 2: Coiled-coil domain-containing protein 105



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

















GLU	LYS	ALA	GLY	GLN	ASP	GLU	LEU	CYS	TYR	ALA	PHE	CYS	HIS	GLN	ARG	ALA	VAL	ASN	VAL	PRO	VAL	GLN	VAL	LEU	PHE	LEU	GLU	PHE	GLU	ARG	GLU	ARG	GLU	GLN	GLU	GLN	GLN	ASP	GLN	ARG	LEU	LEU	GLN	ARG	ALA	GLN	THR	ARG	GLN	GLN	THR	PRO	GLN	PRO	THR	ASP	LYS	ASP	LYS	THR	GLU	GLU	LEU	GLN	GLU	THR	LEU	LEU	ILE	LEU	ALA	ARG	ASP	GLN	VAL	GLN	THR	ALA	GLN	THR	VAL	GLN	THR	VAL	THR	GLN	ASP	ASP	GLN	ASN	ASP	THR	ASP	GLY	ASP	THR	ASP	GLY	LEU	PHE	LEU	GLU	ARG	ALA	ASP	VAL	GLY	PHE	PRO	GLU	LEU	TYR	LEU	GLN	GLN	ASP	GLY	VAL	ALA	GLY	GLY	PRO	LEU	GLU	GLU	LEU	GLY	ASP	MET	ASP
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C661	D662	Q663	Y664	H665	R666	C667	E668	Q669	C670	L671	R672	VAL	LYS	LYS	ASN	CYS	GLY	GLU	GLU	SER	ASN	ILE	TRP	R625	K626	S627	L628	E629	E630	T631	W632	K633	E634	A635	D636	A637	K639	K640	S641	R642	E643	E644	E645	Q646	W647	L648	K649	L650	Q651	S652	S653	Q654	I655	L656	L657	H658	E659	Q660
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● Molecule 4: FAM166C



MET	S2	R3	S4	A5	L8	T11	H12	Q13	R20	L21	M22	H28	C29	M32	K33	F34	D35	Y36	G37	E38	G41	N42	A43	D50	Y51	R52	N58	S59	K60	T61	N65	Q68	F69	D78	D85	R90	P95	Q96	Y97	S98	L99	S100	N101	H104							
D105	E108	D109	I110	N111	D114	K115	E119	E122	K125	D126	T130	V131	G132	R133	V134	M135	E136	F137	L138	R141	Q144	E145	M146	Y147	H148	Q149	D150	S151	A152	L153	I154	D155	E156	H157	V158	D159	M160	R161	E162	E163	A164	S165	T166	N167	M168	A169	R170	N171	I172	P173	V174
E175	R176	M177	S178	I179	P180	P181	I182	R183	T184	F185	S186	K187	S188	S189	T190	V191	R192	D193	R194	A195	M196	R197	D198	V199	H200	Y201	E202	H203	R204																						

● Molecule 4: FAM166C



MET	SER	ARG	SER	ALA	GLY	THR	LEU	GLN	THR	THR	HIS	GLN	ALA	THR	THR	ILE	PRO	PRO	ARG	LEU	MET	GLY	PRO	PRO	TYR	LYS	GLY	HIS	CYS	PRO	THR	THR	MET	LYS	PHE	ASP	TYR	GLY	GLU	THR	TYR	GLY	ASN	ALA	THR	ALA	ALA	CYS	LEU	GLN	ASP	TYR	ARG	THR	THR	THR	LEU	ASN	SER	SER	LYS
THR	ASN	TYR	SER	ASN	GLY	G67	Q68	Y73	N76	P77	D78	C82	A83	R84	D85	R86	T87	R88	E89	A90	F91	A92	T93	T94	P95	Q96	Y97	S98	L99	S100	M101	H104	D105	E108	D109	D114	K115	E122	K125	D126	G132	R133	V134	M135	R136	F137	L138	I139	P140	R141											
Q144	E145	M146	Y147	H148	Q149	D150	S151	A152	L153	I154	D155	E156	H157	V158	D159	M160	R161	E162	E163	S165	T166	M167	M168	A169	R170	N171	I172	P173	V174	E175	R176	M177	S178	I179	P180	P181	I182	R183	T184	F185	S186	K187	S188	S189	T190	V191	R192	D193	R194	A195	M196	R197	D198	V199	H200	Y201	E202				
H203	R204																																																												

● Molecule 5: Protein FAM166B







GLU	SER	GLY	LEU	VAL	ALA	GLN	GLU	PRO	PRO	ILE	GLY	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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Molecule 6: CFAP144(FAM183A)



MET	ALA	ALA	ALA	ALA	GLN	GLU	ALA	LYS	LYS	PRO	GLU	GLY	HIS	ASP	P13	V14	M15	I16	V17	H18	Q19	N20	A21	I22	L23	C24	E25	K84	T26	I27	K28	K29	E30	N31	E32	C33	Q34	R35	L36	Y37	T38	N39	Y40	S41	L42	M43	P44	P45	F45	K46	K47	M48	Y49	T50	L51	T52	G53	K54	P55	N56	S57	L58	H59	D60
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SER	ALA	GLY	GLU	E66	D67	D68	N69	F70	L71	R72	I73	I74	K75	R76	S77	T78	Q79	E80	P81	K83	G82	K83	R84	F85	E86	F87	P88	Q89	T90	E91	A92	Q93	E94	G95	G96	W97	Y98	Y99	K100	P101	L102	L103	P104	Q105	D106	R107	G108	D109	K110	E111	R116	Q117	E120	I121	T122	K123	Y124
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M125	D126	E127	A128	W129	Q131	K132	E133	Q134	Q135	E136	ASN	LEU	GLN
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Molecule 7: Outer dense fiber protein 3



MET	ASN	SER	SER	CYS	TYR	ASN	THR	PRO	THR	ILE	PRO	ARG	ALA	ALA	PRO	ILE	ALA	HIS	PHE	THR	GLY	GLY	PRO	GLY	PRO	ASN	VAL	MET	LEU	PRO	LYS	SER	CYS	LEU	GLY	ALA	ASN	GLY	THR	THR	ALA	ILE	ASN	GLY	PRO	VAL	ARG	HIS	LYS	SER	TYR	THR	THR	ASP	TYR	SER
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PRO	GLY	CYS	HIS	ASN	PHE	PRO	VAL	THR	ARG	THR	LYS	GLY	ASN	ASP	GLY	THR	PRO	LYS	THR	PRO	GLY	THR	LEU	TYR	VAL	ALA	ARG	SER	LEU	GLY	THR	ALA	PHE	GLY	THR	THR	THR	PRO	GLY	ALA	LYS	THR	THR	ALA	GLY	ARG	VAL	ARG	HIS	LYS	TYR	THR	THR	ASP	TYR	SER
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G121	S122	R123	T124	K125	G126	I127	T128	F129	D130	K131	S132	P133	A134	P135	N136	N137	Y138	S139	L140	P141	S142	I143	L144	G145	G146	R147	S148	C149	V150	K151	P152	S153	K154	P155	V156	Y157	S158	M159	R160	G161	R162	N163	K164	M165	G166	G167	F168	D169	E170	D171	L172	Q173	T175	P176	G177	P178	G179	S180
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Y181	D182	V183	V184	P186	A187	I188	Y189	K190	N191	K192	S193	P194	A194	M195	Y196	S197	I198	T199	G200	R201	N202	Q203	L204	P205	C206	D207	S208	T209	R210	R211	P214	G215	P219	E220	K221	V222	T223	V224	N225	K226	R227	M228	A229	P230	K231	F232	S233	F234	G235	H238	S239	Q240	Y241	T242
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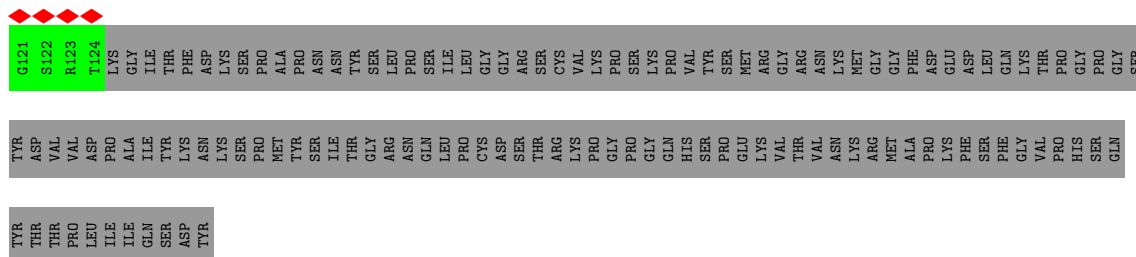
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Molecule 7: Outer dense fiber protein 3

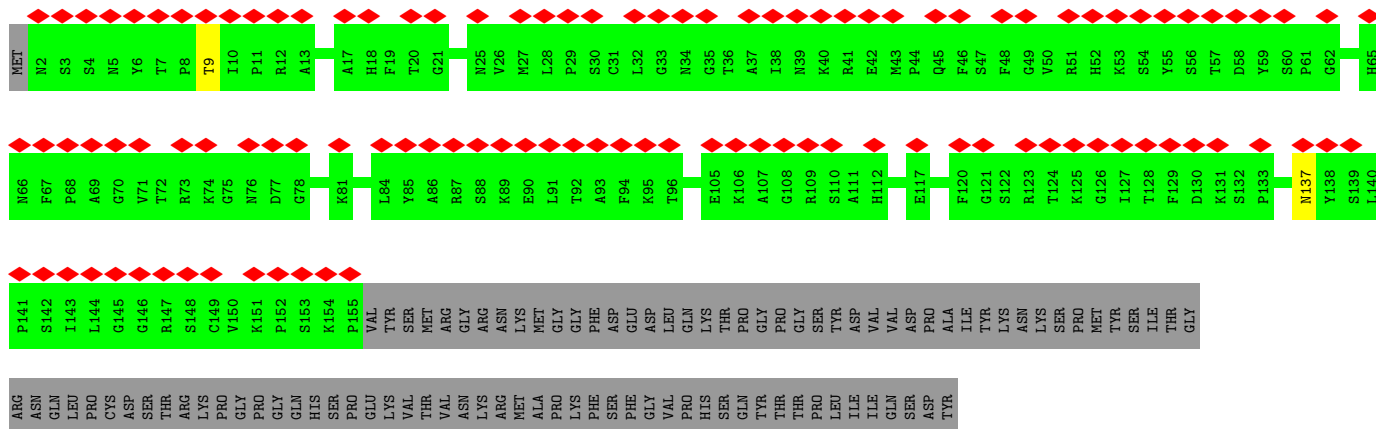
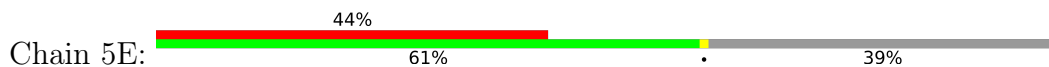


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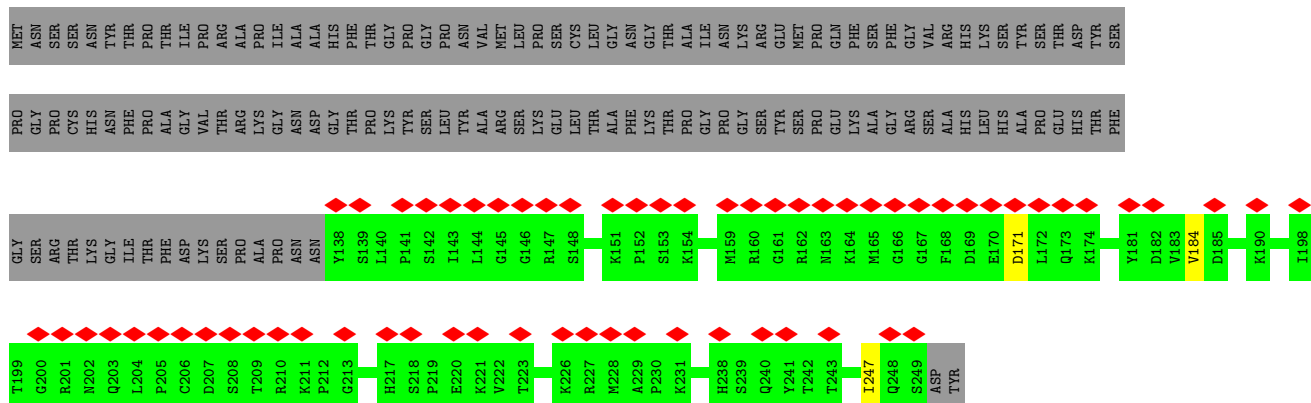
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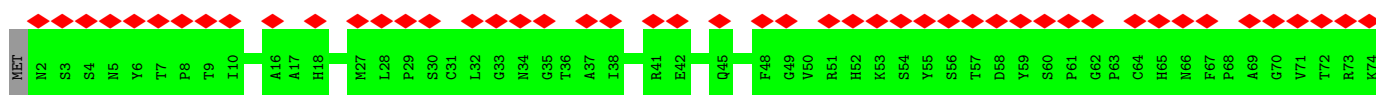
• Molecule 7: Outer dense fiber protein 3

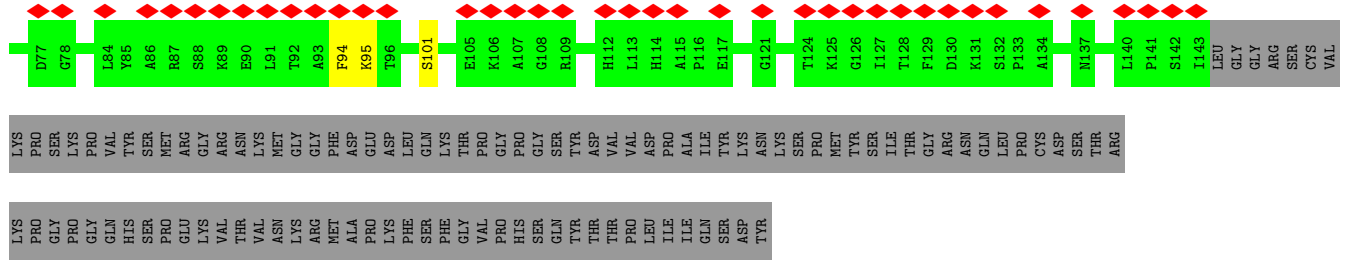


• Molecule 7: Outer dense fiber protein 3

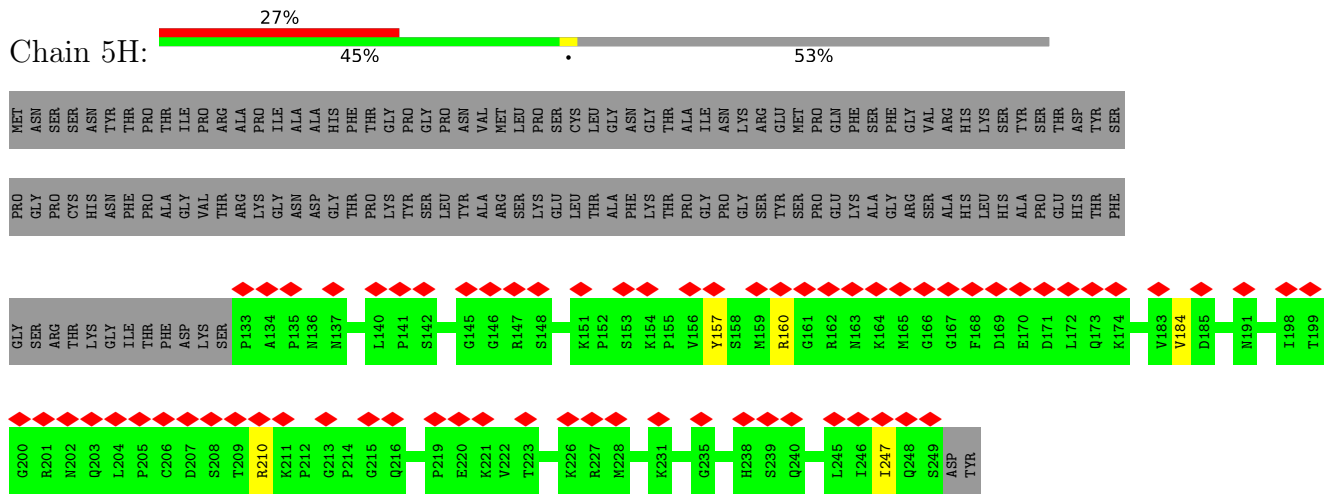


• Molecule 7: Outer dense fiber protein 3

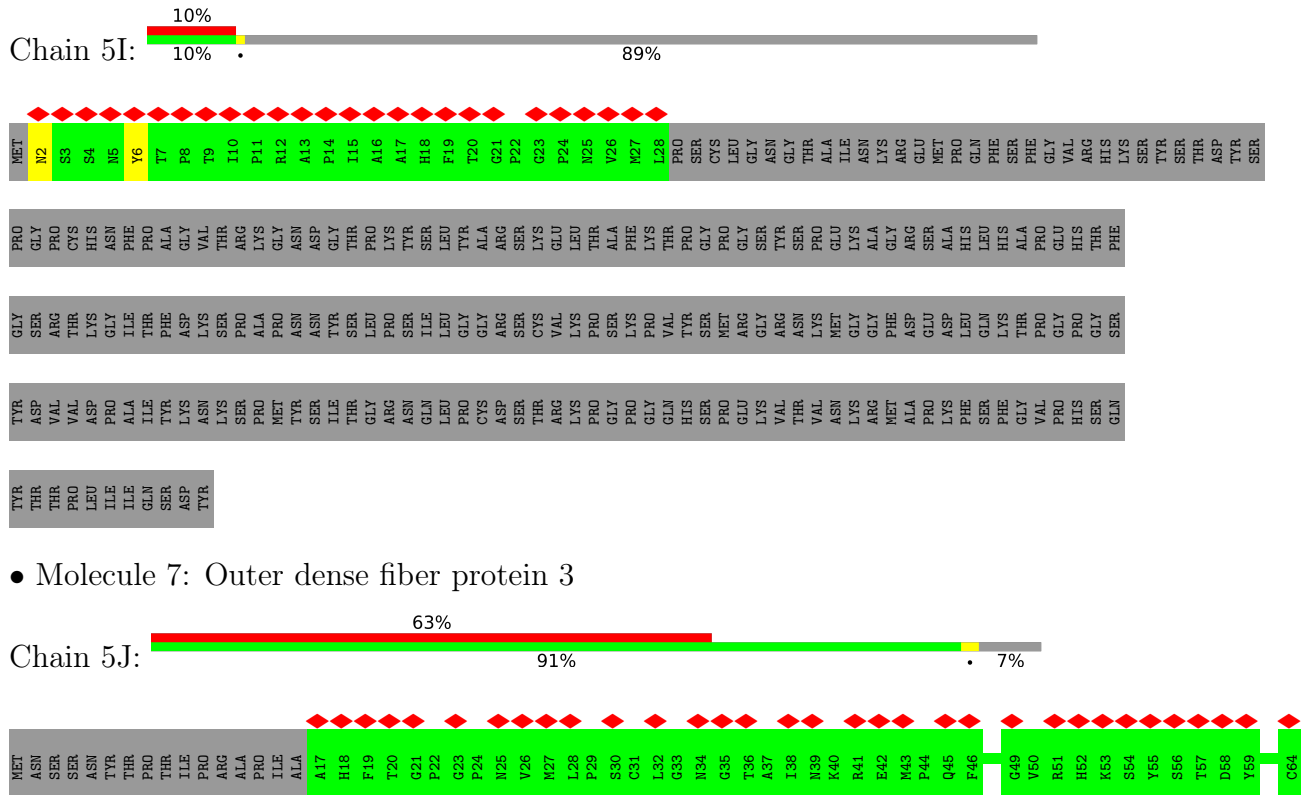


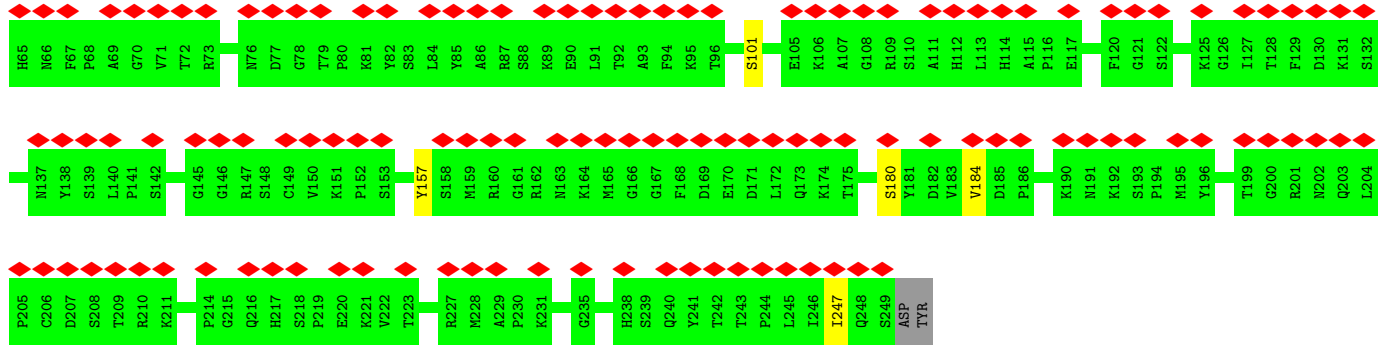


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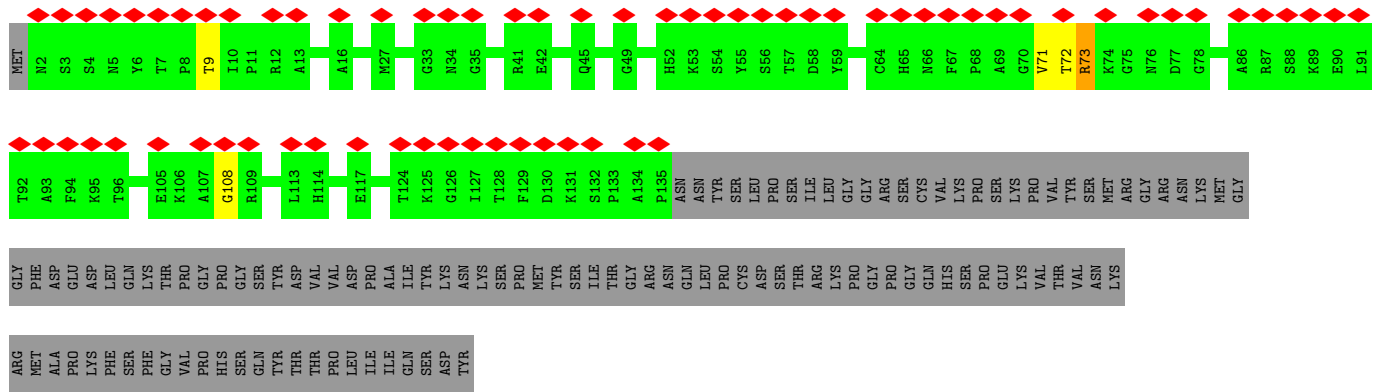


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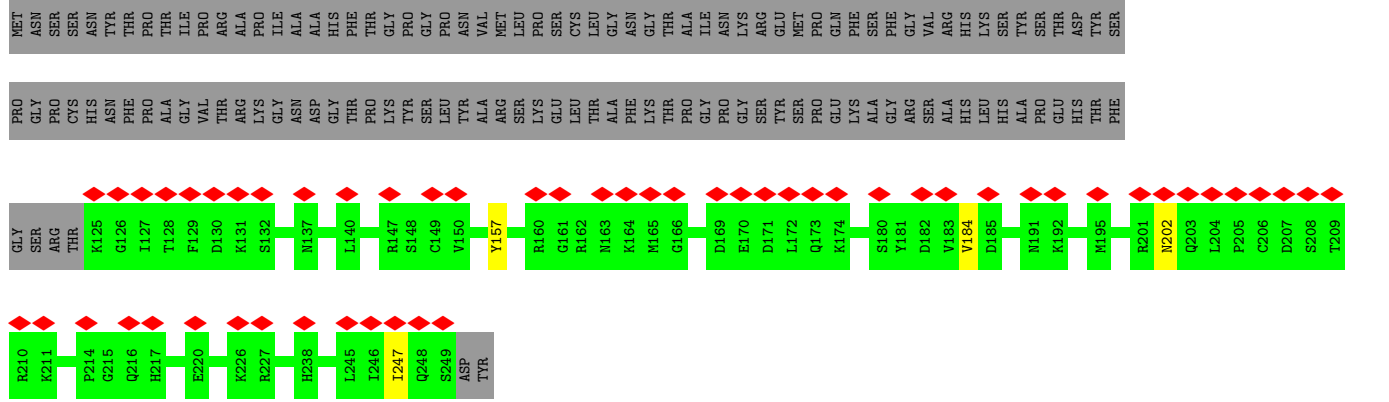




• Molecule 7: Outer dense fiber protein 3

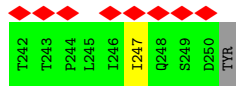
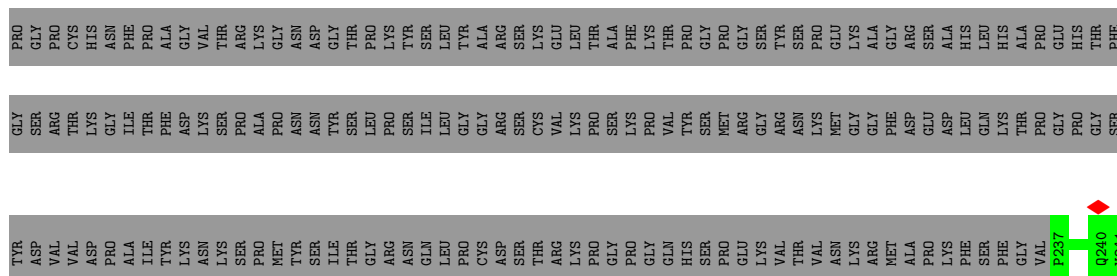


• Molecule 7: Outer dense fiber protein 3

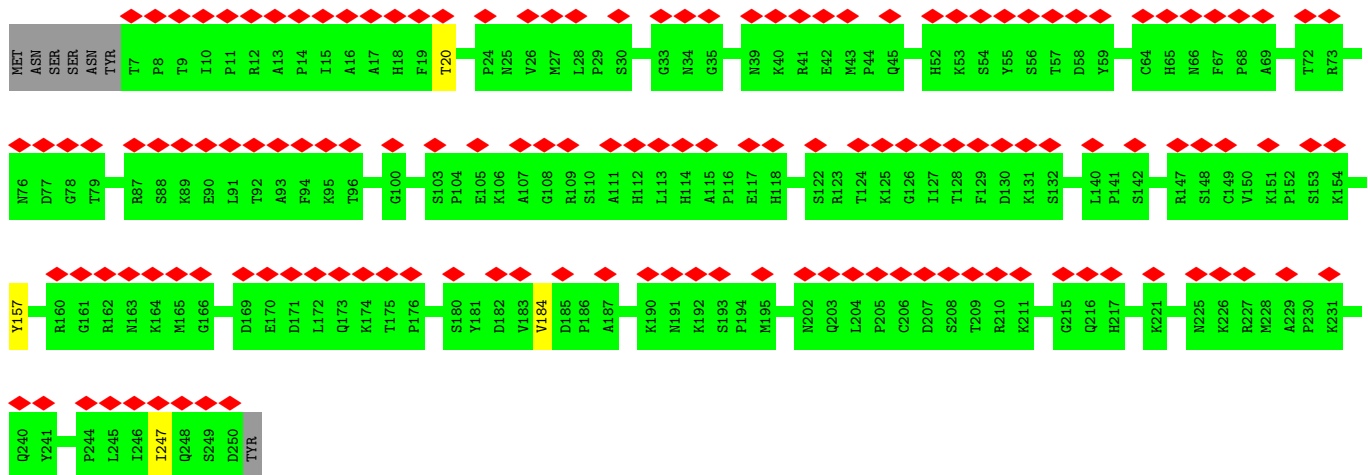


• Molecule 7: Outer dense fiber protein 3

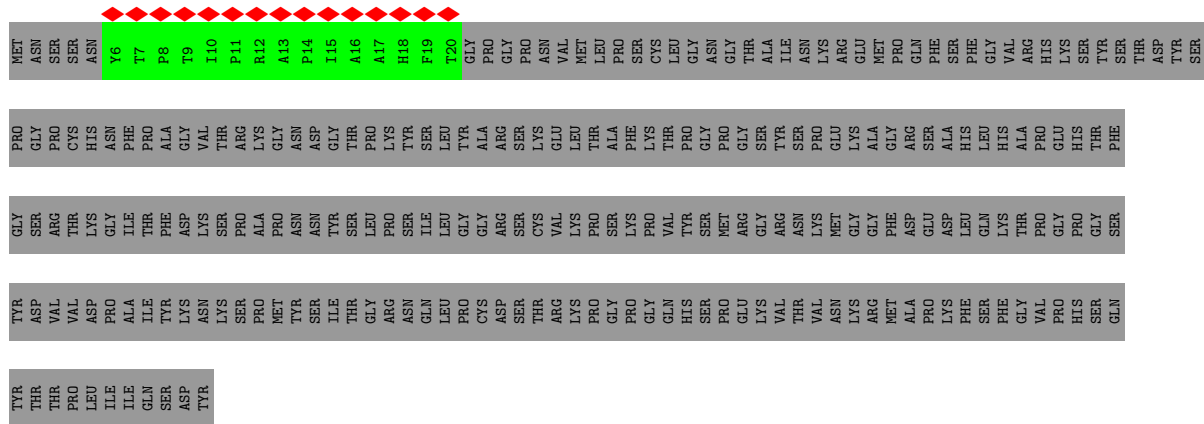




• Molecule 7: Outer dense fiber protein 3



• Molecule 7: Outer dense fiber protein 3

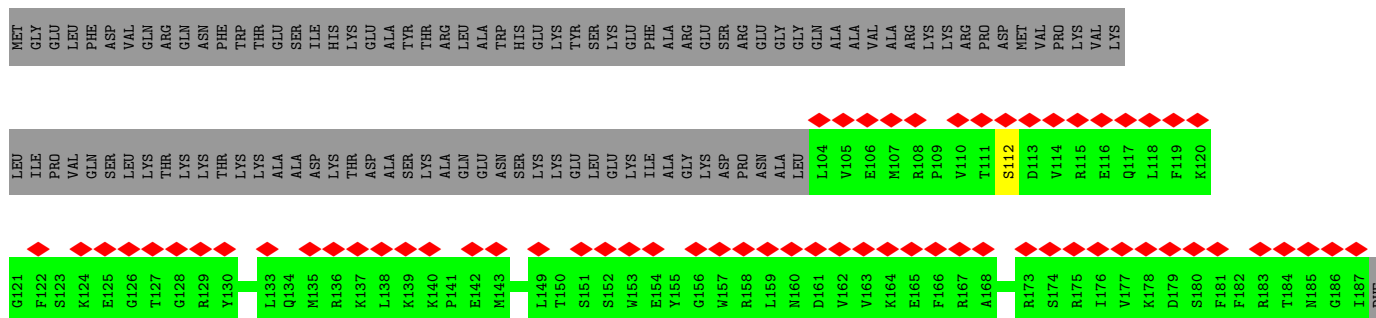


• Molecule 8: Tex33

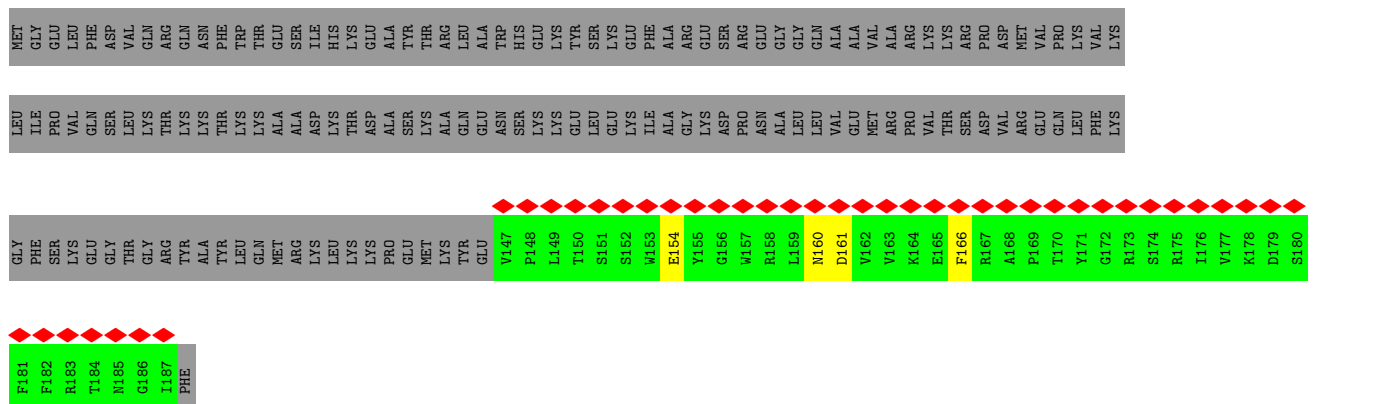




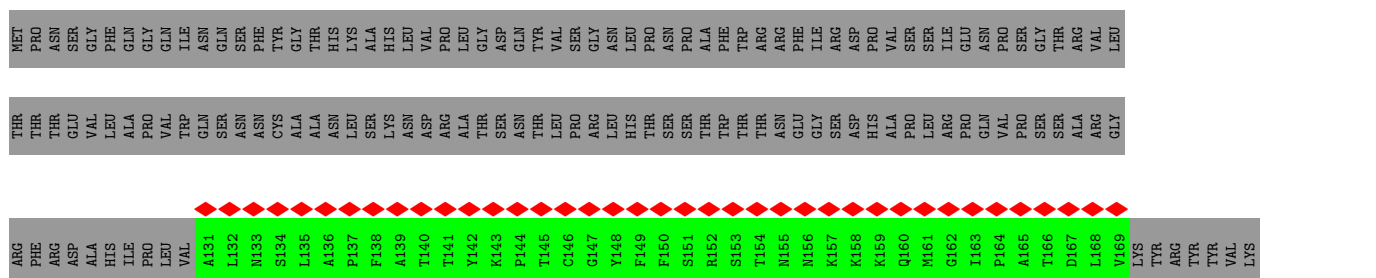




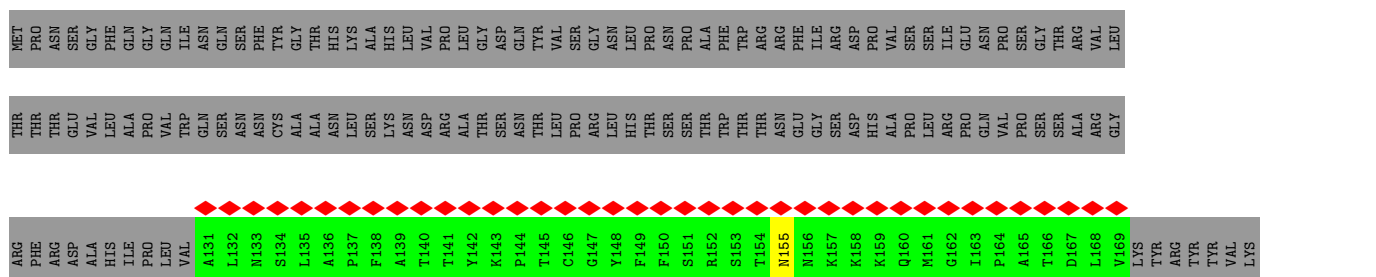
• Molecule 10: ATP6V1FNB



• Molecule 11: Tex26(LOC100888047)

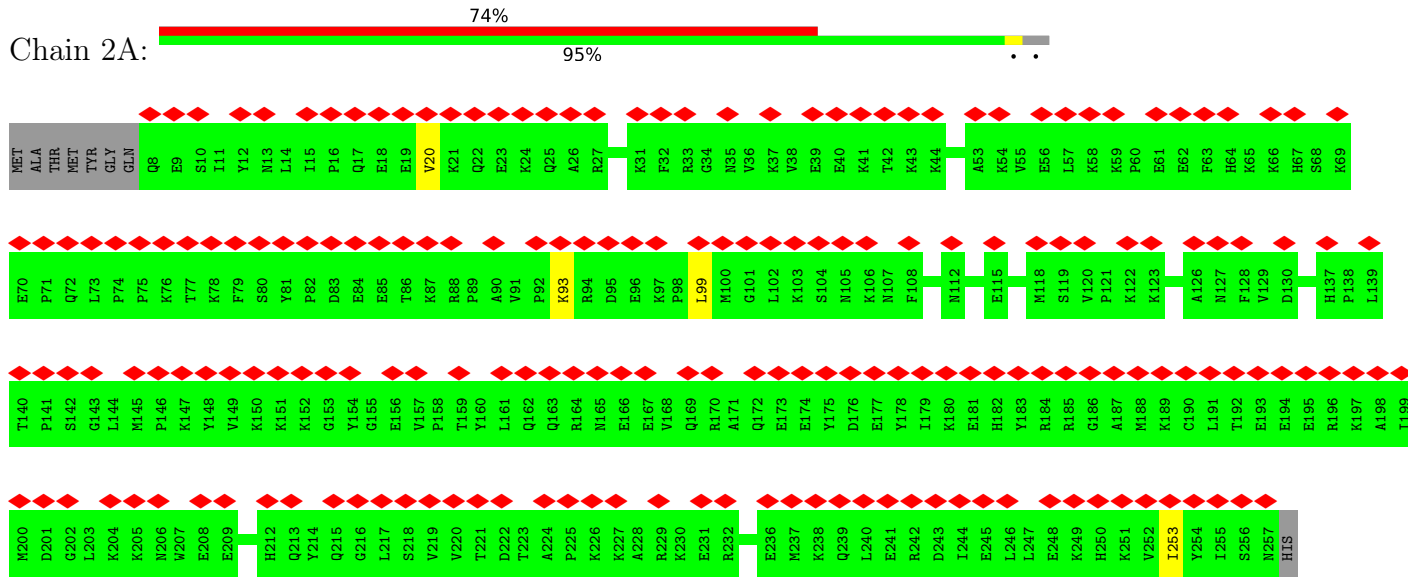


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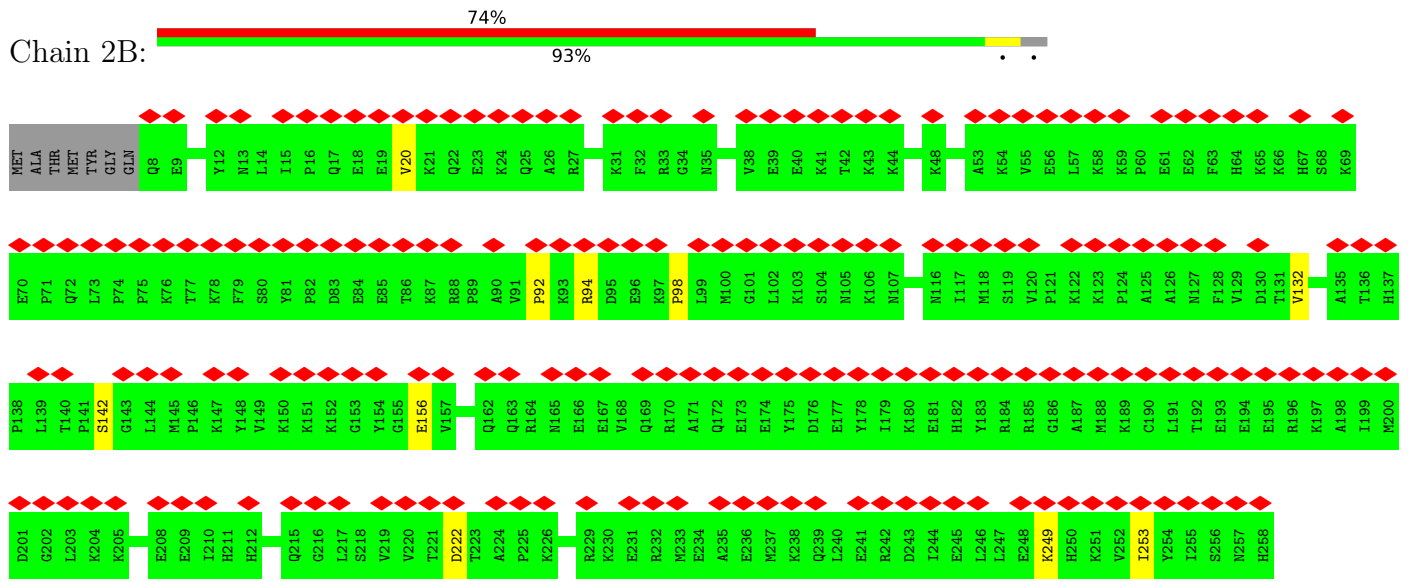




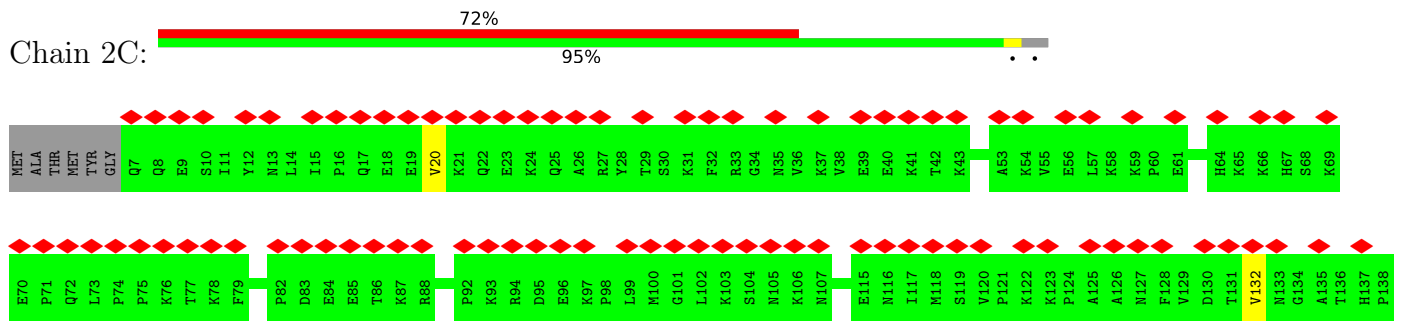
• Molecule 13: Enkurin domain-containing protein

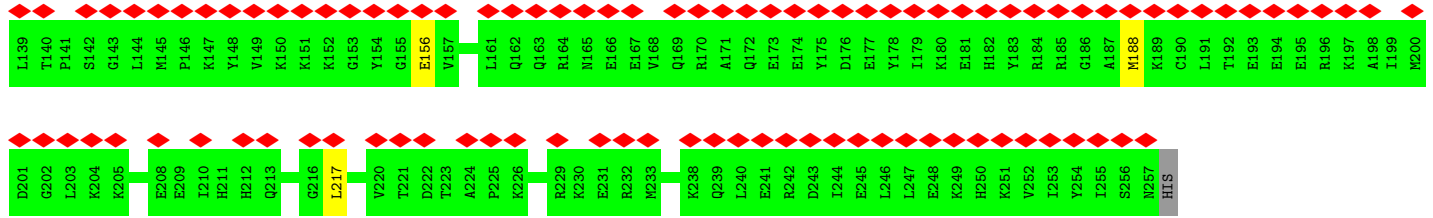


• Molecule 13: Enkurin domain-containing protein

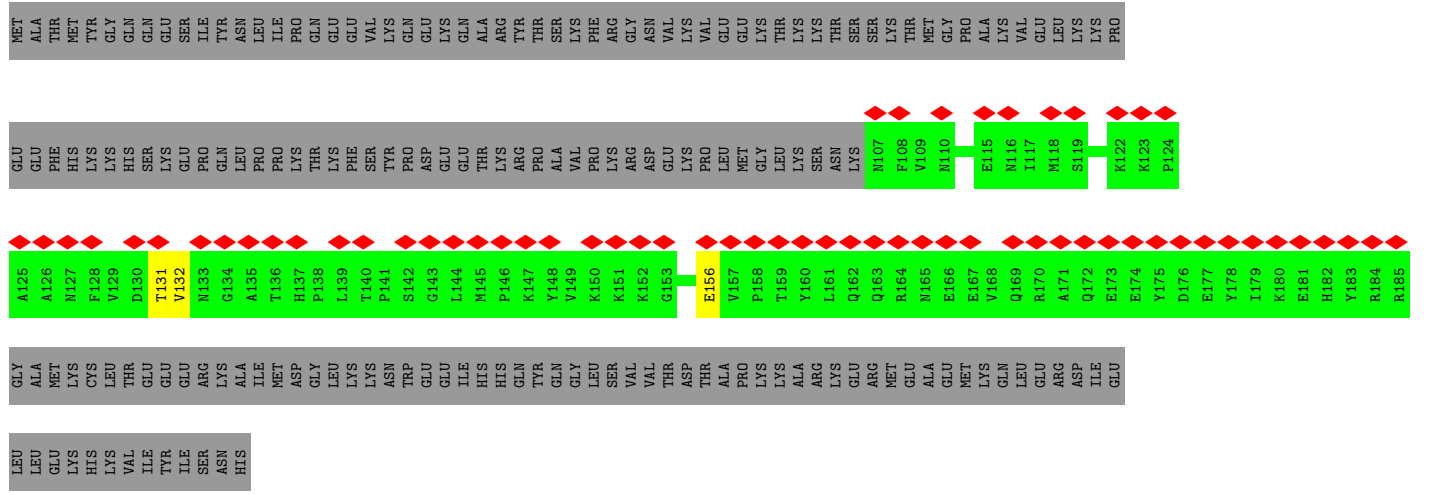


• Molecule 13: Enkurin domain-containing protein

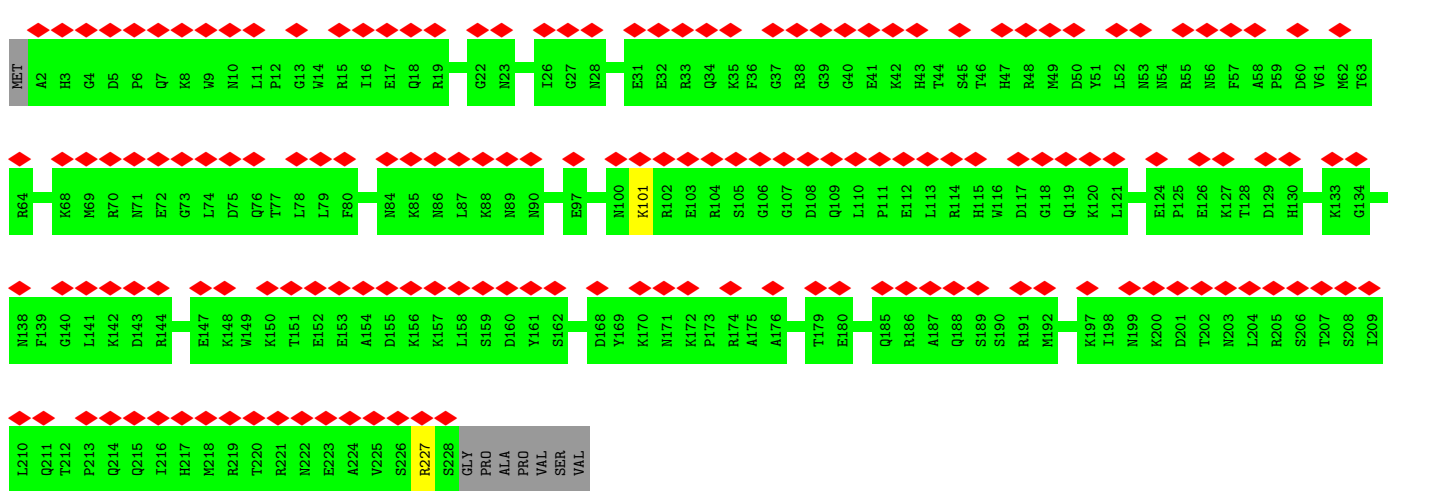




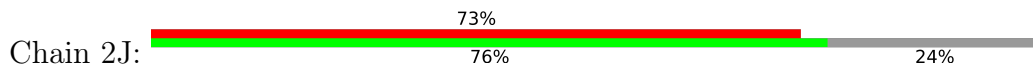
• Molecule 13: Enkurin domain-containing protein

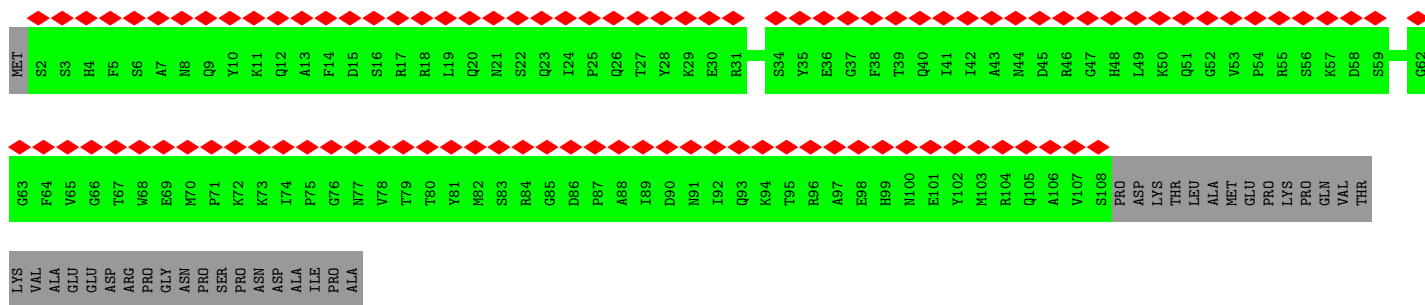


• Molecule 14: CFAP107

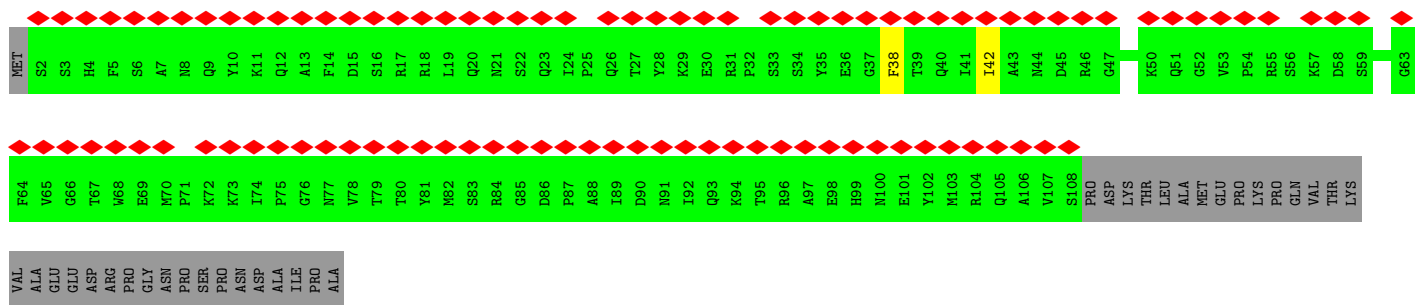
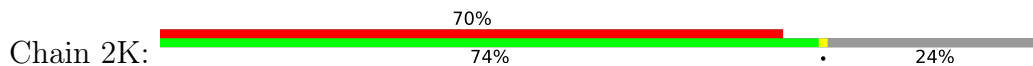


• Molecule 15: Cilia- and flagella-associated protein 126

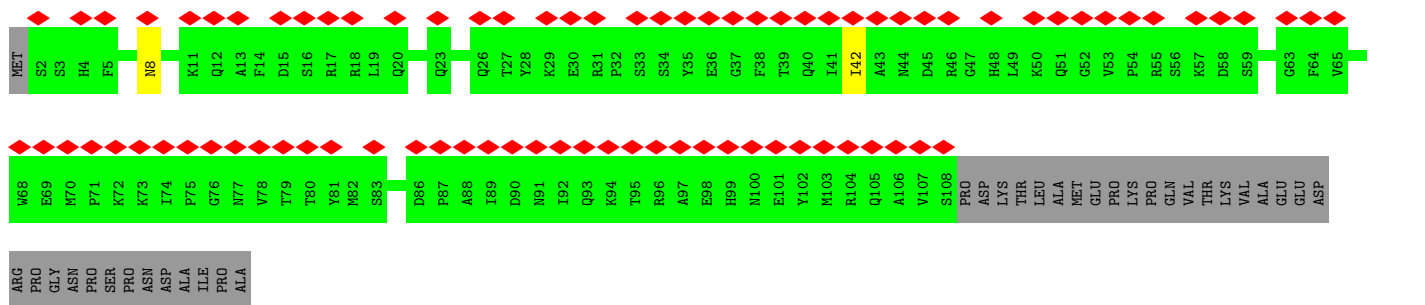
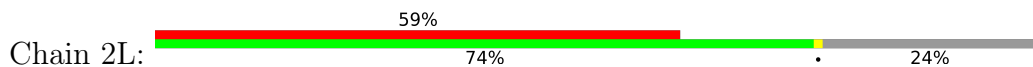




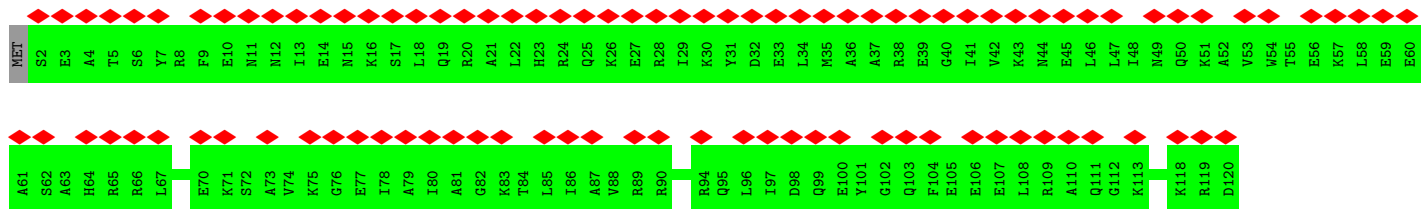
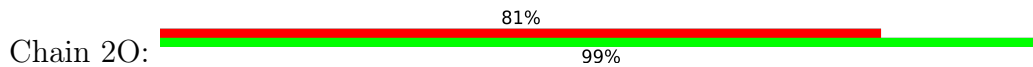
• Molecule 15: Cilia- and flagella-associated protein 126



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



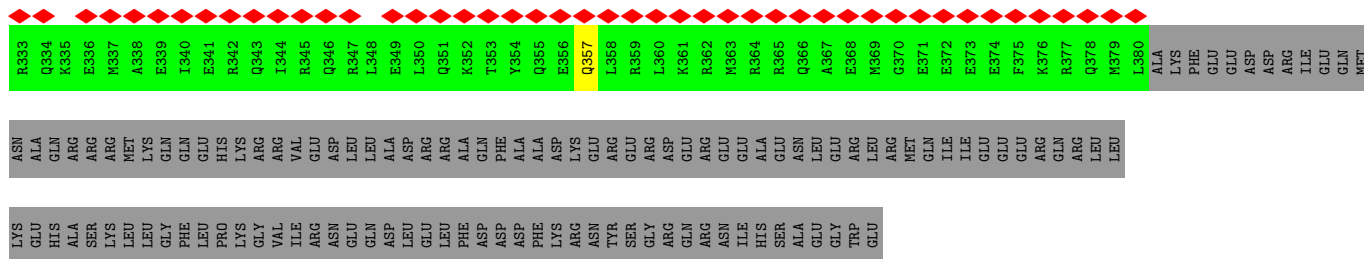
• Molecule 16: Flagellar FliJ protein



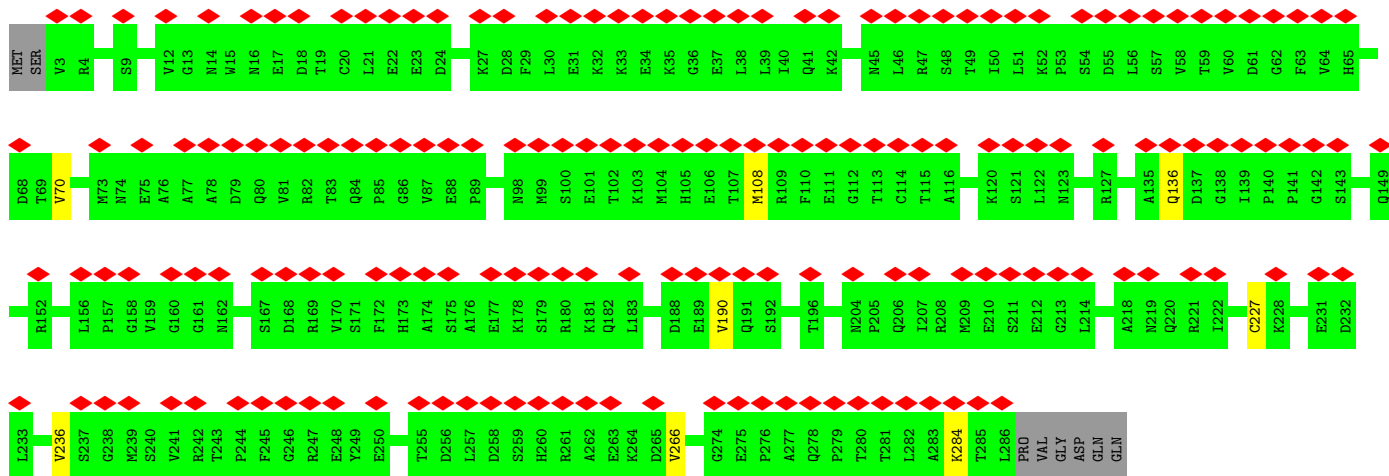
• Molecule 17: Meiosis-specific nuclear structural protein 1



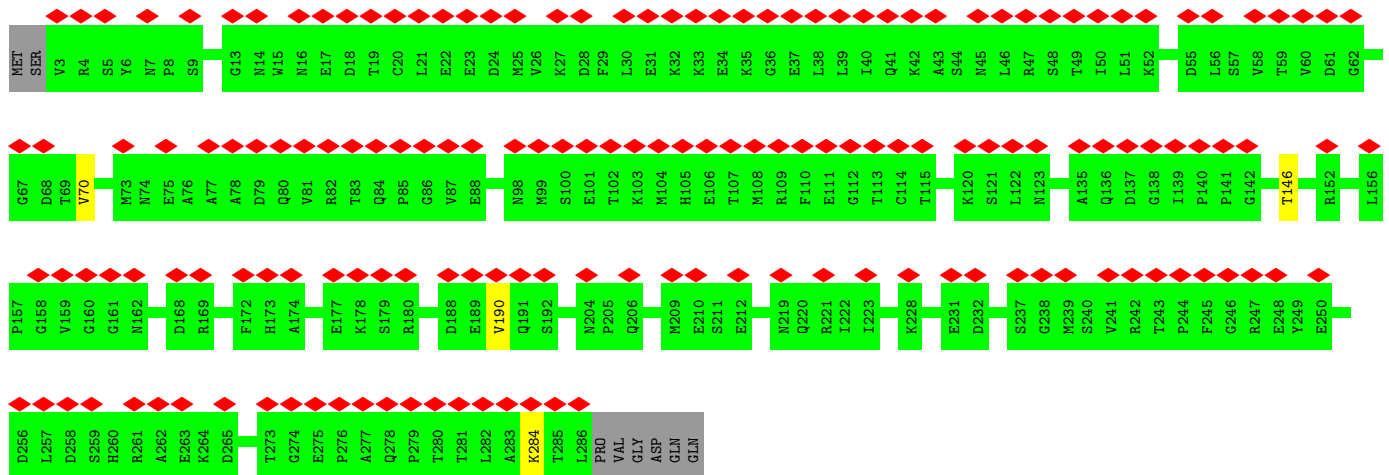




• Molecule 18: Cilia- and flagella-associated protein 161

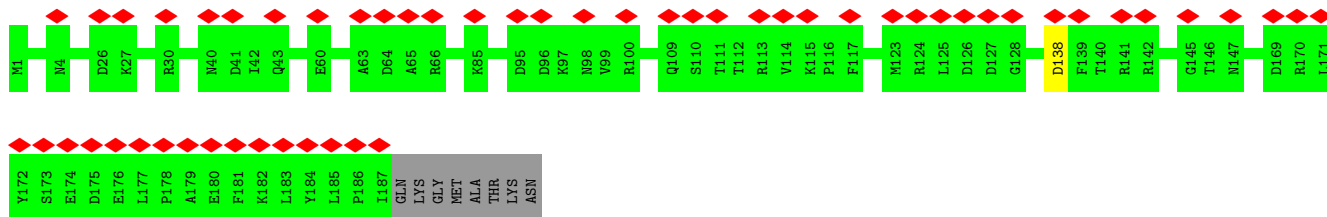


• Molecule 18: Cilia- and flagella-associated protein 161

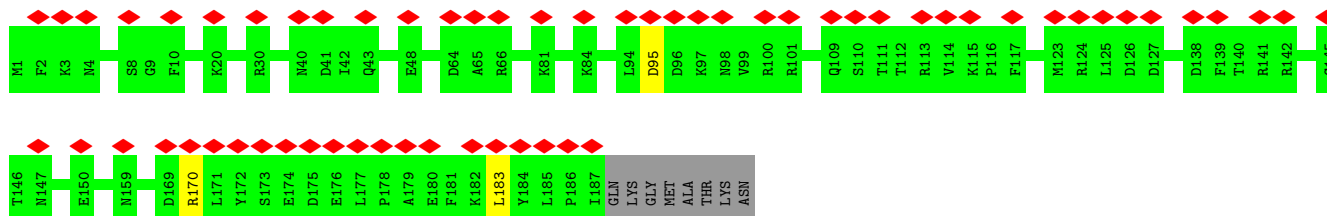


• Molecule 19: CFA20 domain-containing protein

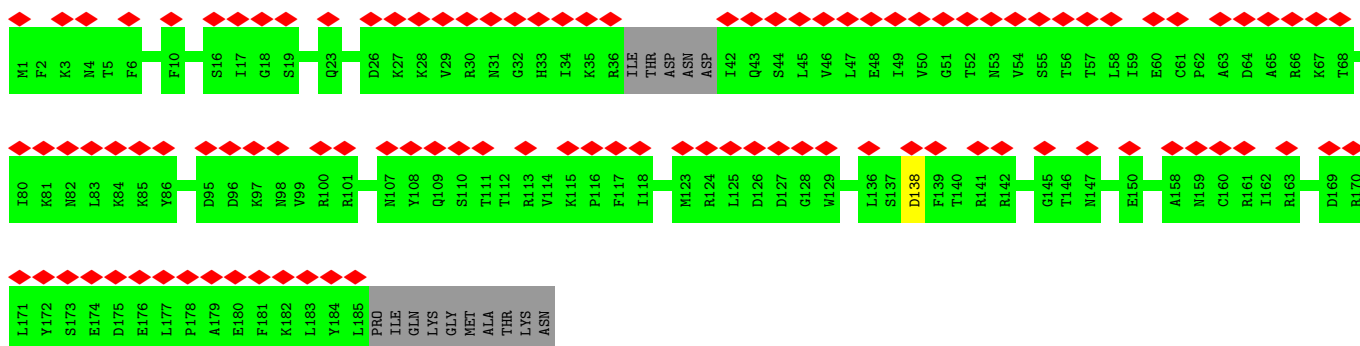
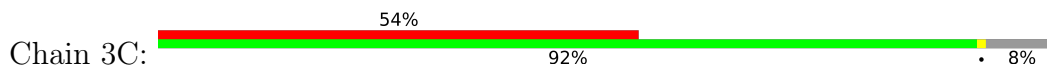




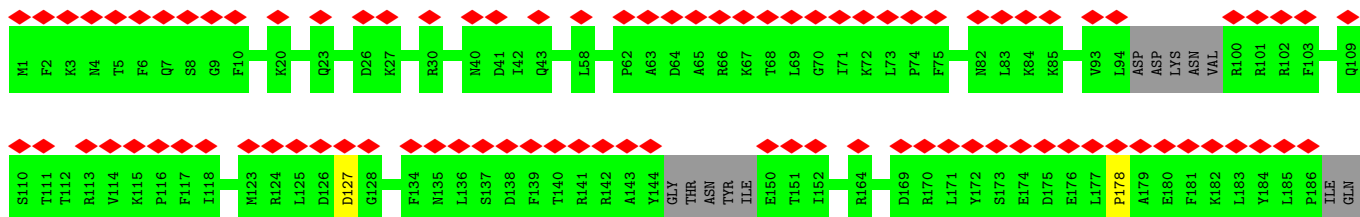
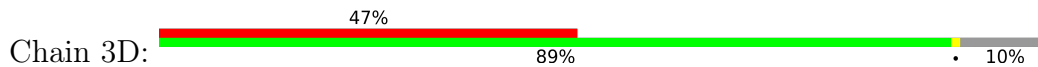
• Molecule 19: CFA20 domain-containing protein



• Molecule 19: CFA20 domain-containing protein

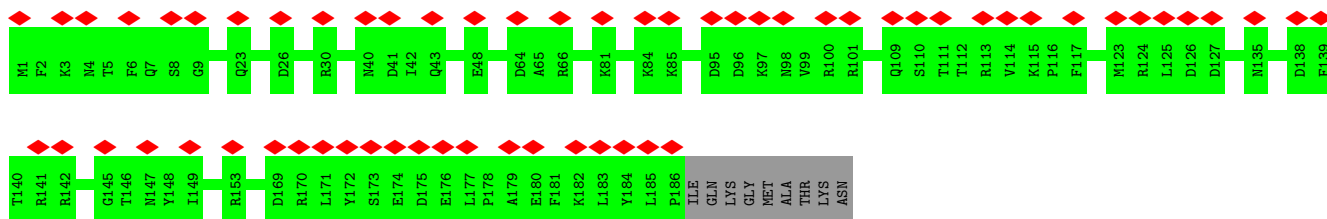


• Molecule 19: CFA20 domain-containing protein

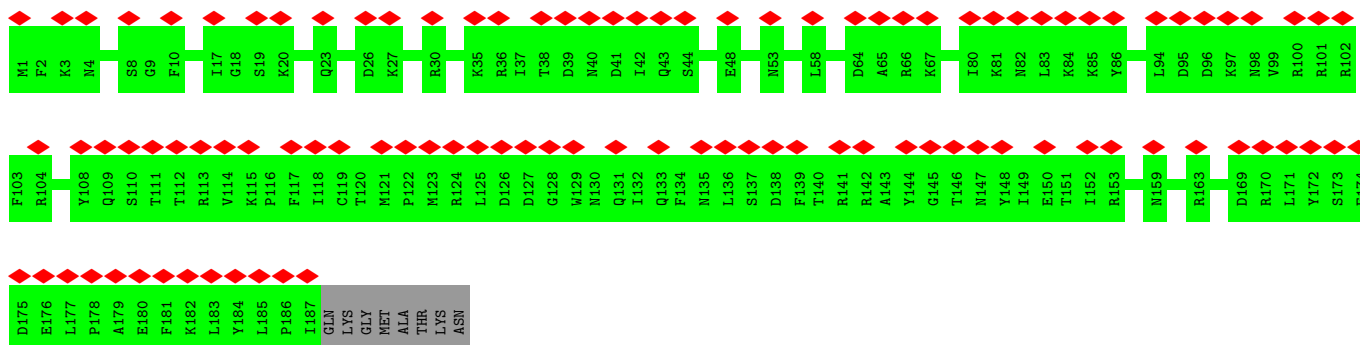


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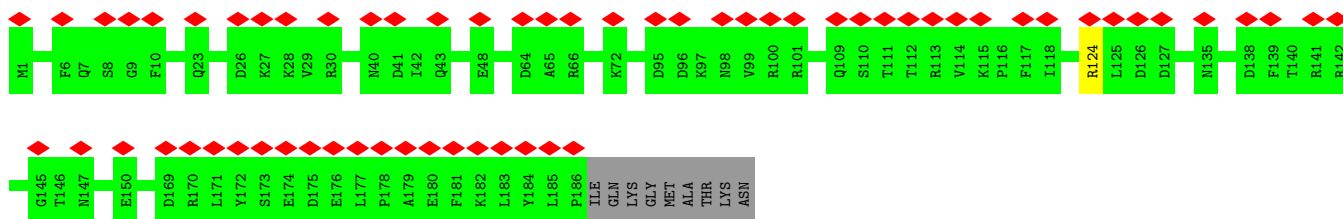




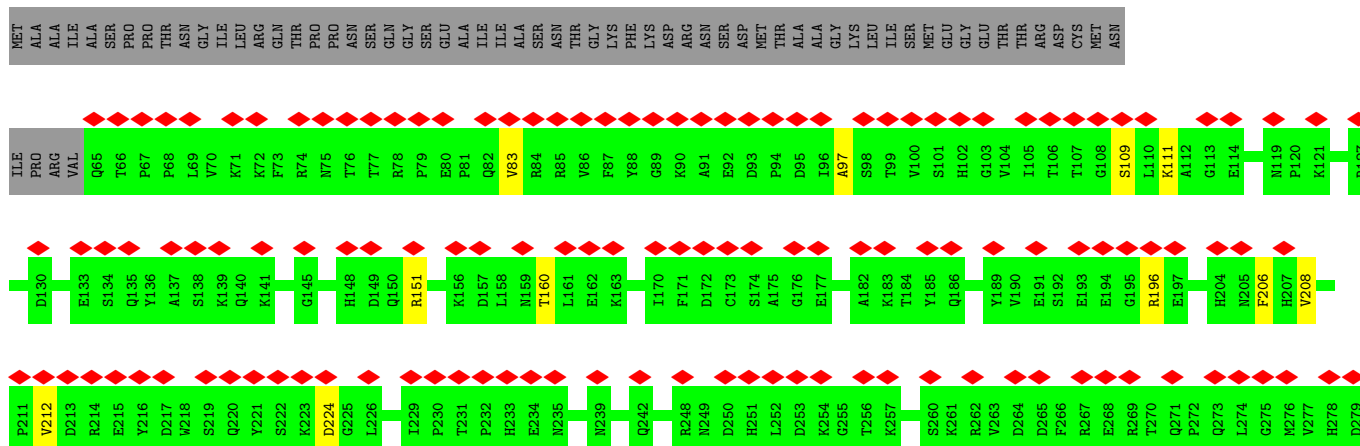
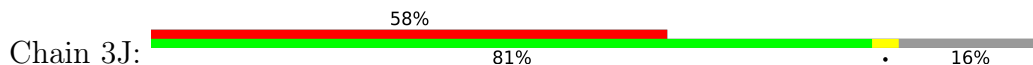
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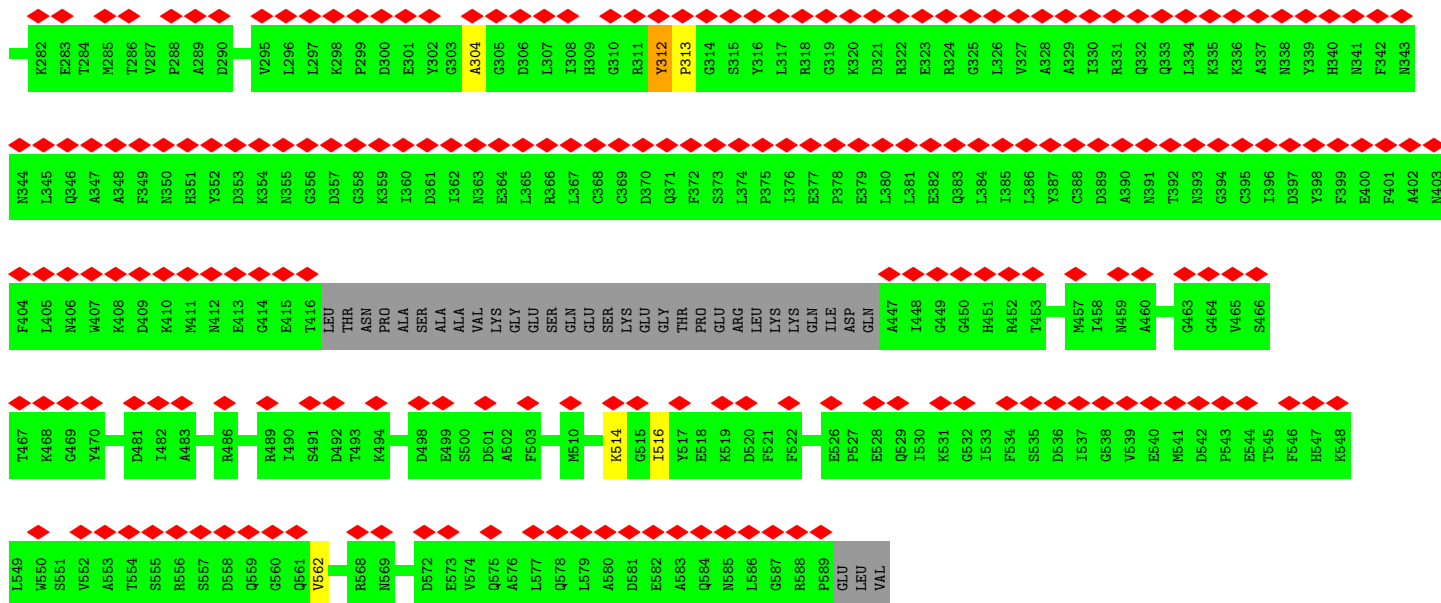


• Molecule 19: CFA20 domain-containing protein

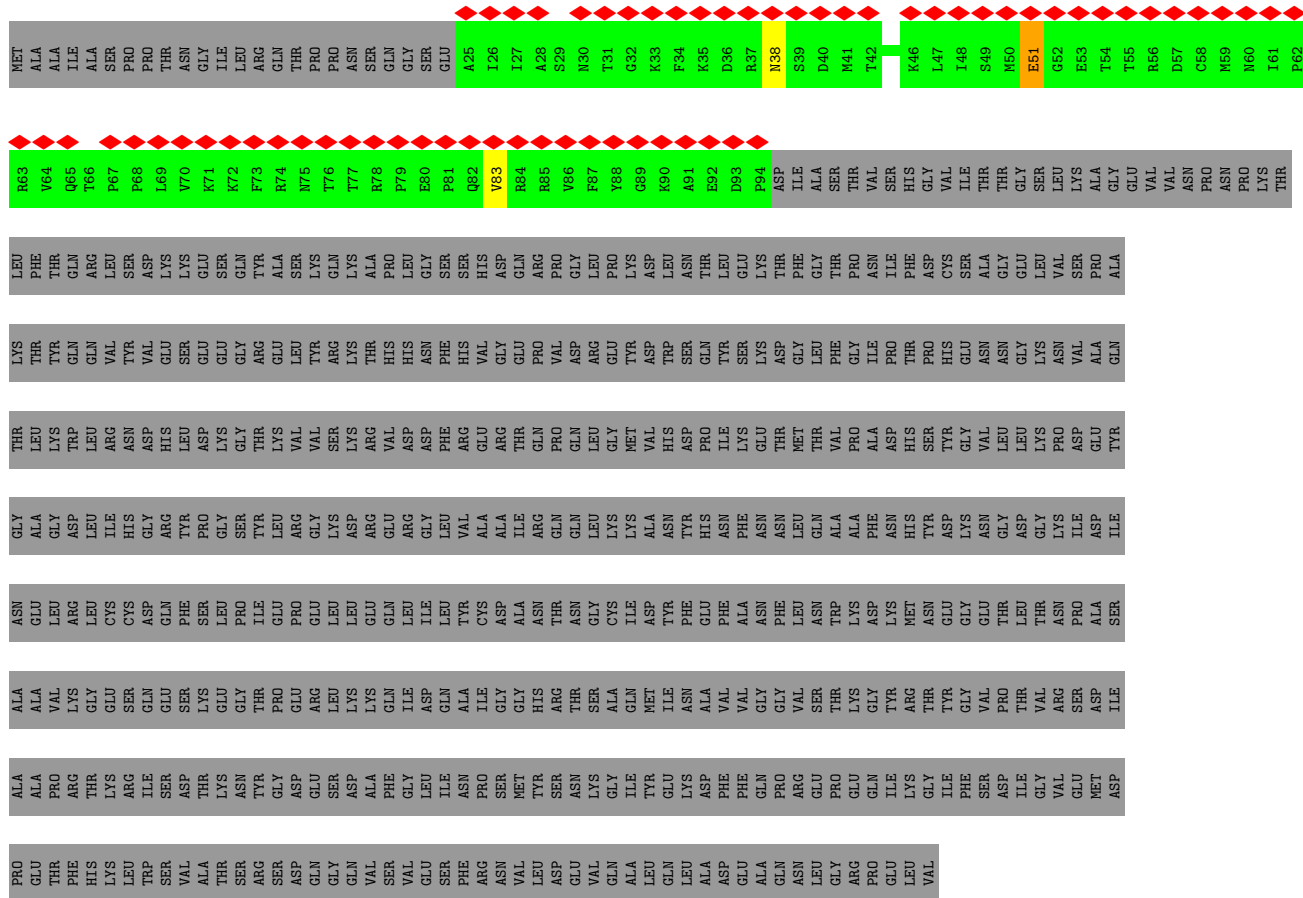


• Molecule 20: CFAP21





• Molecule 20: CFAP21

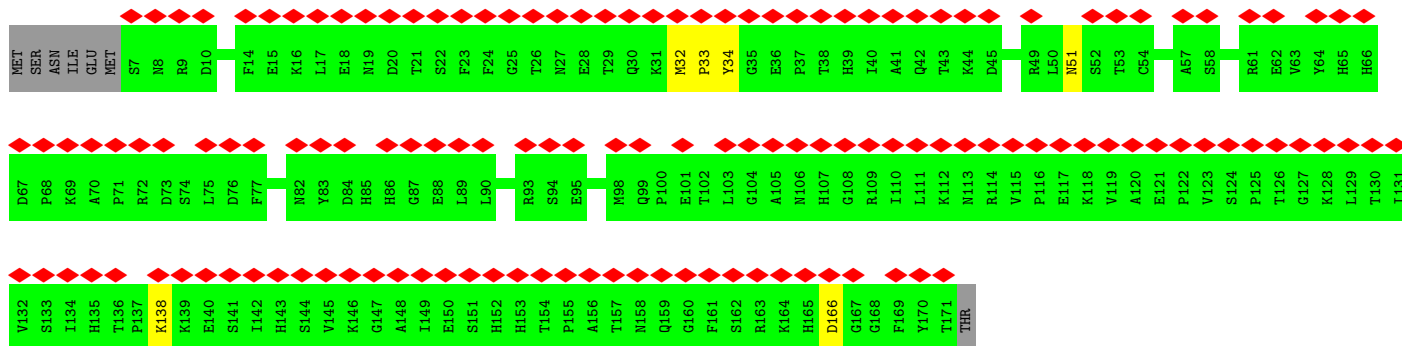
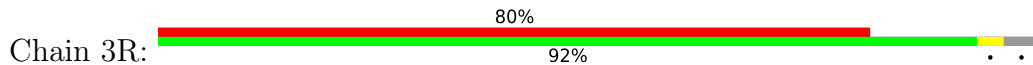


• Molecule 21: Trichohyalin-plectin-homology domain-containing protein

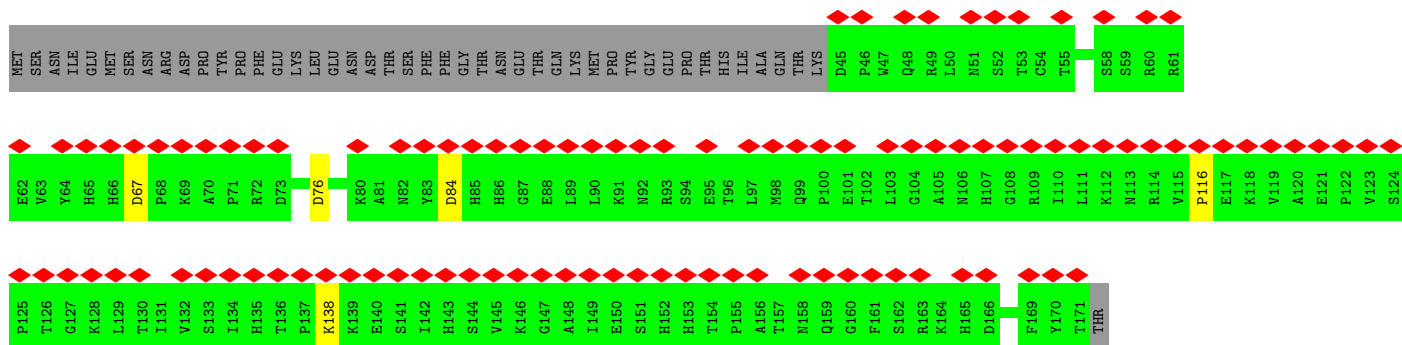
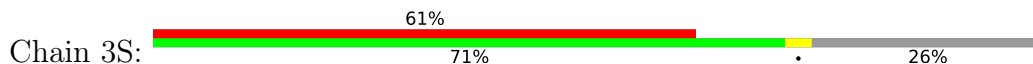


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ALA	GLY	VAL	ILE	LYS	HIS	CYS	LYS	ALA	HIS	ILE	GLY	ARG	GLU	ARG	ASN	VAL	TYR	THR	ARG	LEU	LYS	GLY	PHE	ALA	ARG	GLN	ILE	GLY	HIS	GLY	LEU	PRO	VAL	THR	ARG	GLY	LEU	VAL	PHE	ASP	GLY	ARG	ALA	GLY	GLN	LEU	VAL	PHE	ASP	THR	LYS	LYS	ASN	ILE	ASP	ASP	ARG	LEU	VAL	ALA	LEU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

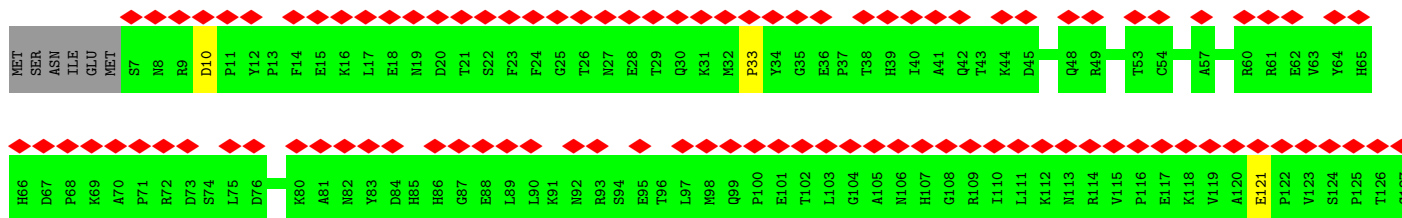
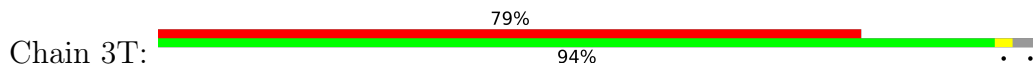
• Molecule 22: CFAP276

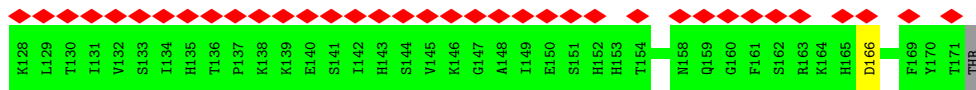


• Molecule 22: CFAP276

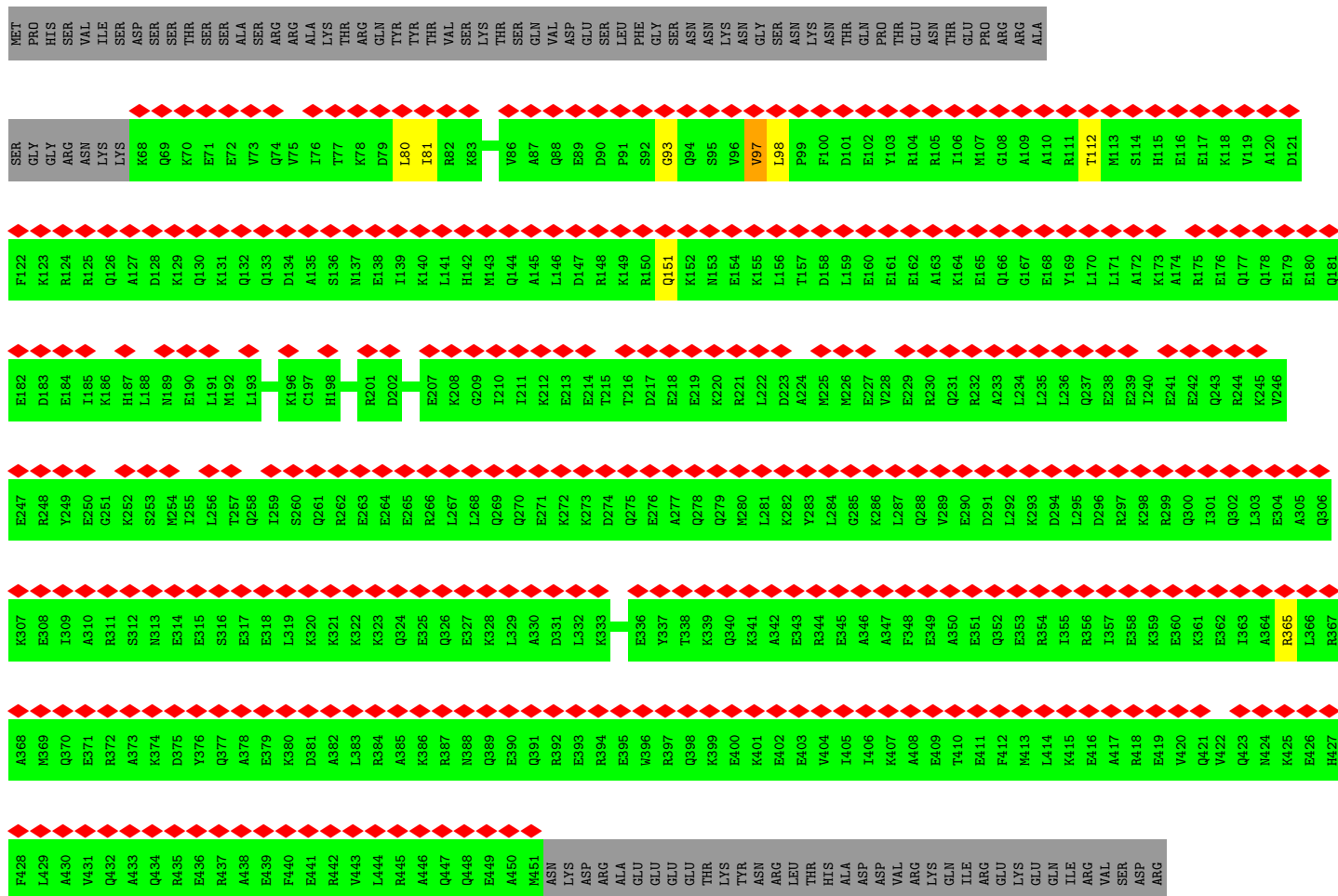
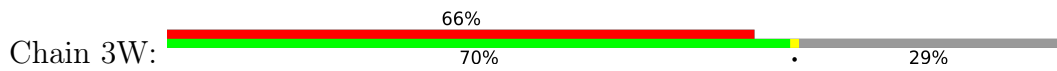


• Molecule 22: CFAP276

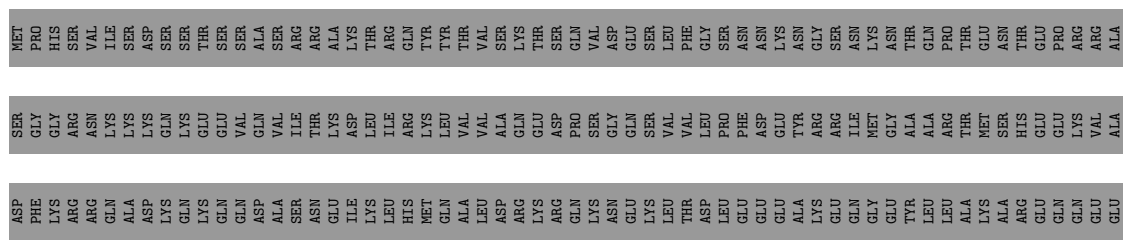




• Molecule 23: Cilia- and flagella-associated protein 45



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



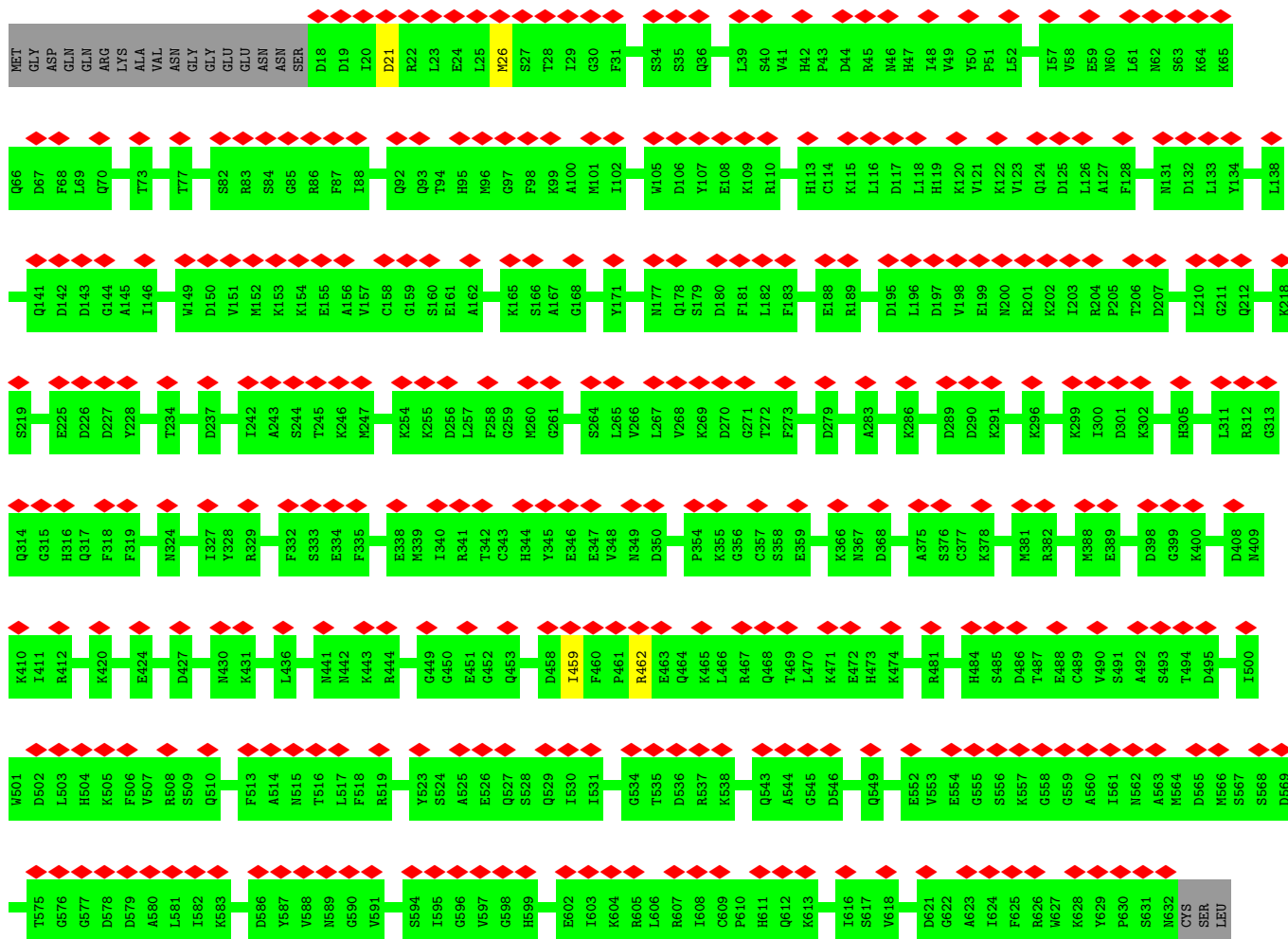




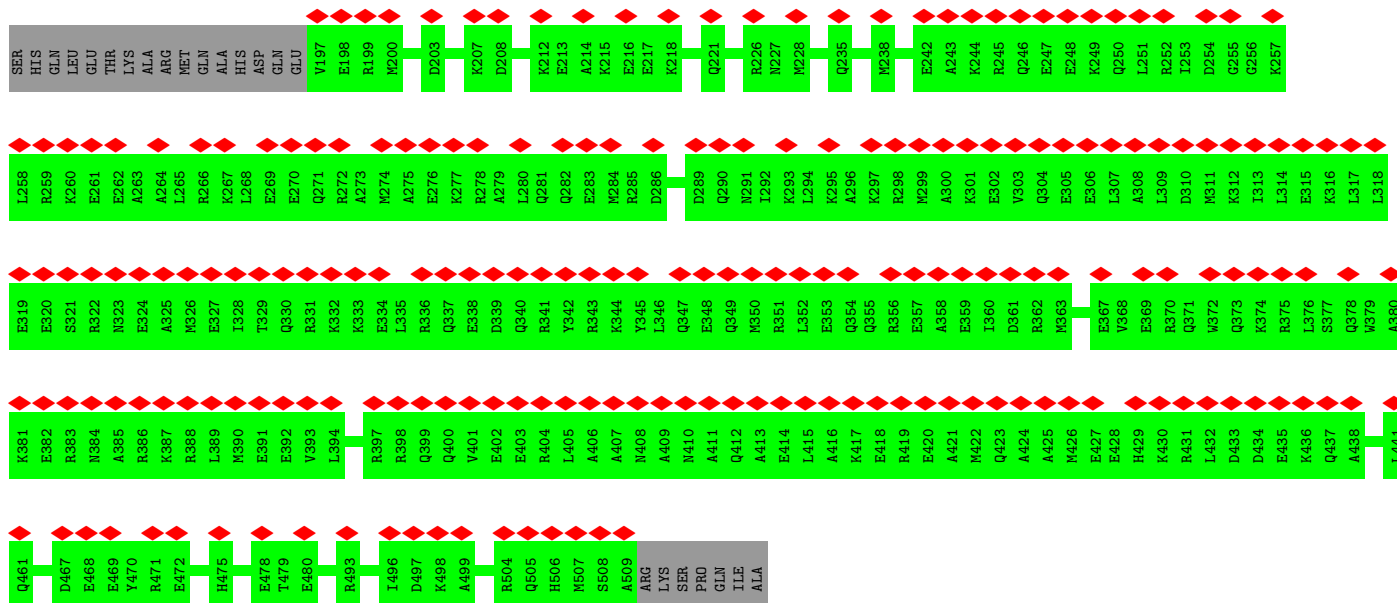




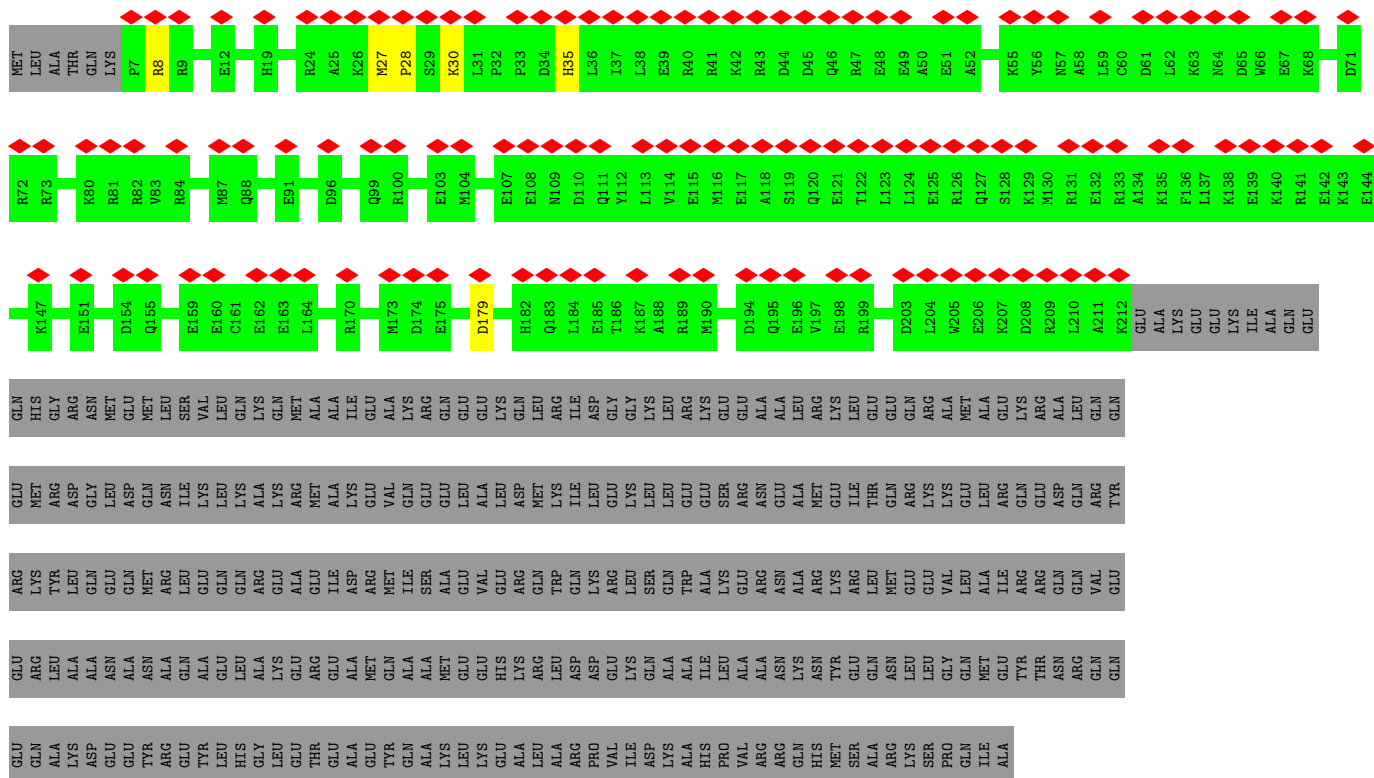
● Molecule 24: Cilia- and flagella-associated protein 52





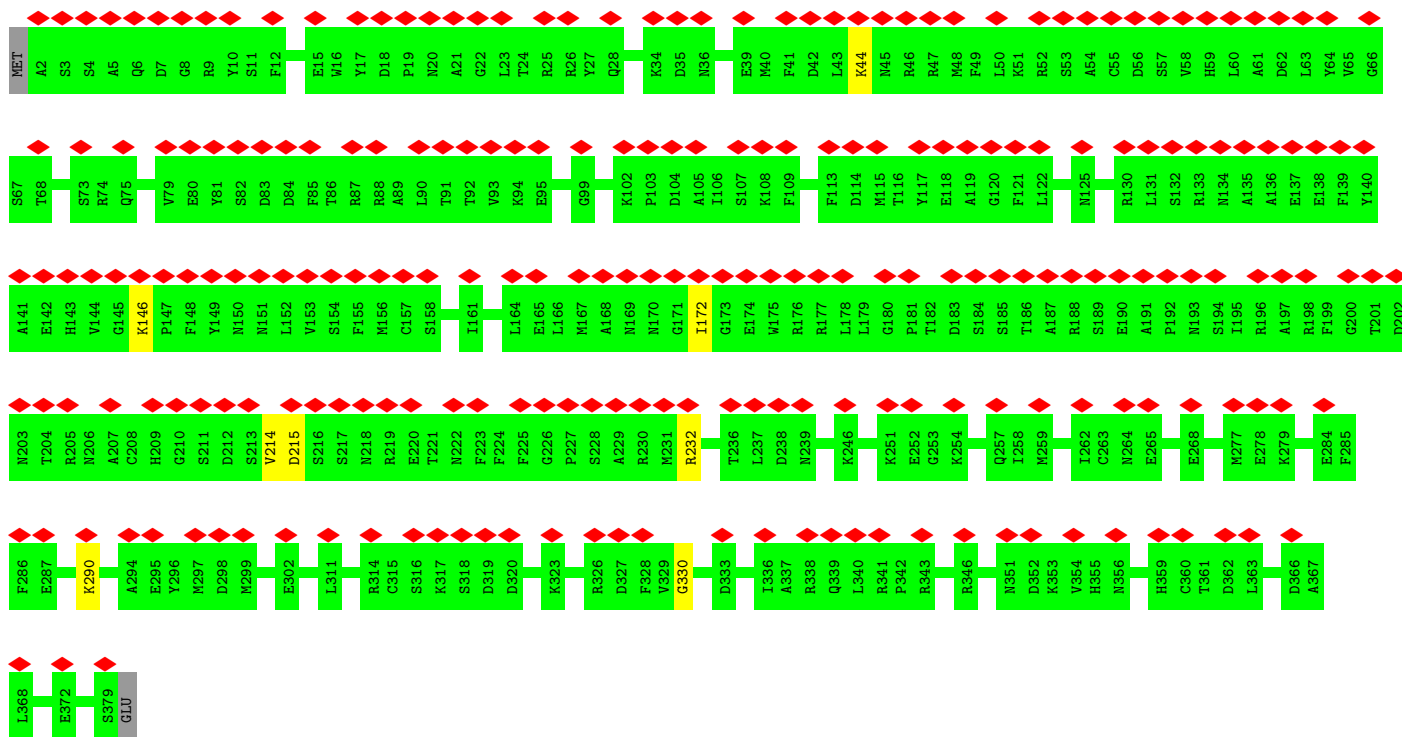


• Molecule 25: Trichohyalin-plectin-homology domain-containing protein

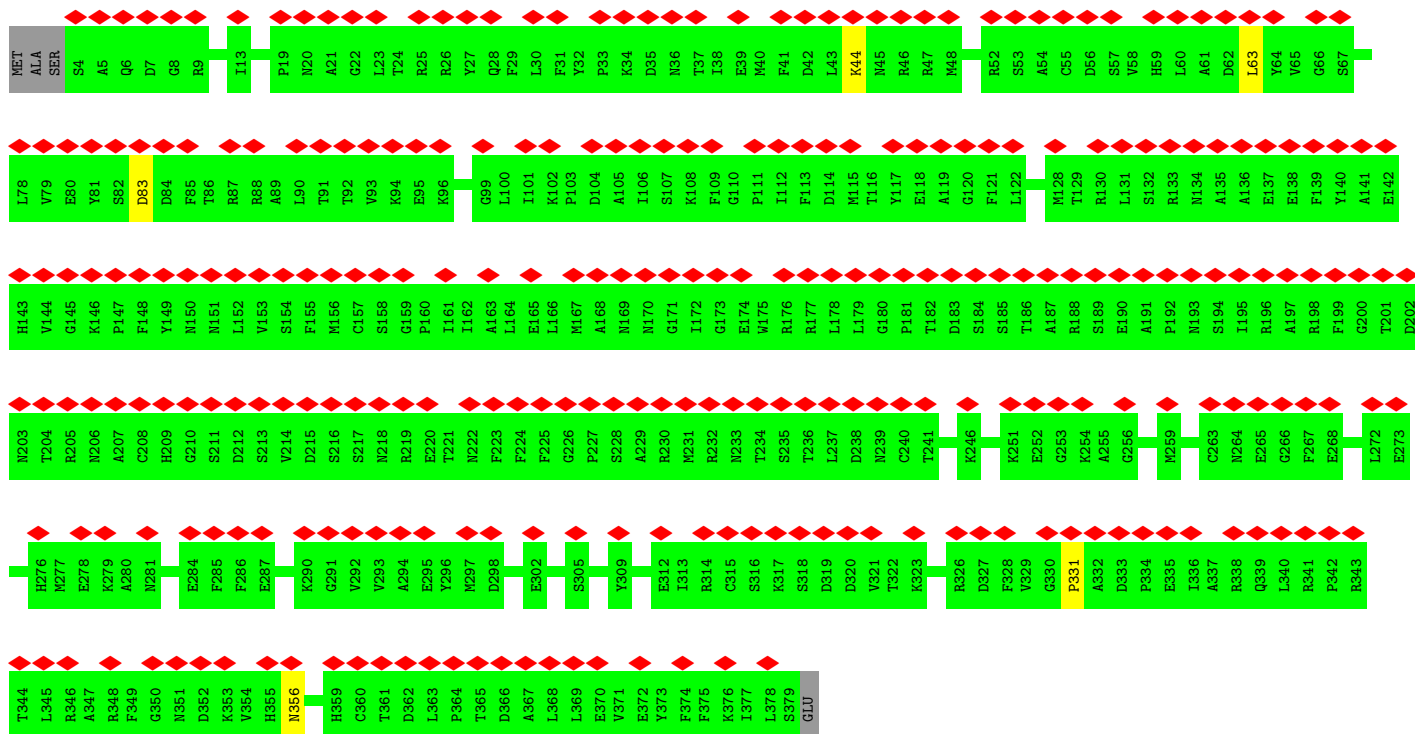
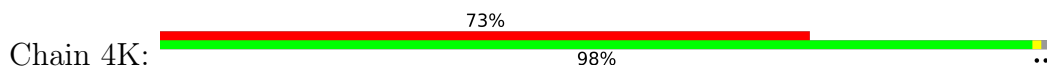


• Molecule 26: Nucleoside diphosphate kinase

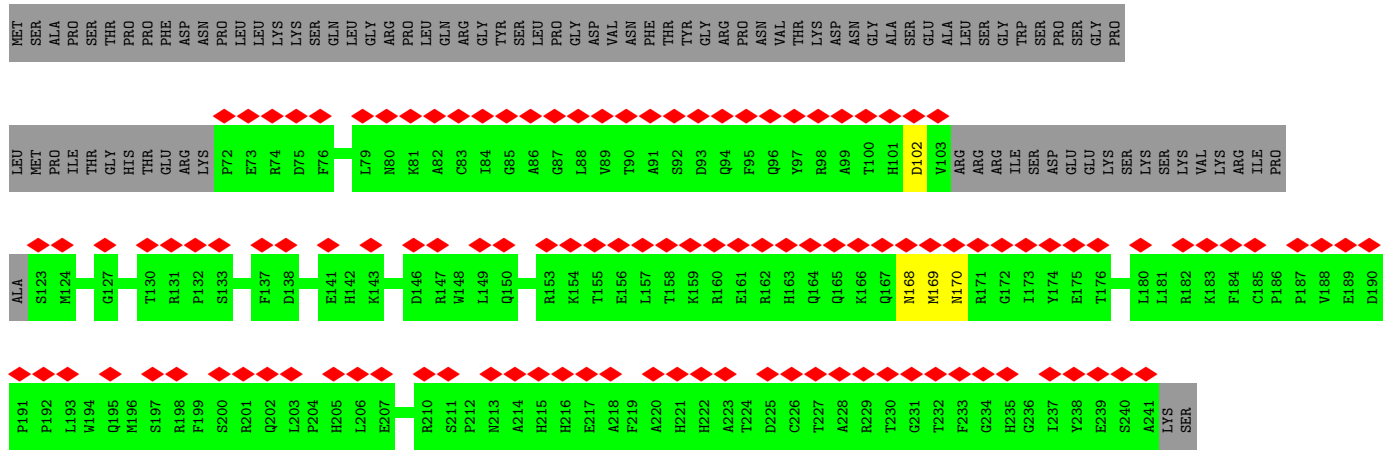




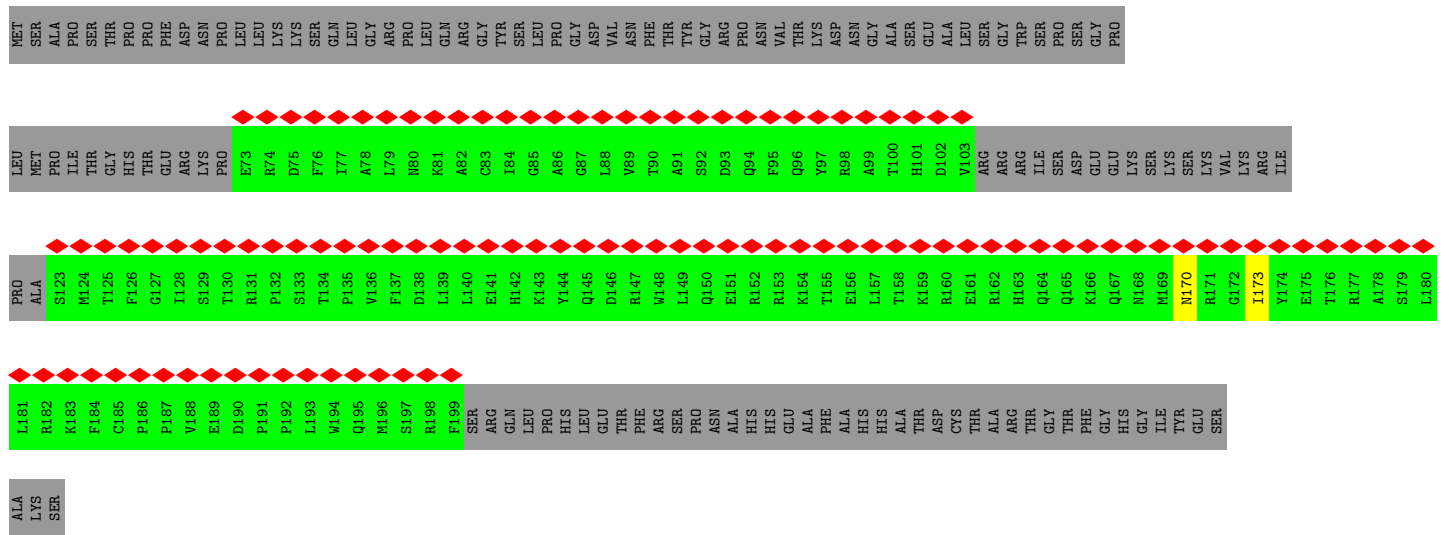
• Molecule 26: Nucleoside diphosphate kinase



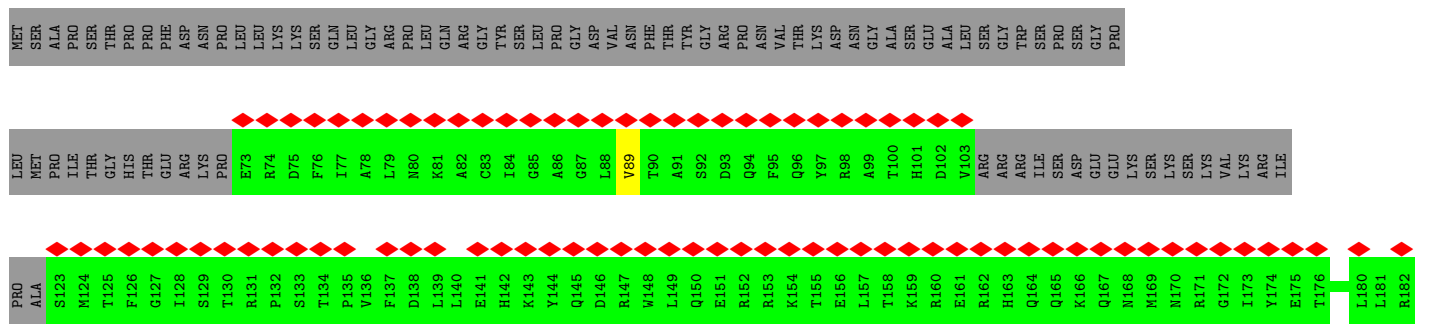
• Molecule 27: Cilia- and flagella-associated protein 77

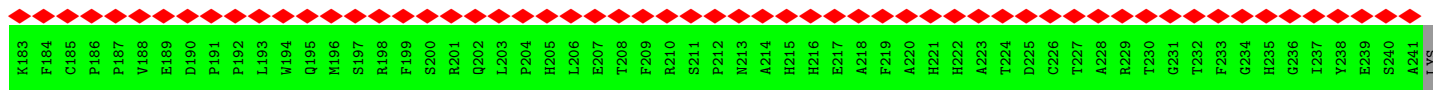


• Molecule 27: Cilia- and flagella-associated protein 77



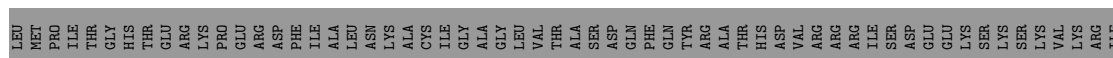
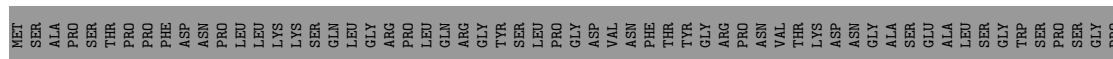
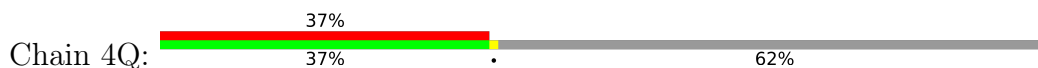
• Molecule 27: Cilia- and flagella-associated protein 77





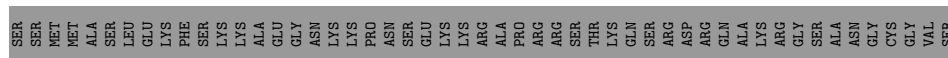
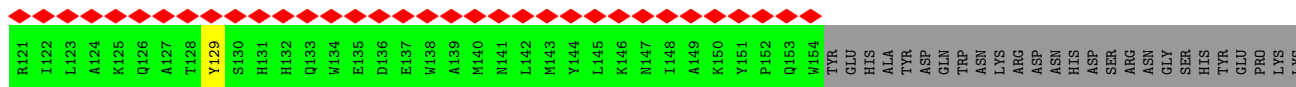
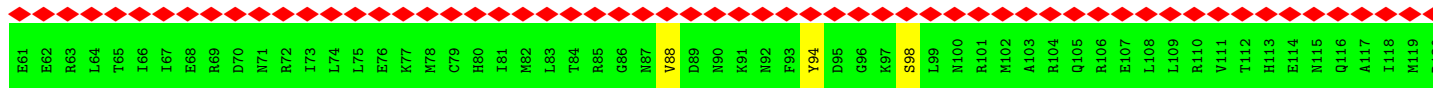
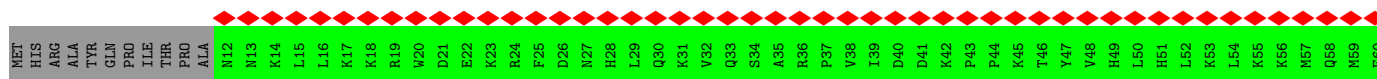
SER

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

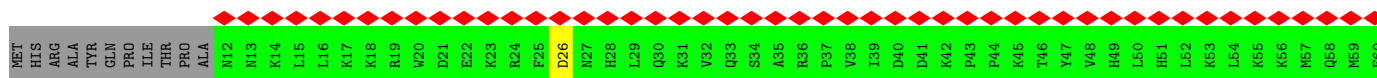


A241  
LYS  
SER

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

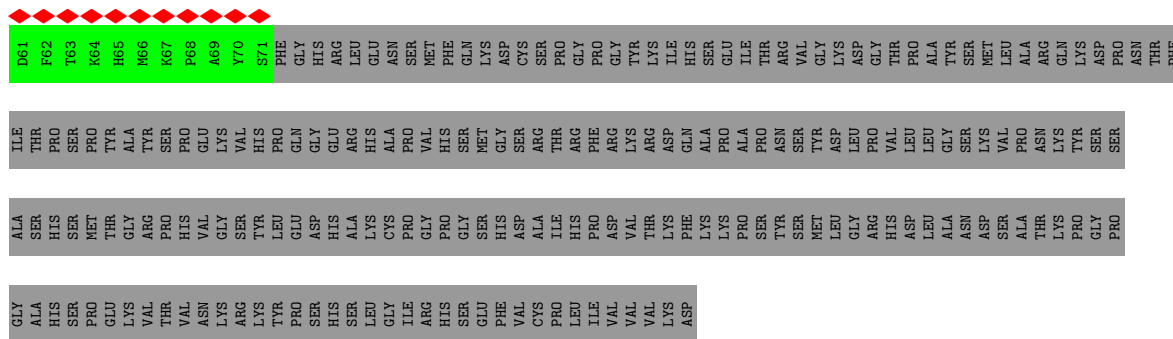


• Molecule 28: Cilia- and flagella-associated protein 97

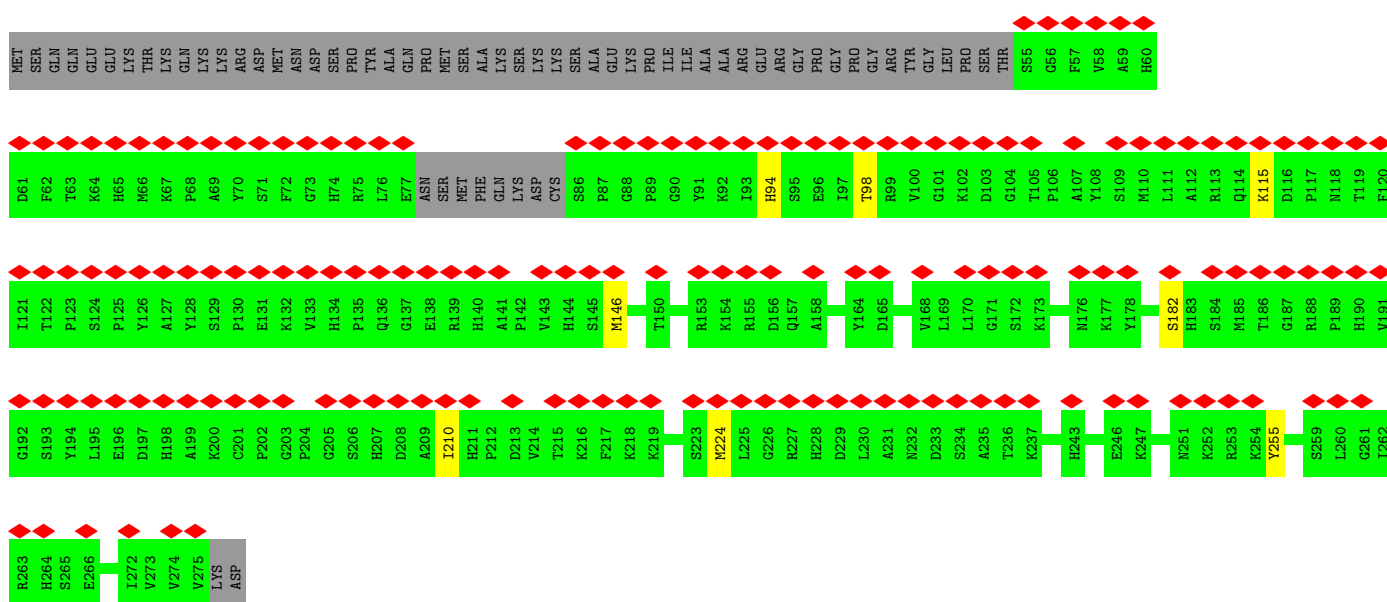




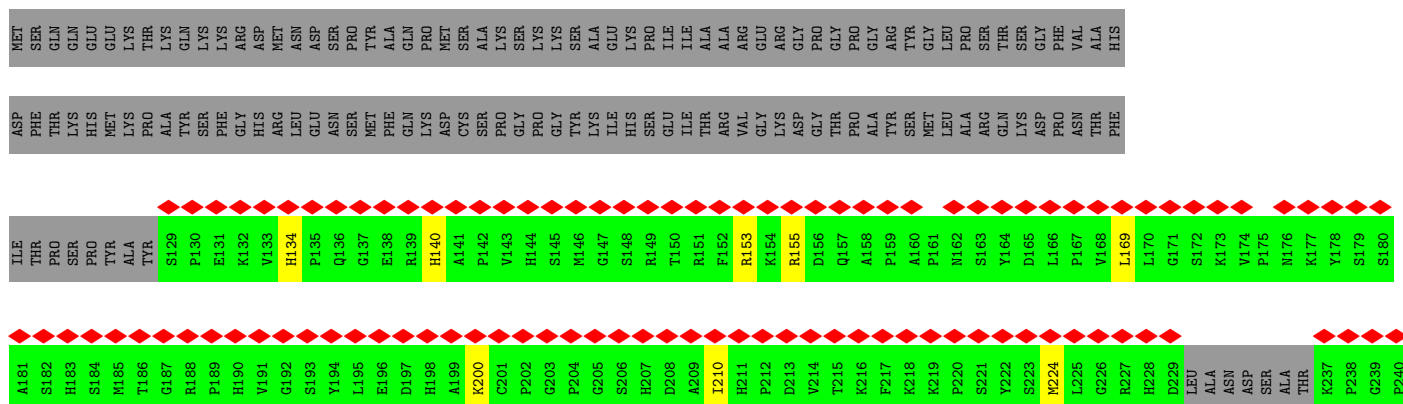


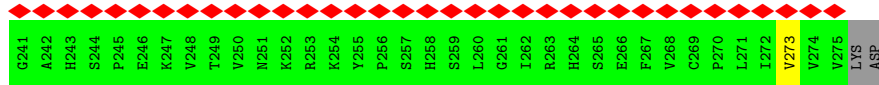


• Molecule 30: Outer dense fiber protein 3

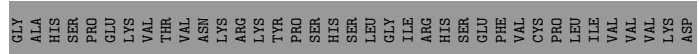
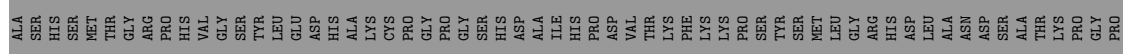
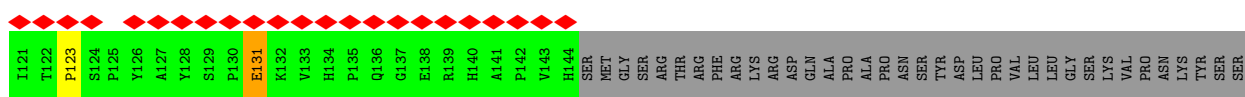
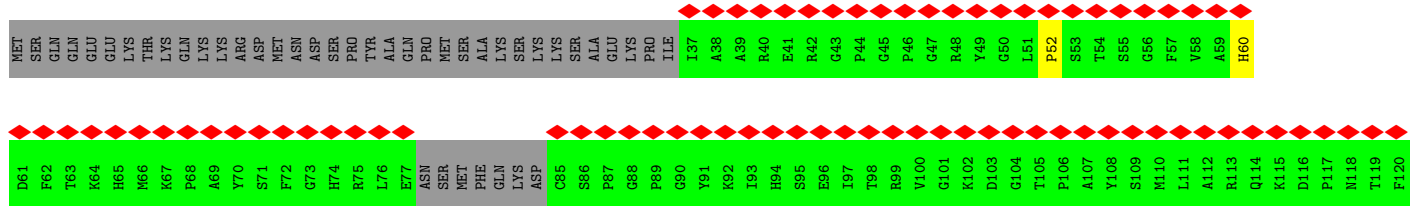


• Molecule 30: Outer dense fiber protein 3

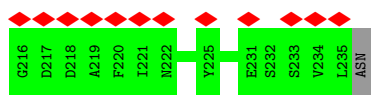
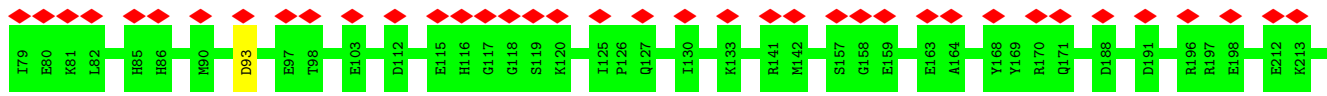
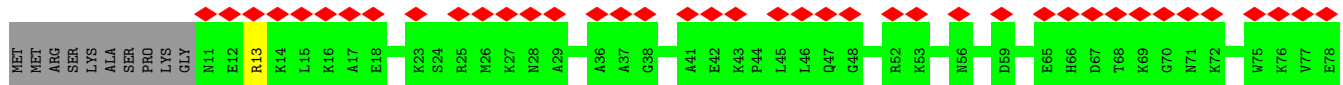




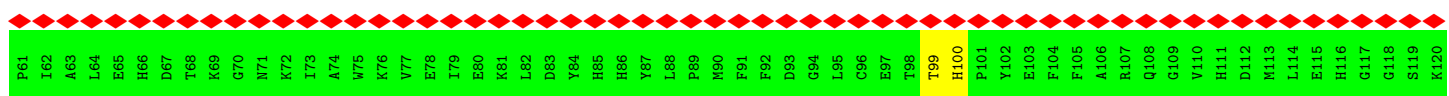
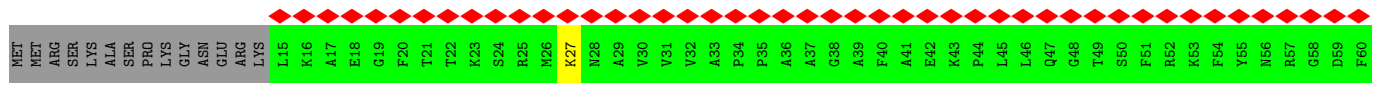
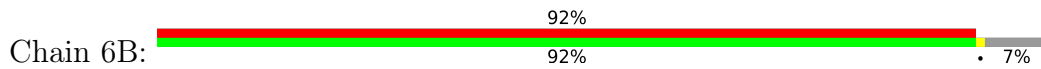
• Molecule 30: Outer dense fiber protein 3

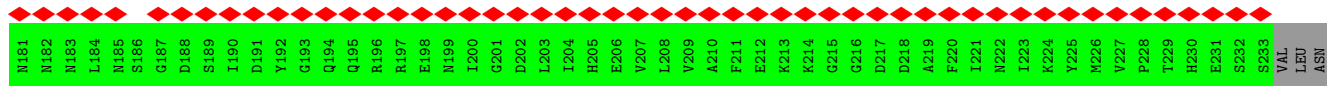
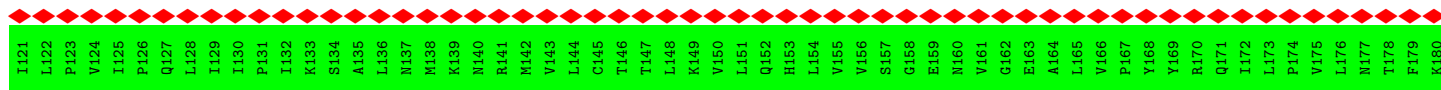


• Molecule 31: PACRG

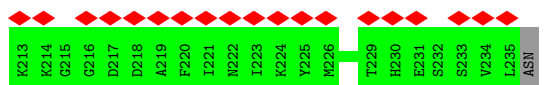
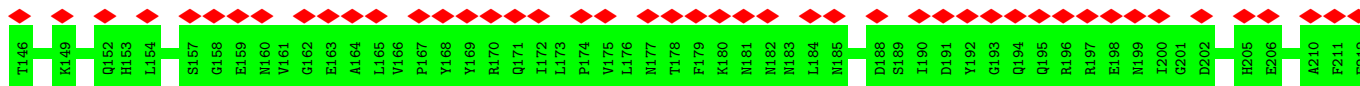
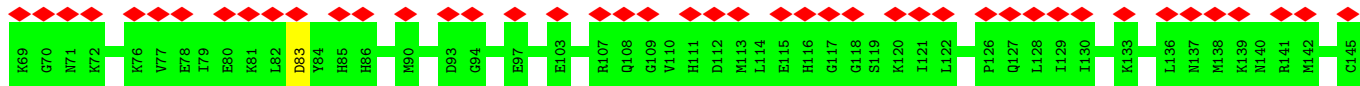
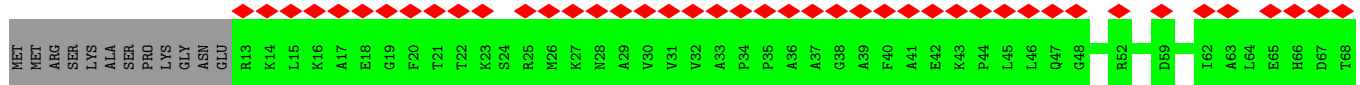


• Molecule 31: PACRG

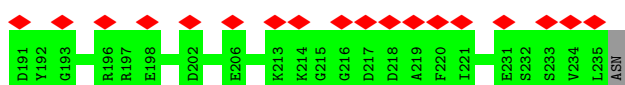
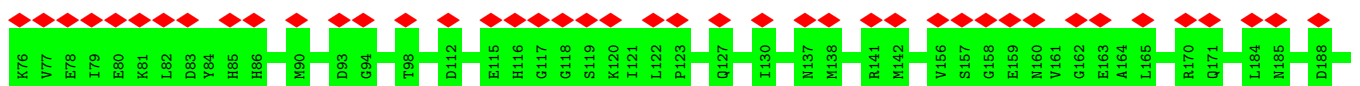
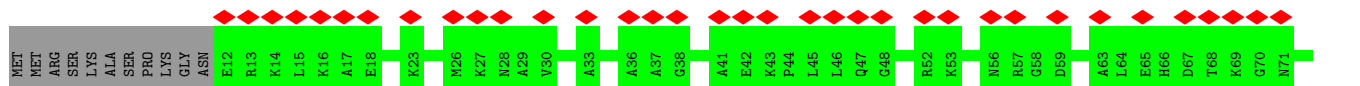
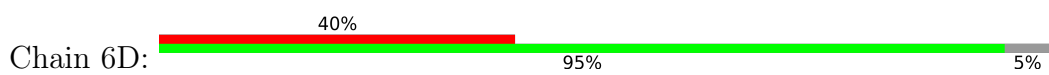




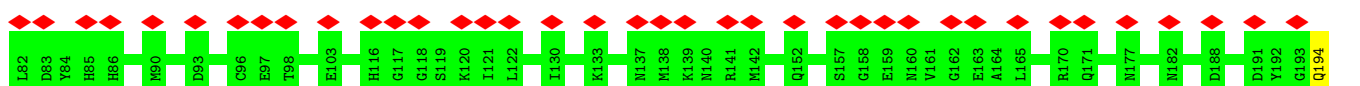
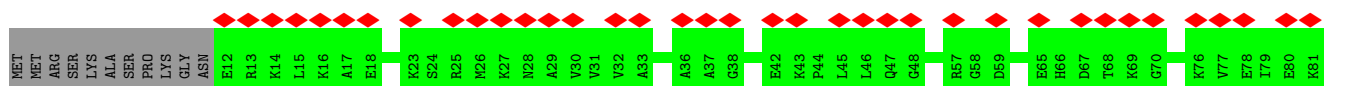
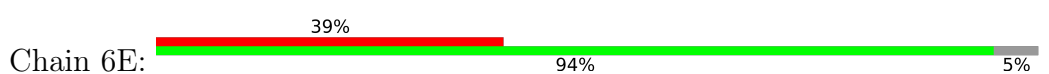
• Molecule 31: PACRG

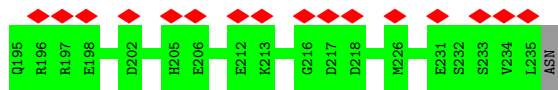


• Molecule 31: PACRG

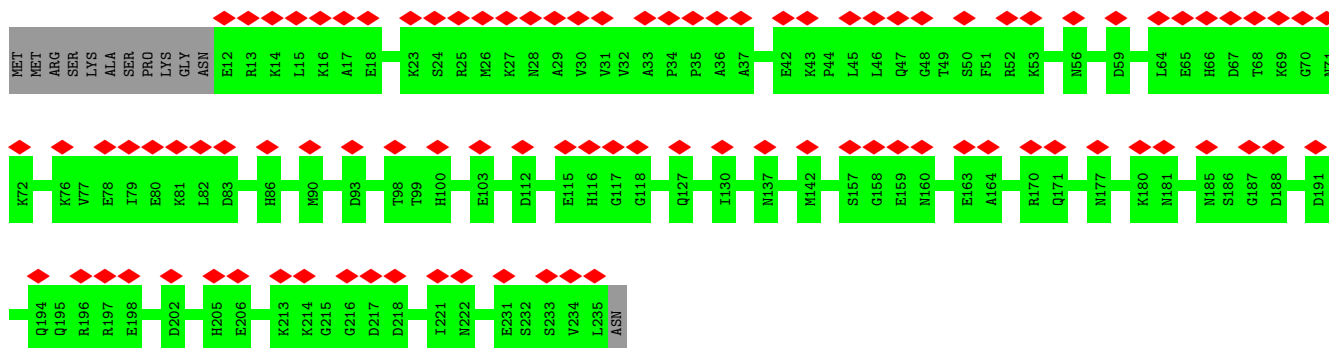
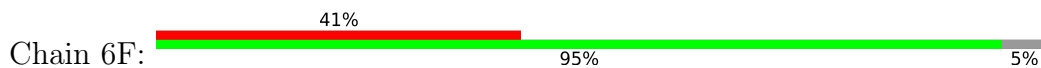


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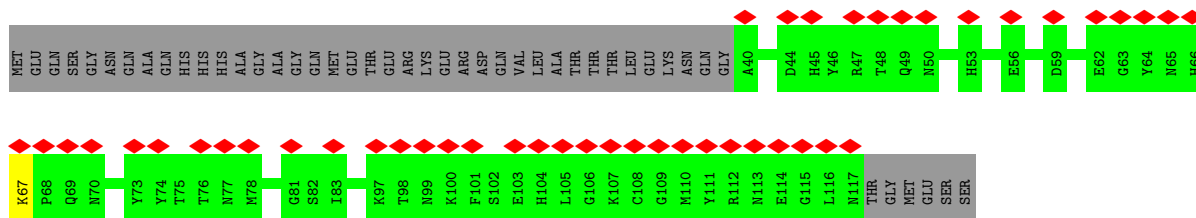




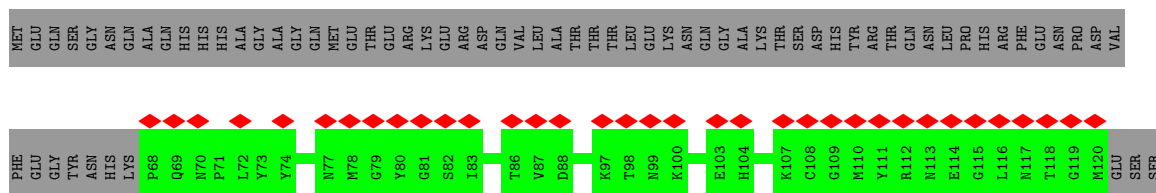
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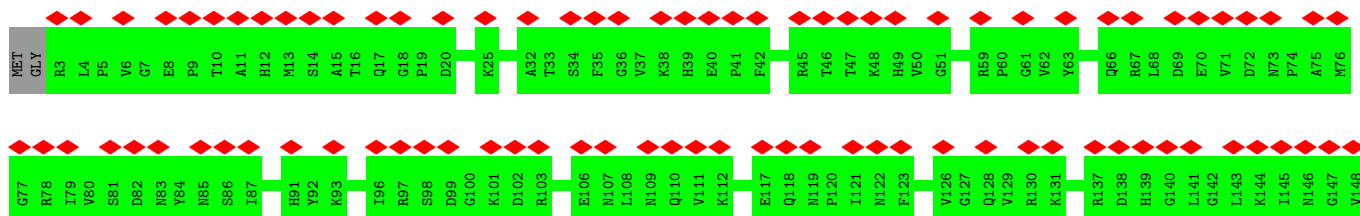
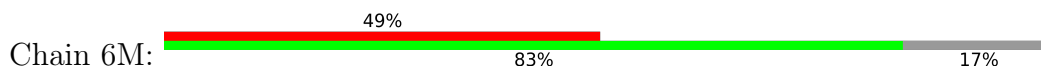
• Molecule 32: Piercel



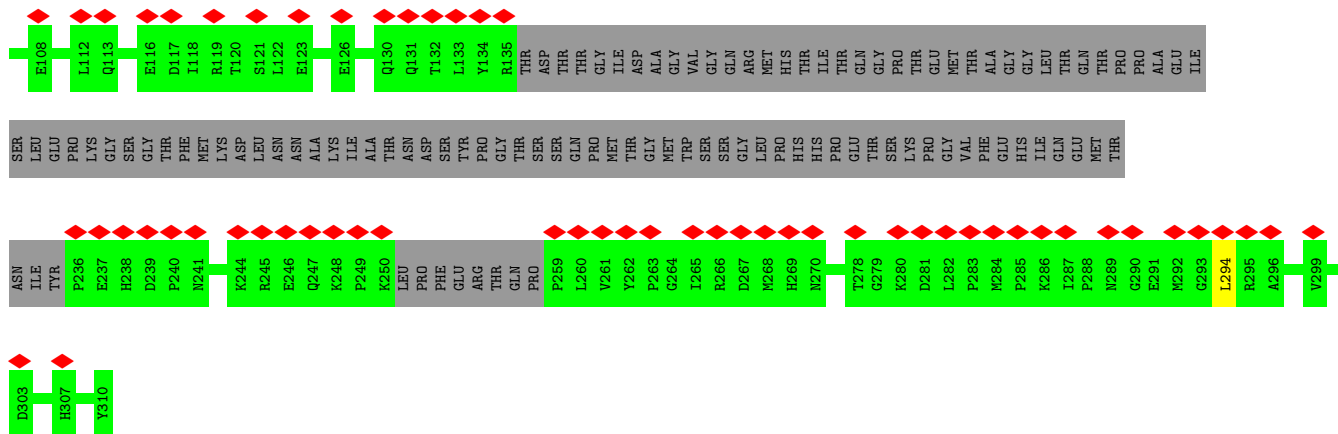
• Molecule 32: Piercel



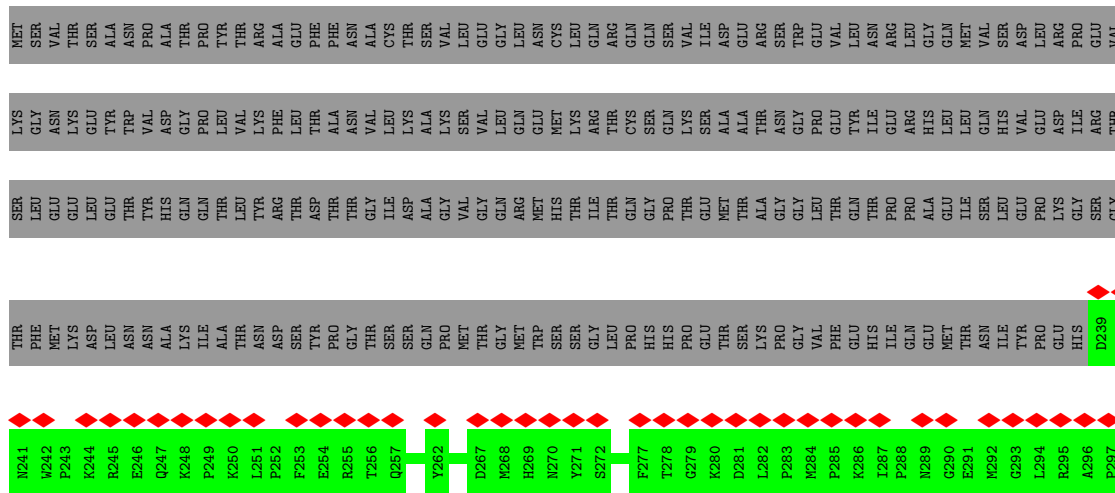
• Molecule 33: Protein phosphatase 1 regulatory subunit 32



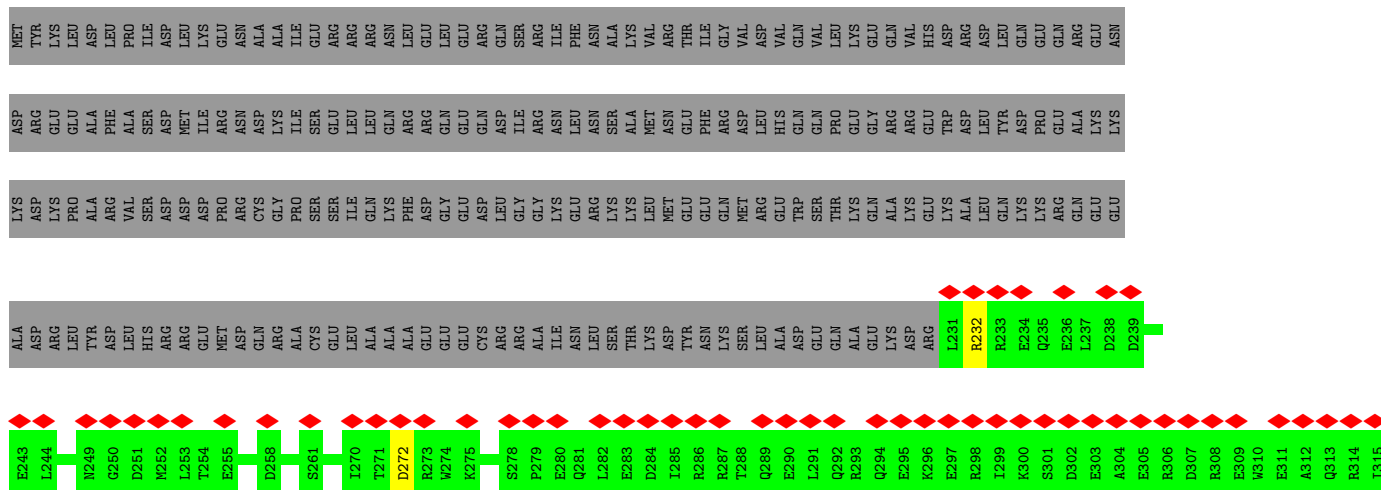




• Molecule 34: RIB35

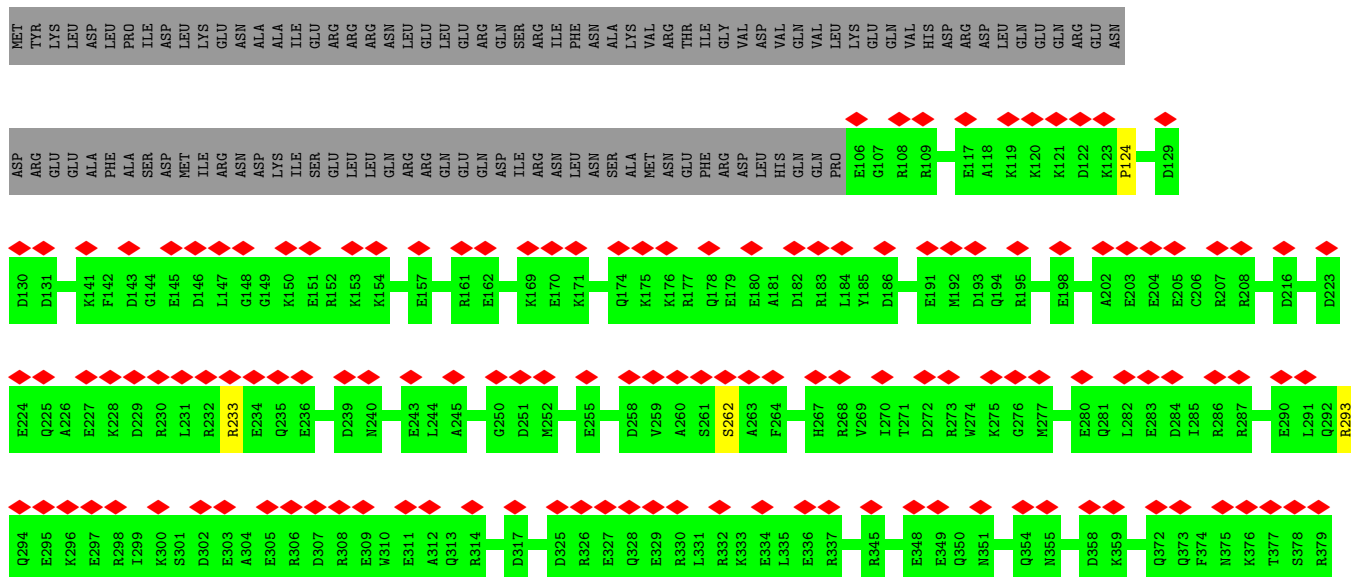
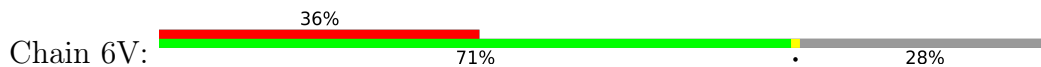


• Molecule 35: RIB43A-like with coiled-coils protein 2

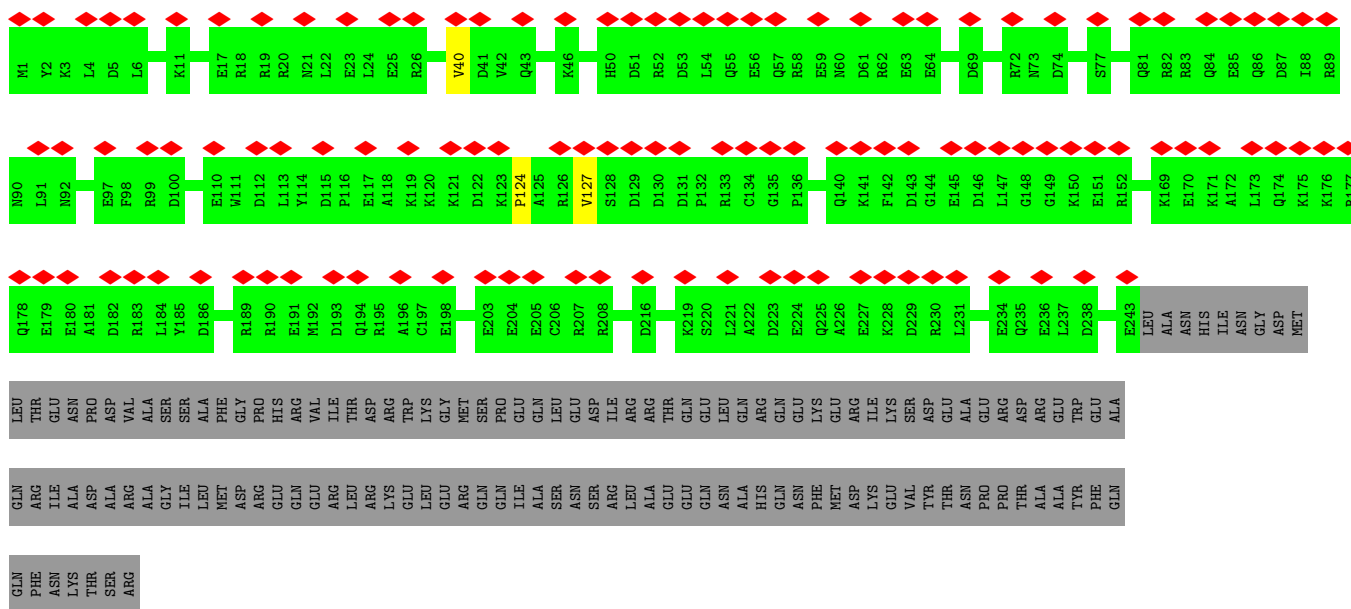




• Molecule 35: RIB43A-like with coiled-coils protein 2

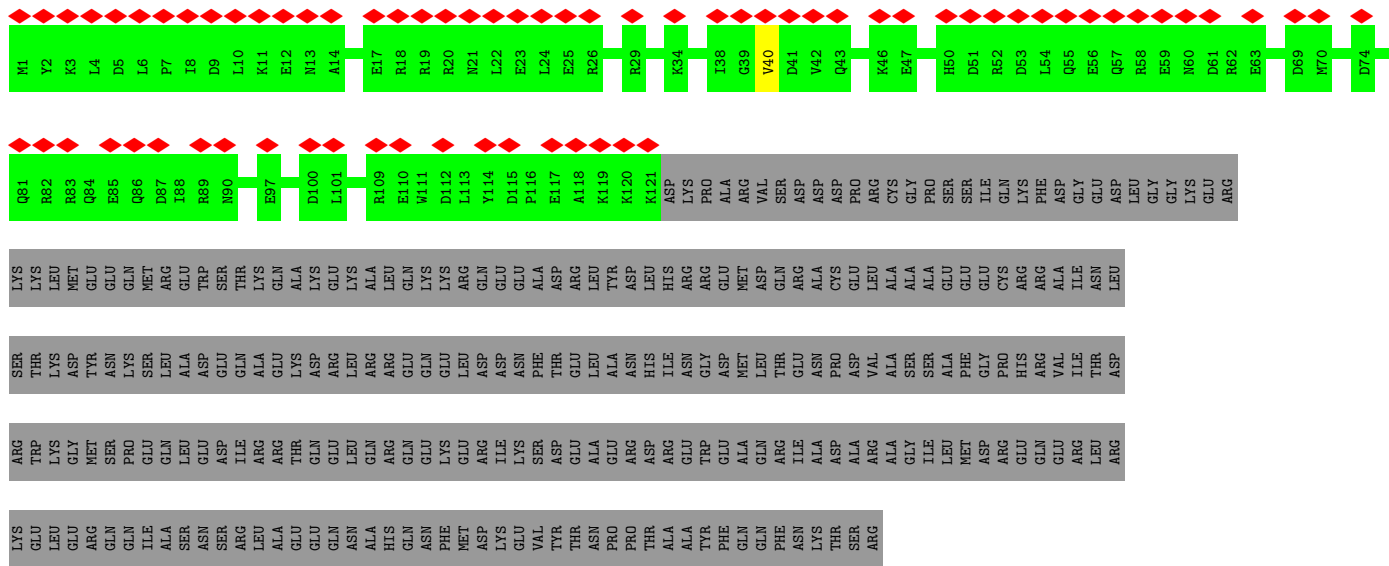


• Molecule 35: RIB43A-like with coiled-coils protein 2

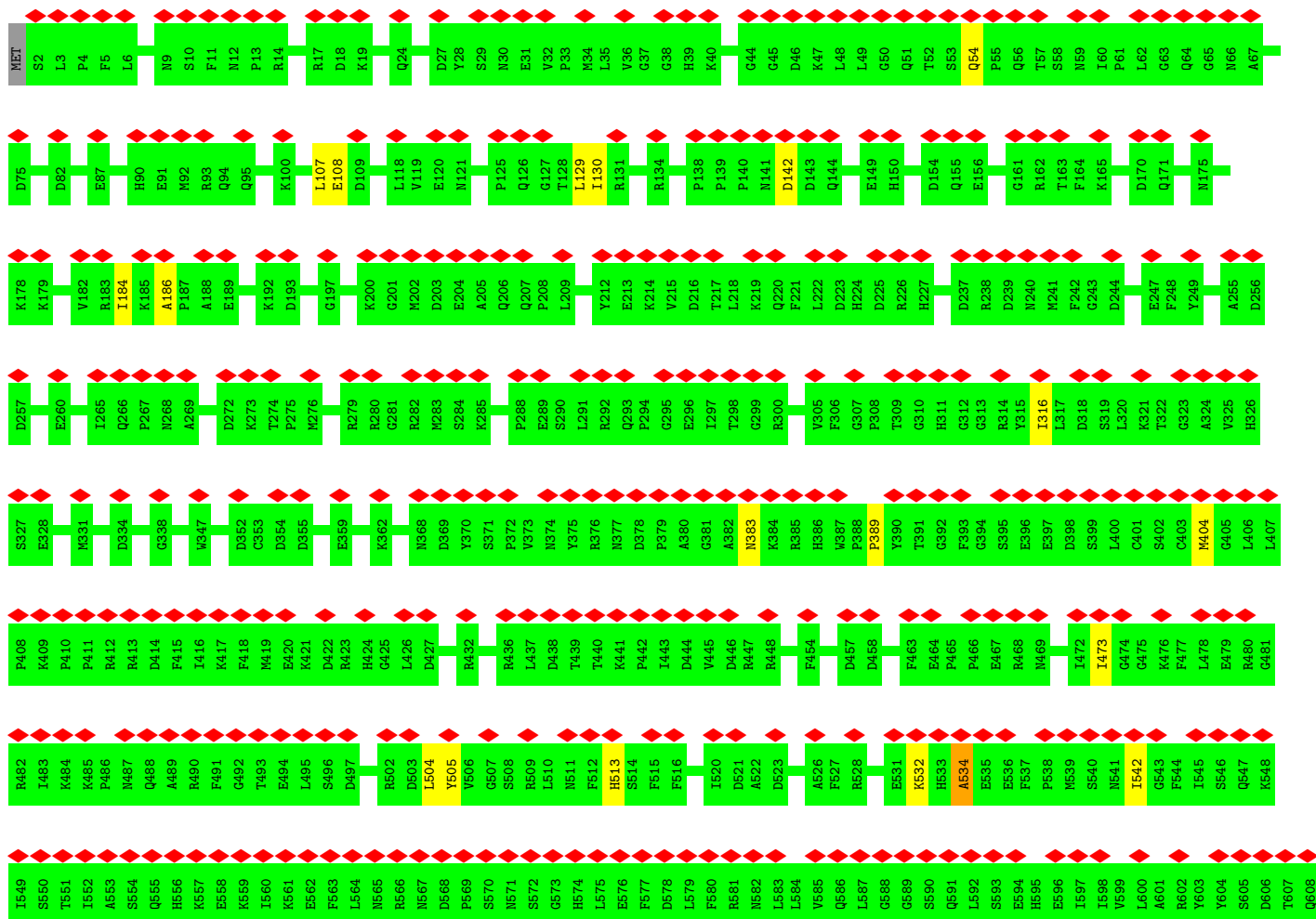


• Molecule 35: RIB43A-like with coiled-coils protein 2

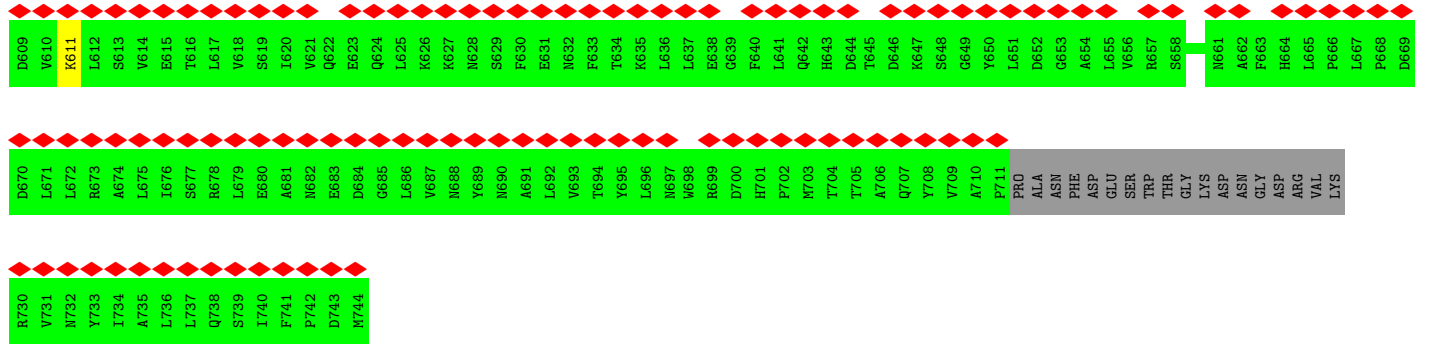




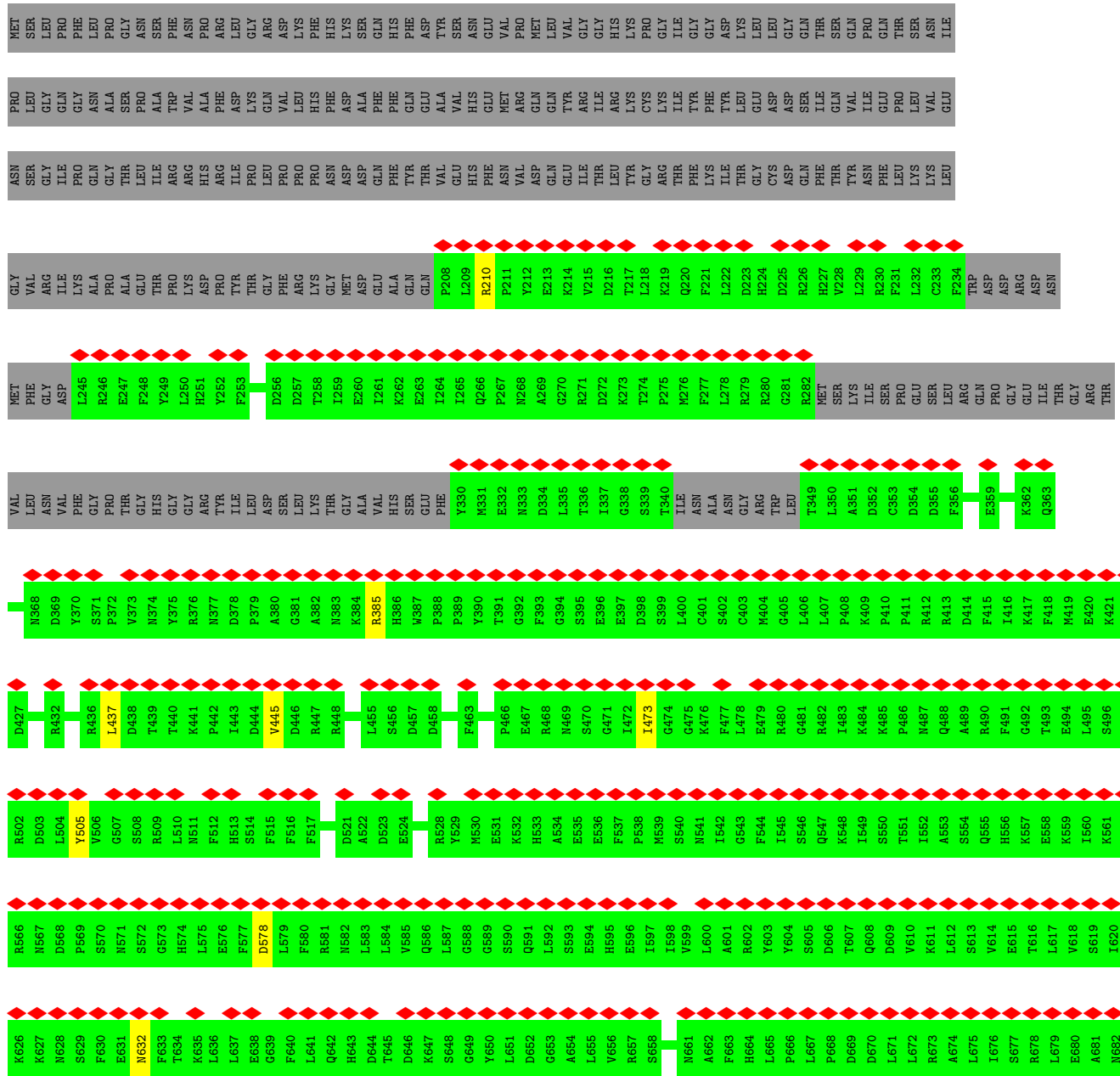
• Molecule 36: EF-hand domain-containing family member C2





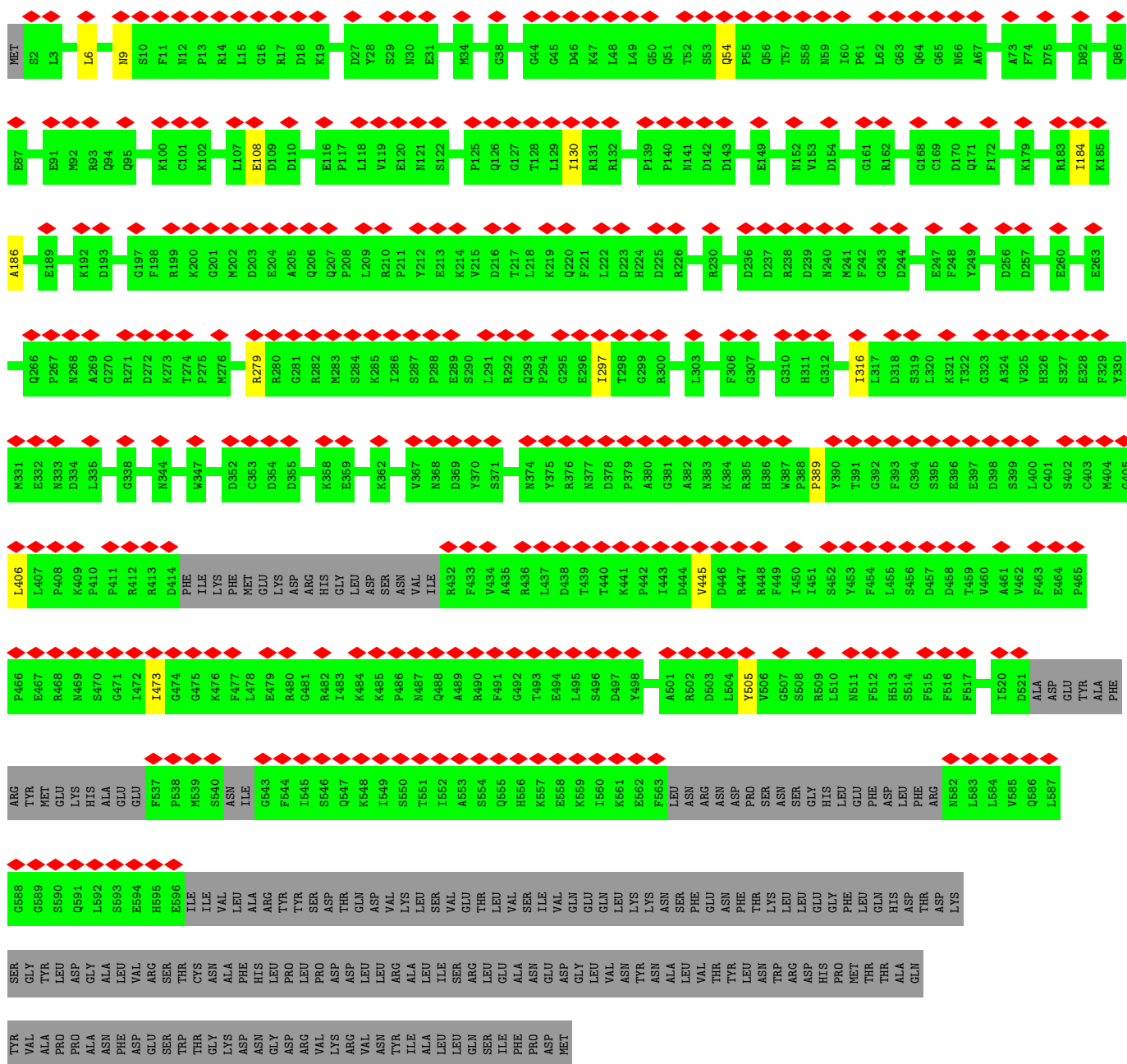
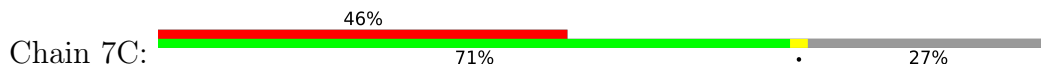


• Molecule 36: EF-hand domain-containing family member C2



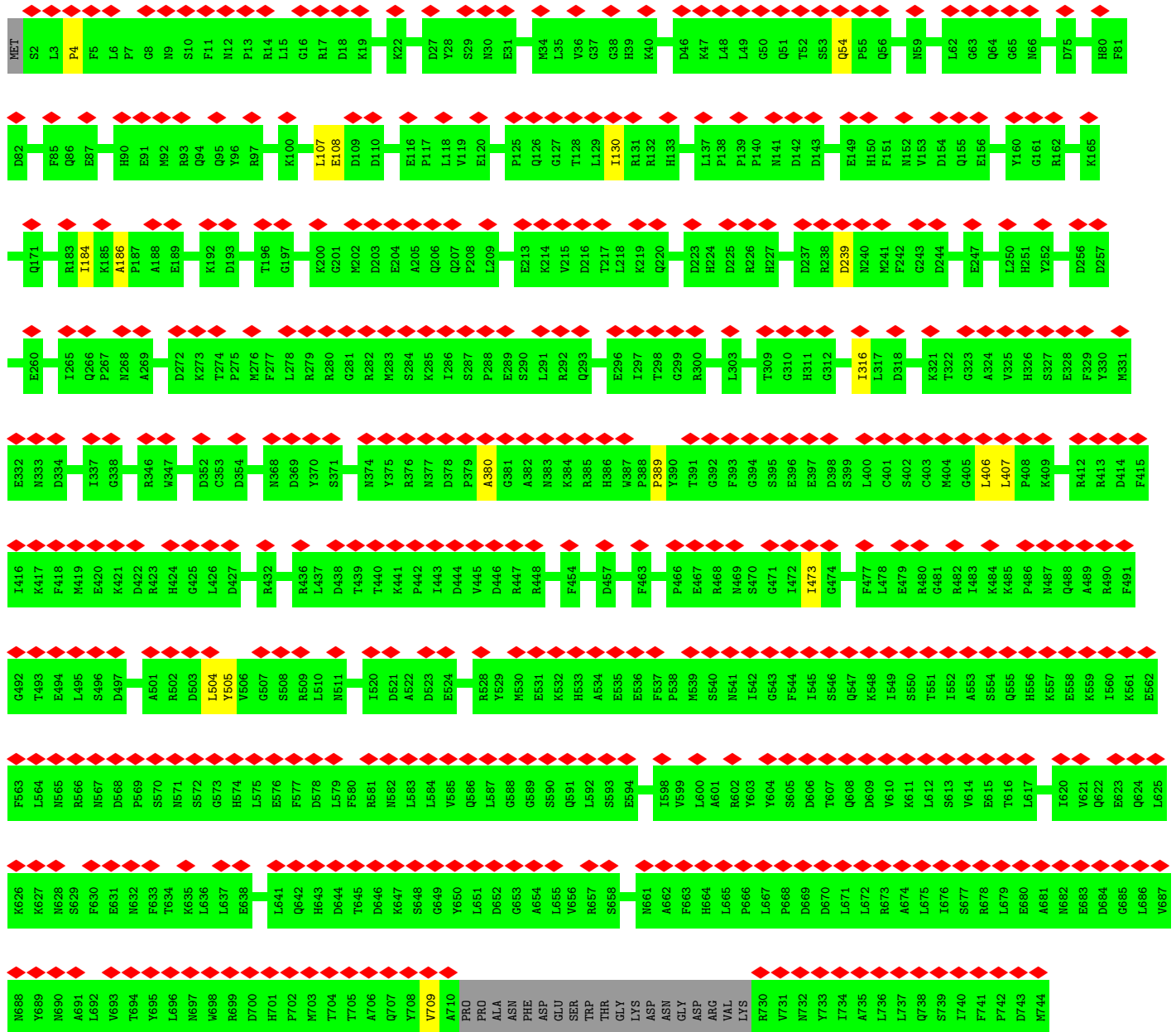


• Molecule 36: EF-hand domain-containing family member C2

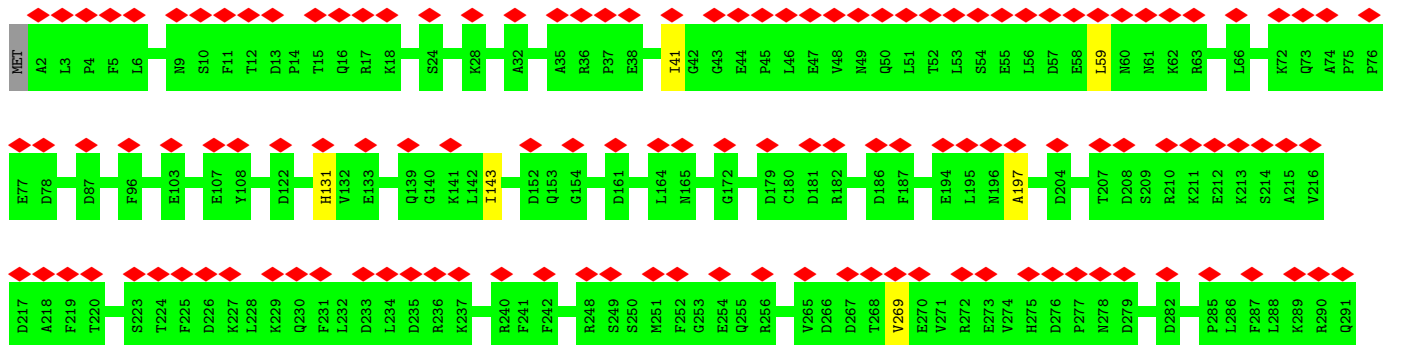
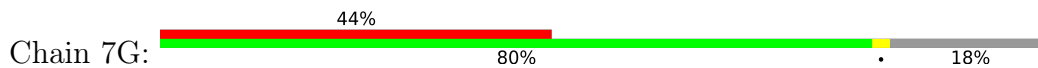


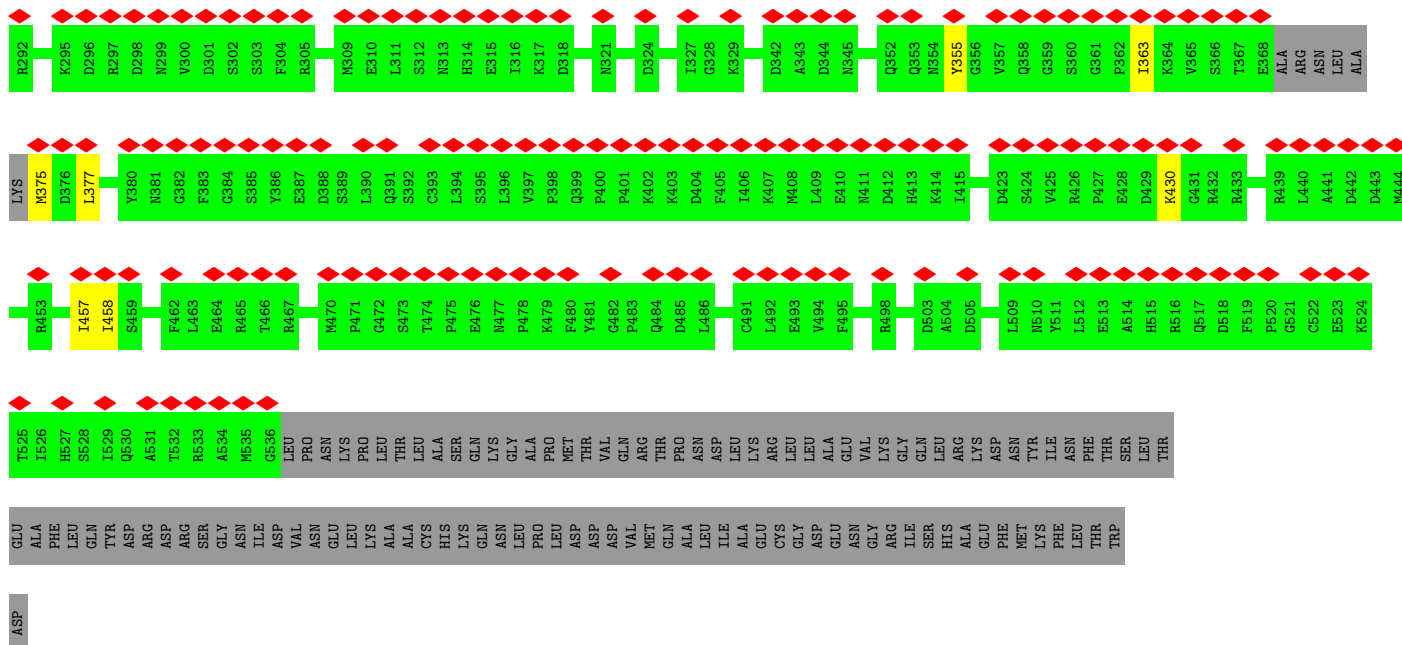
• Molecule 36: EF-hand domain-containing family member C2



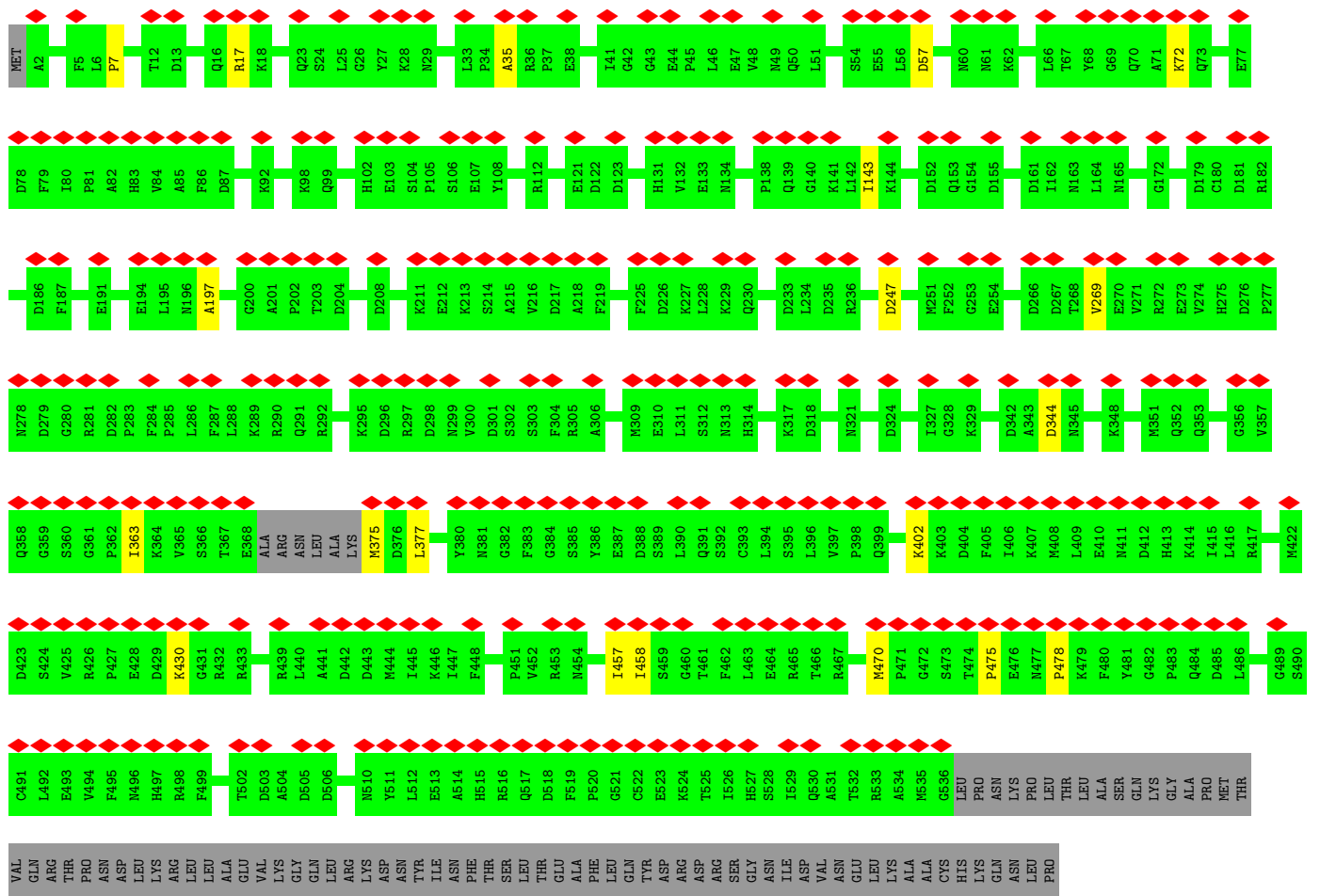
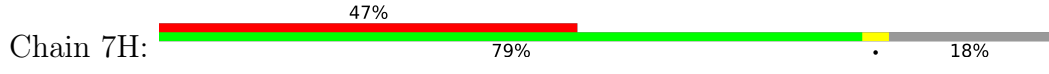


● Molecule 37: Flagellar protofilament ribbon protein rib74



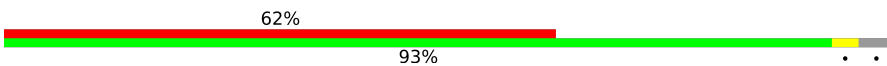


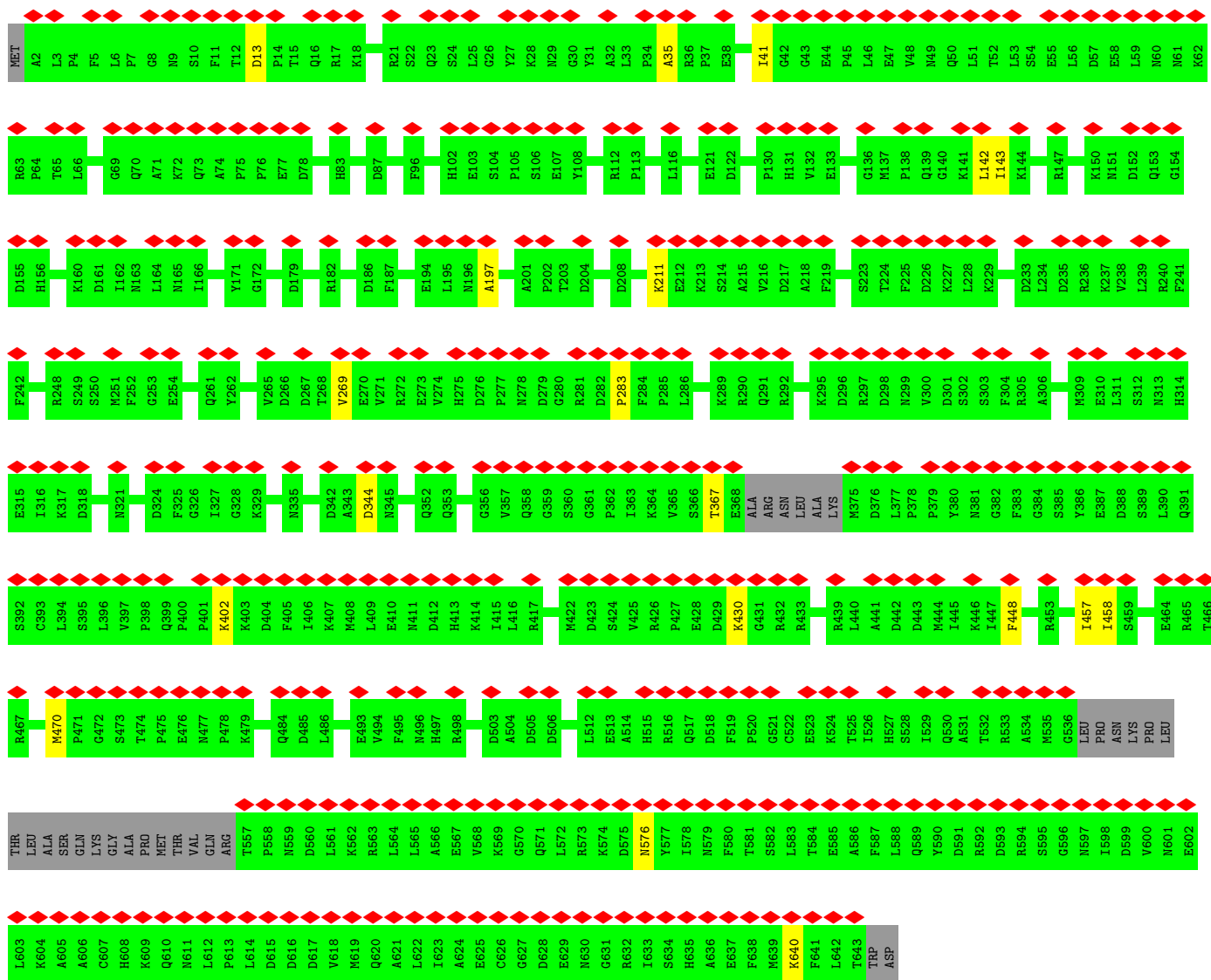
● Molecule 37: Flagellar protofilament ribbon protein rib74




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

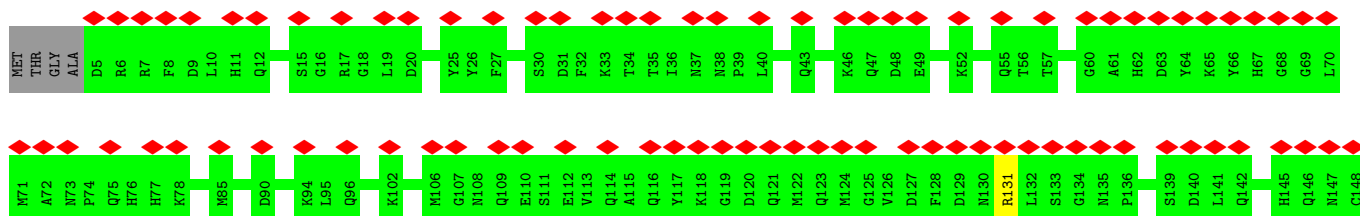
• Molecule 37: Flagellar protofilament ribbon protein rib74

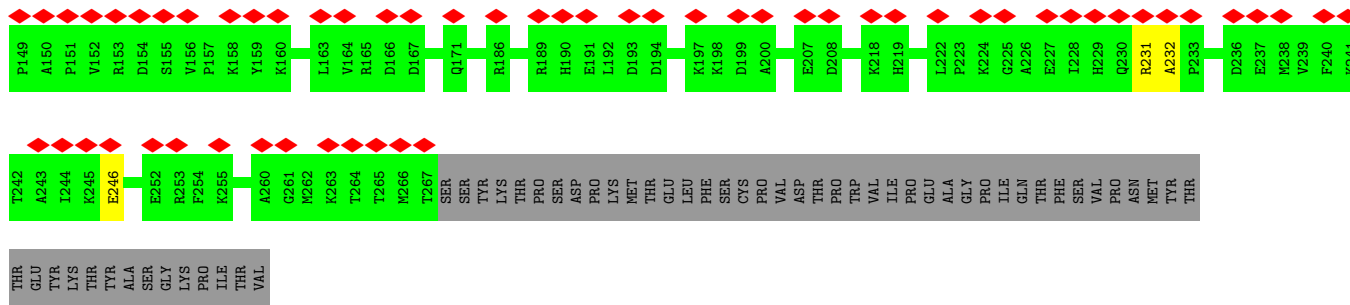
Chain 7I: 



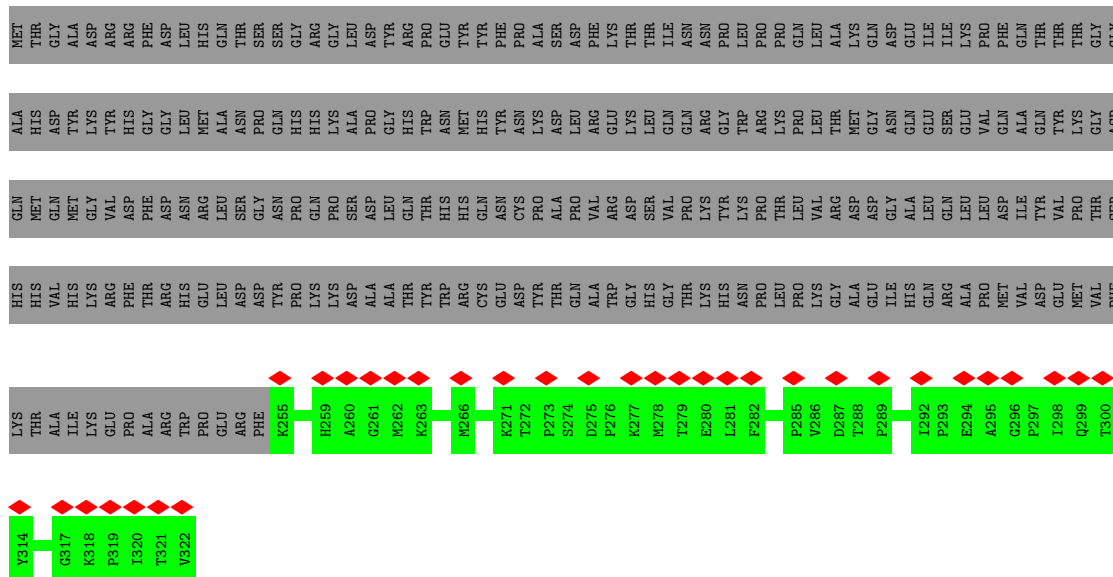
• Molecule 38: SAXO3(LOC115918676)

Chain 7M: 

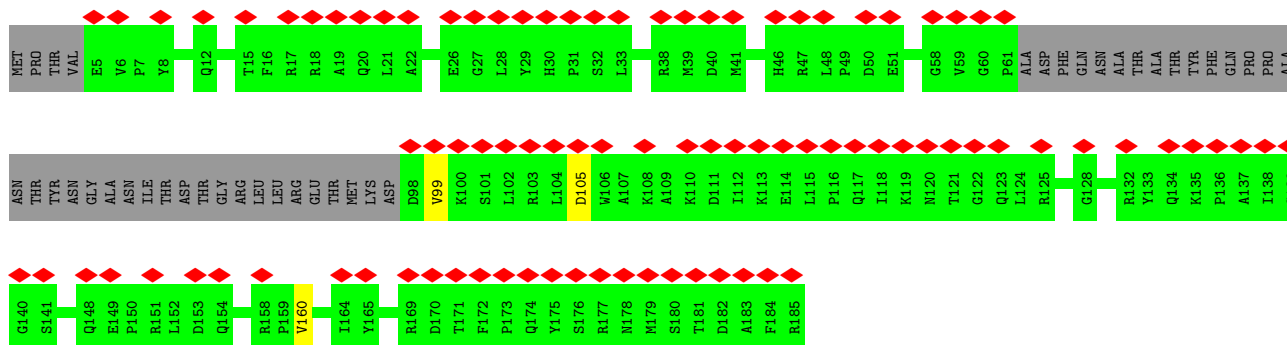
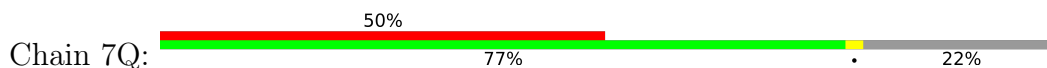




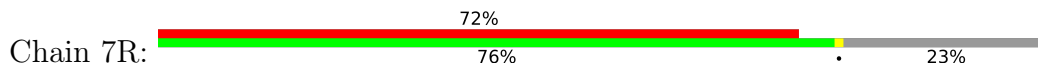
• Molecule 38: SAXO3(LOC115918676)



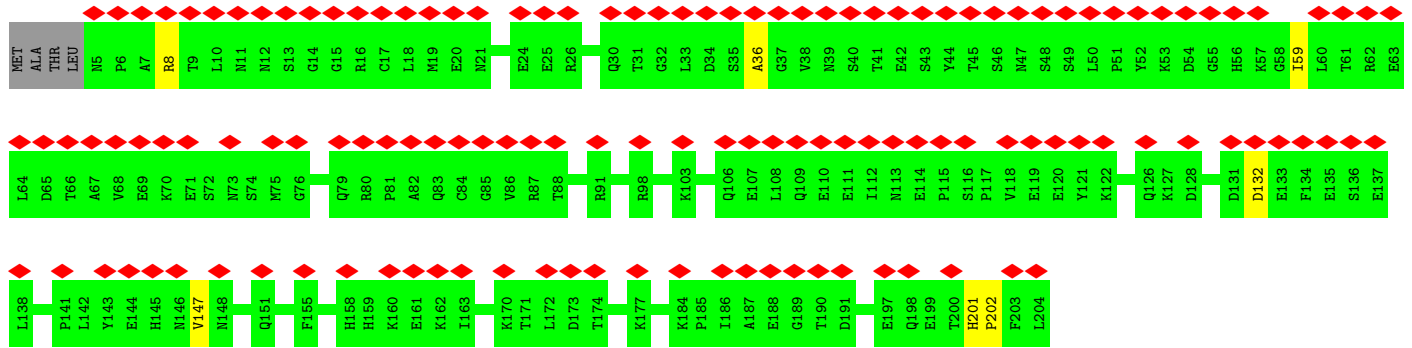
• Molecule 39: TEPP protein



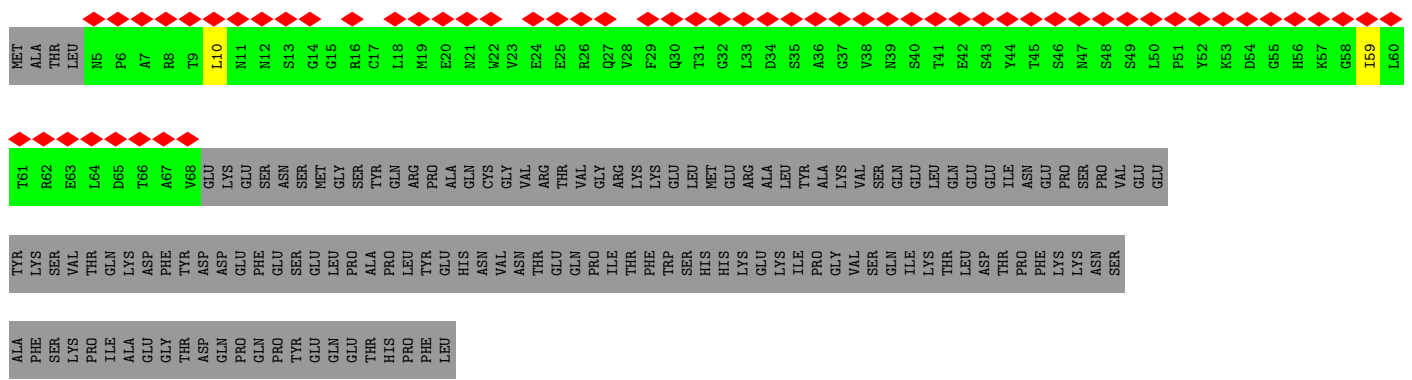
• Molecule 39: TEPP protein



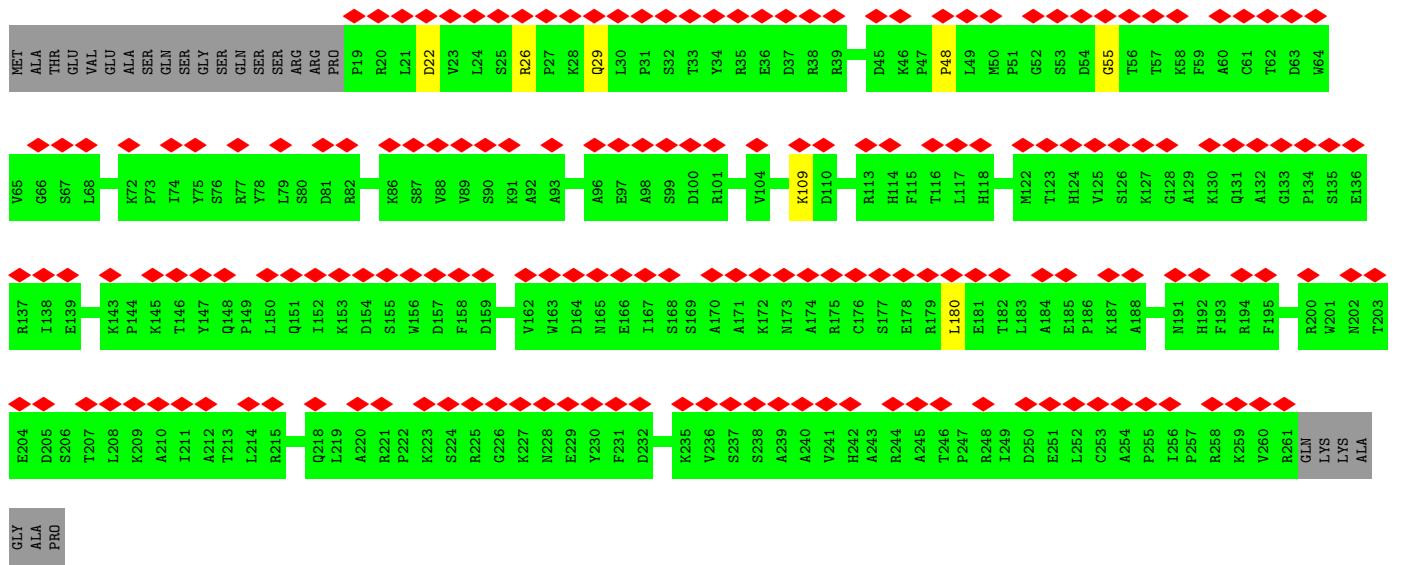




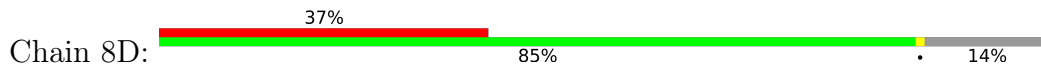
• Molecule 41: Sperm-associated antigen 8



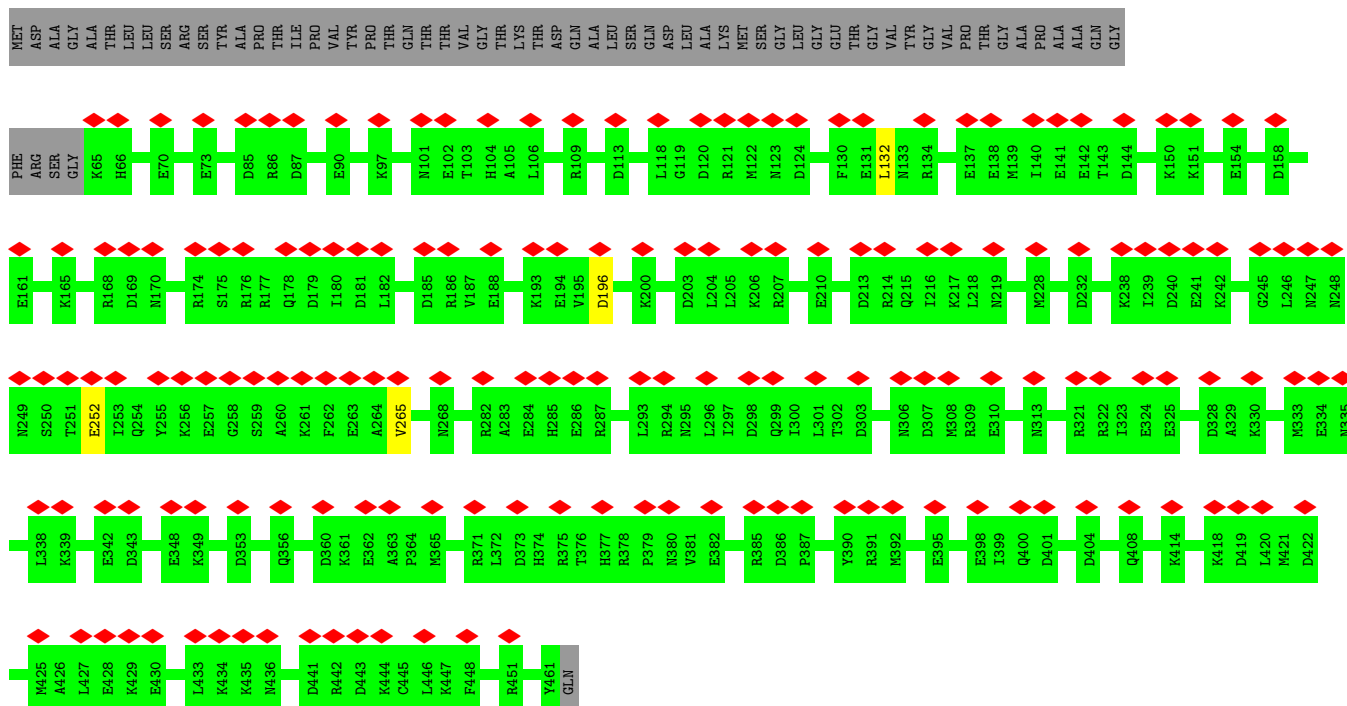
• Molecule 42: Testicular haploid expressed gene protein-like



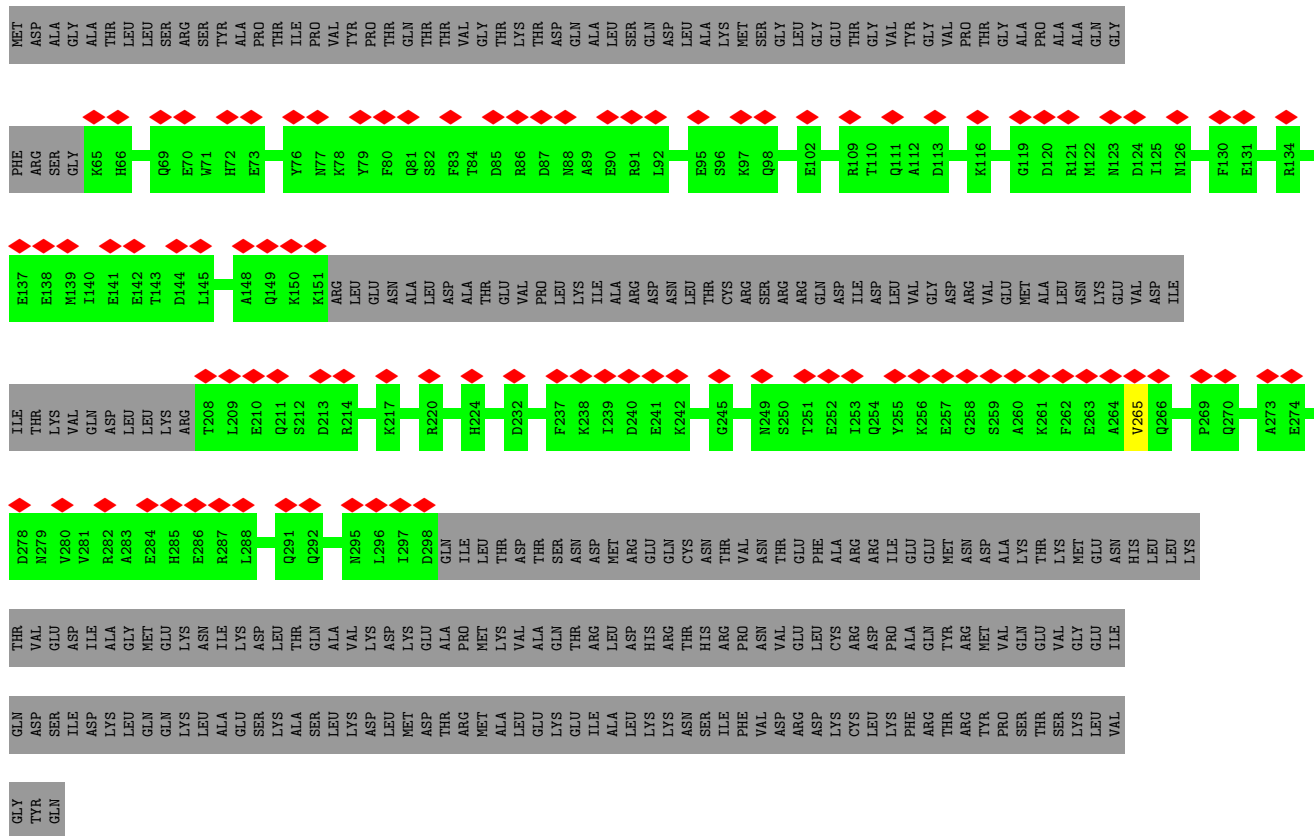
• Molecule 43: Tektin A1





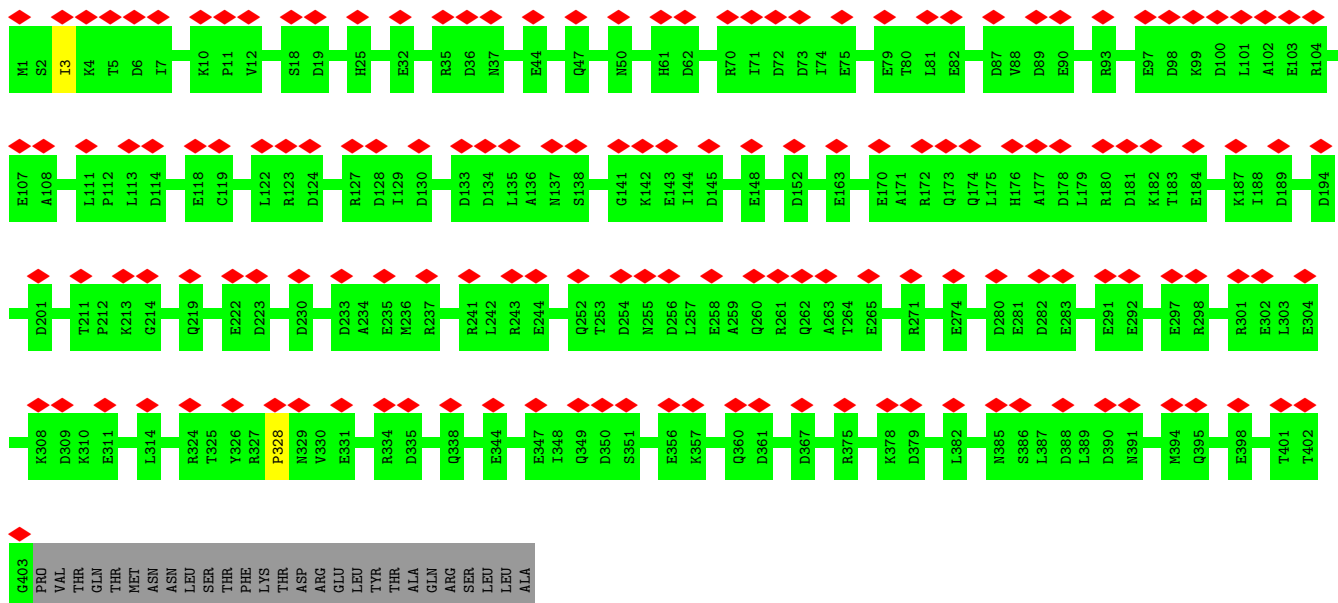


- Molecule 43: Tektin A1

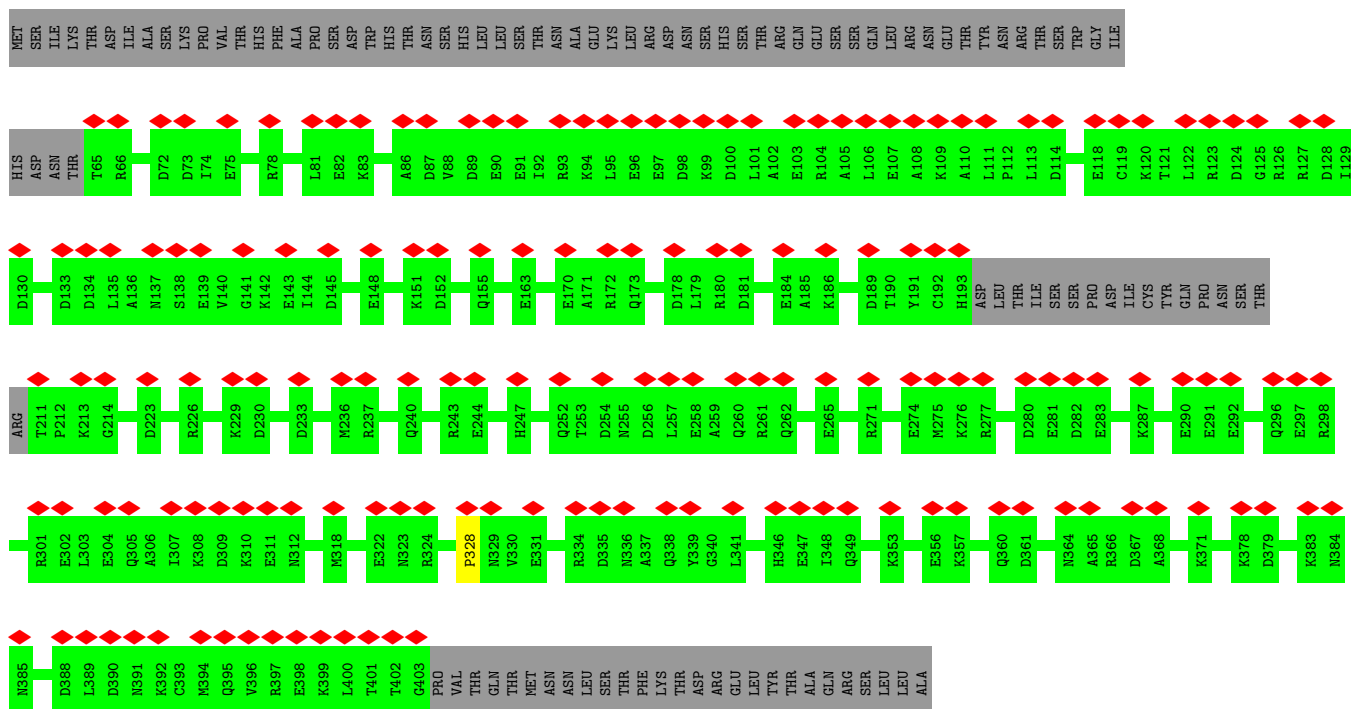
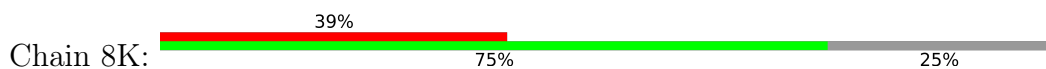


- Molecule 43: Tektin A1

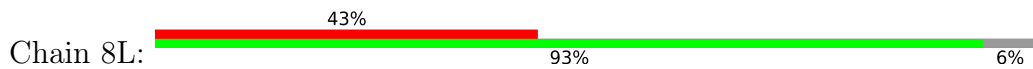




• Molecule 44: Tektin B1

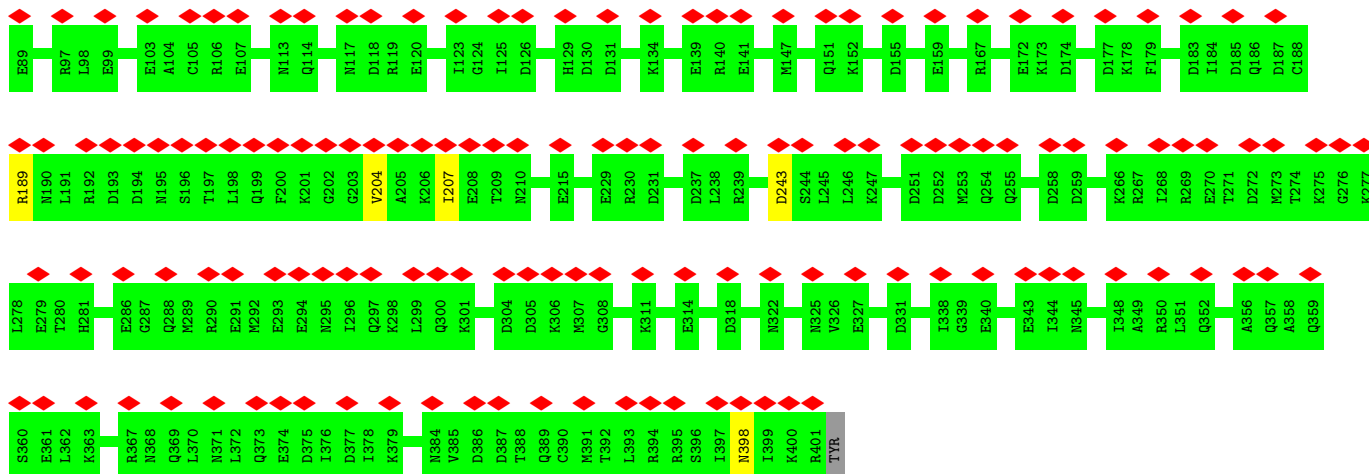


• Molecule 44: Tektin B1

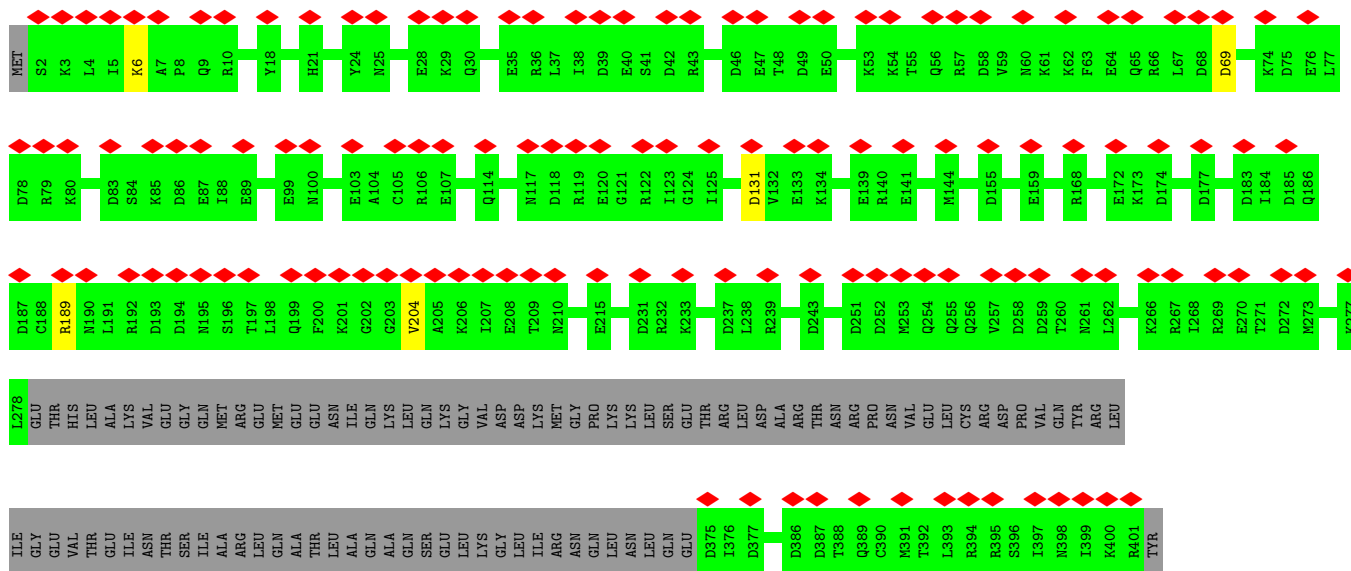
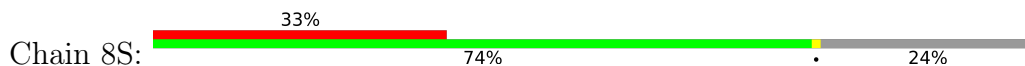




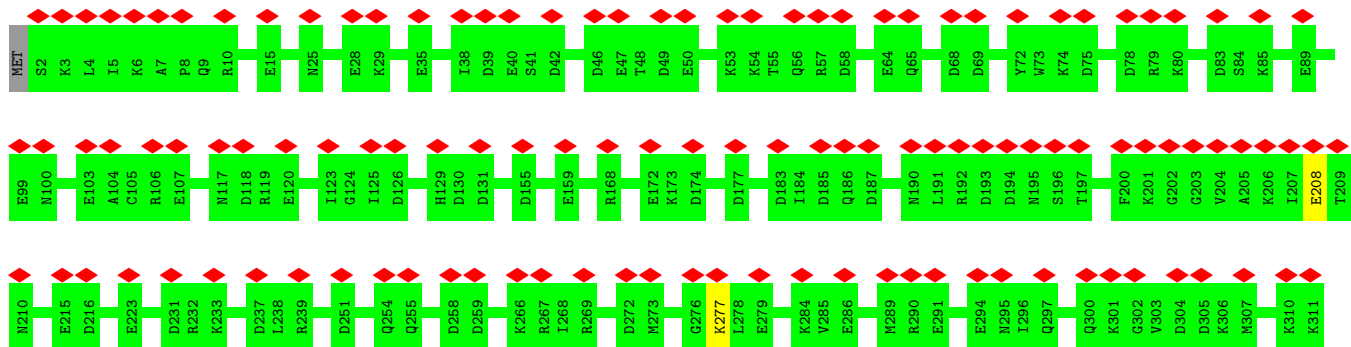
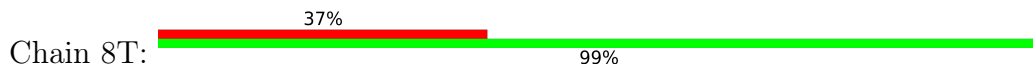


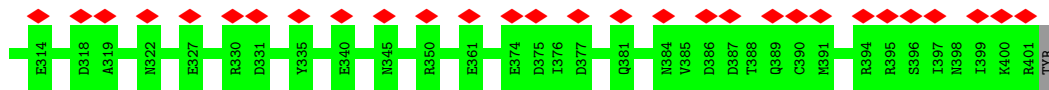


• Molecule 45: Tektin C1

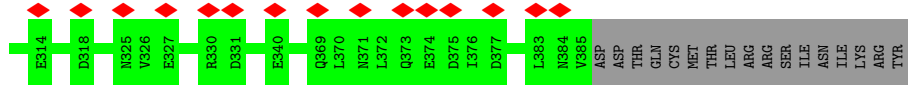
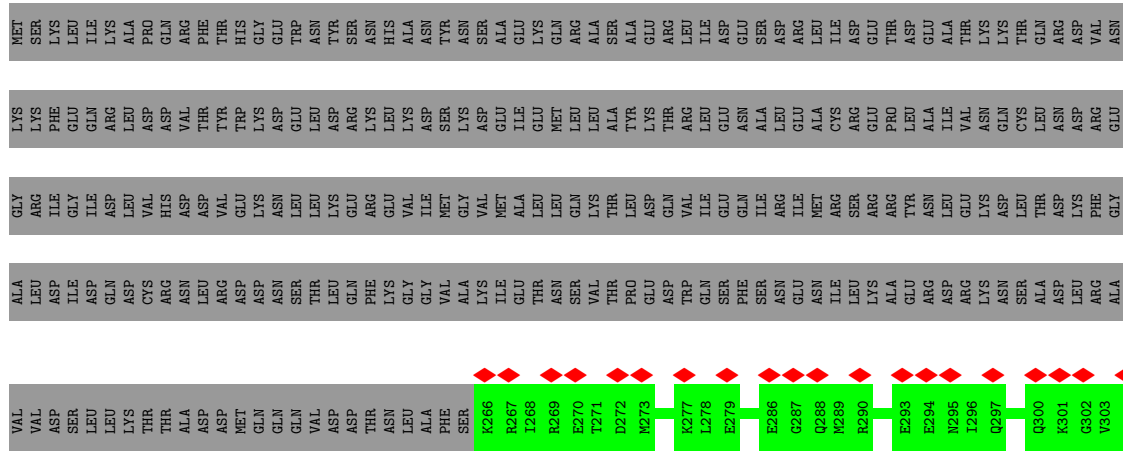


• Molecule 45: Tektin C1

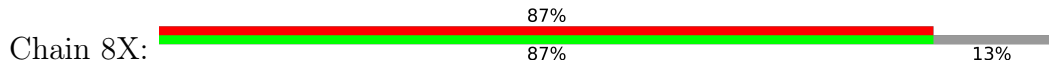




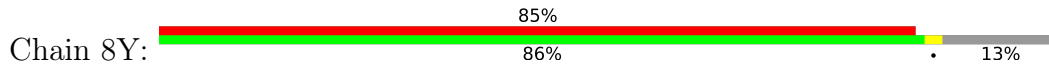
• Molecule 45: Tektin C1



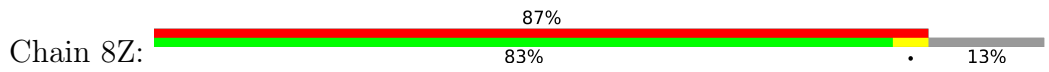
• Molecule 46: Tex43



• Molecule 46: Tex43



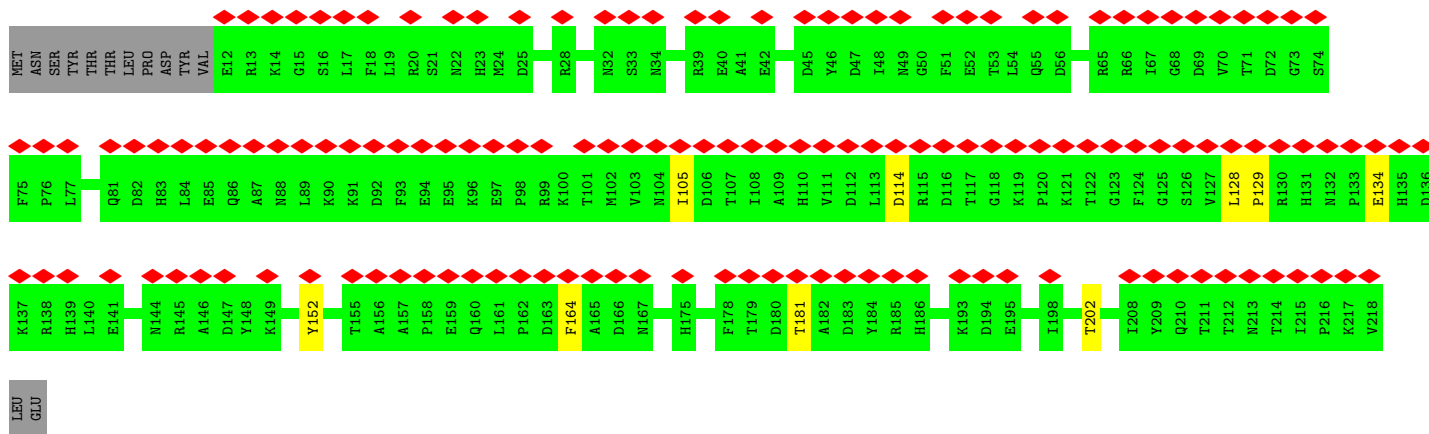
• Molecule 46: Tex43





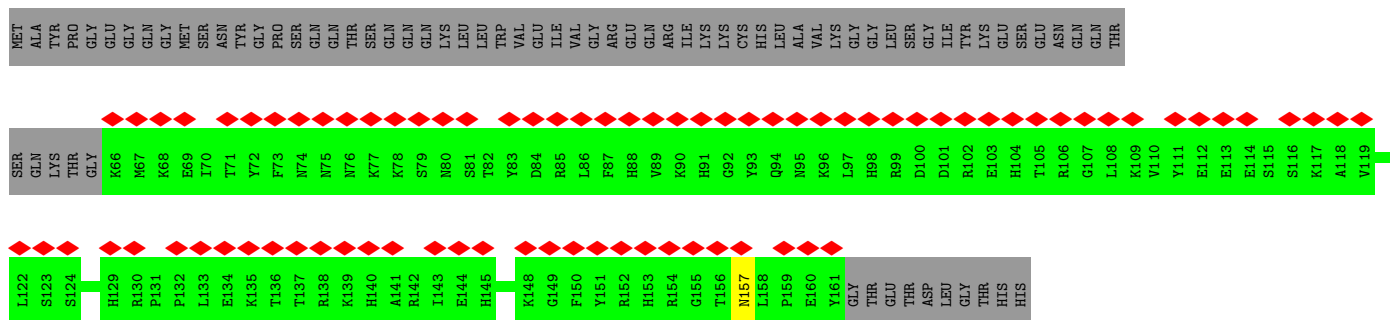
- Molecule 47: Tex36(CFAP95, C9orf135)

Chain 9A: 65% 90% 6%



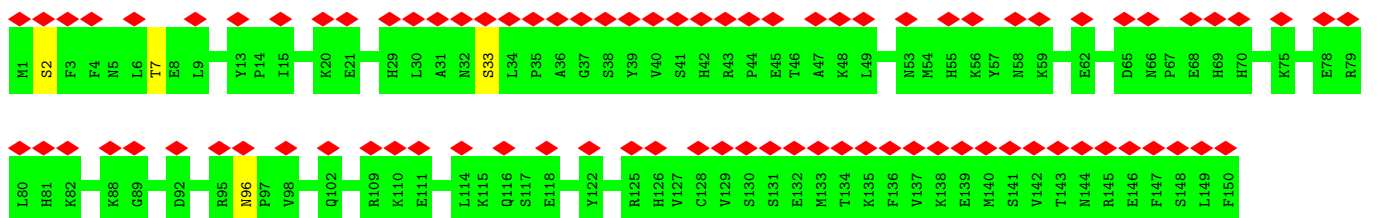
- Molecule 48: CFAP90(C5orf49)

Chain 9D: 47% 56% 44%



- Molecule 49: Tex49

Chain 9G: 57% 97%

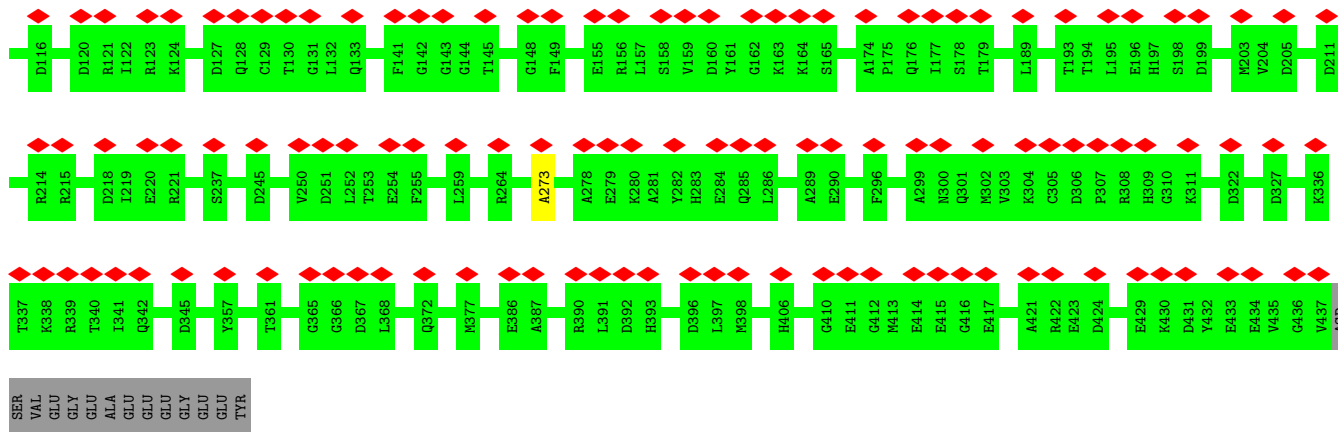


- Molecule 50: Tex49\_homologue(LOC580808)

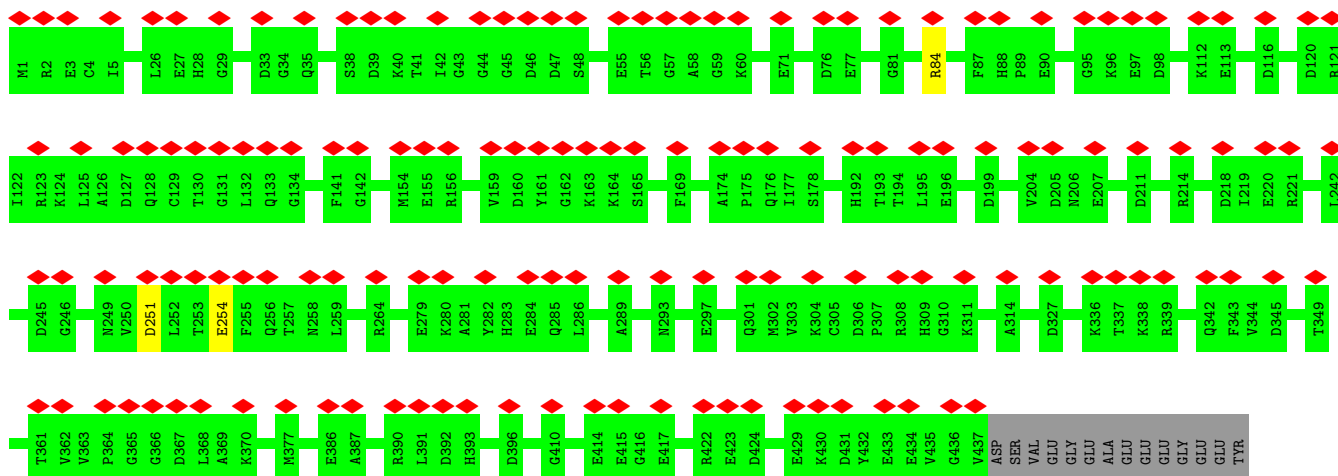




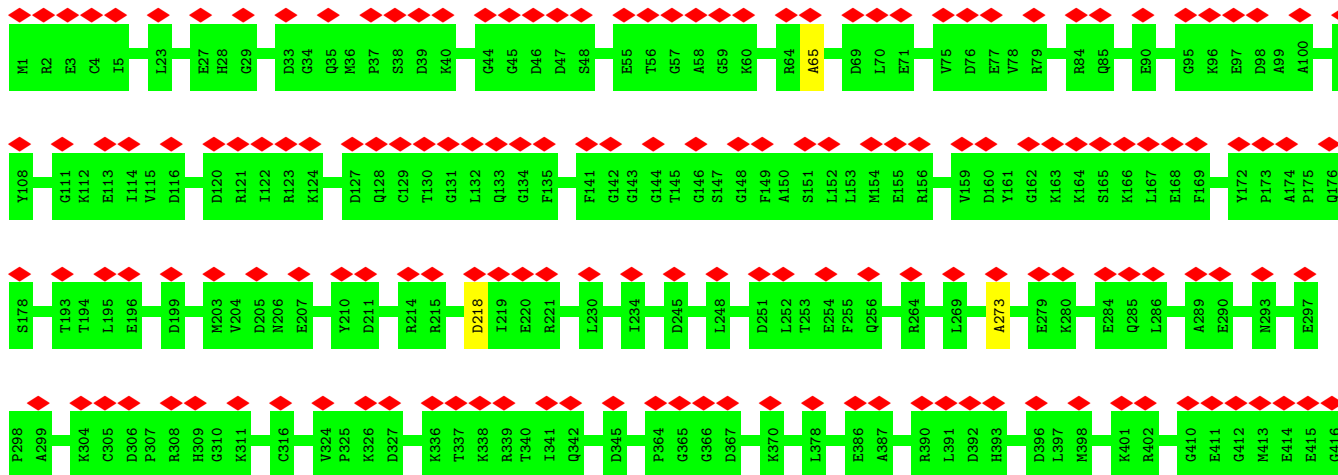
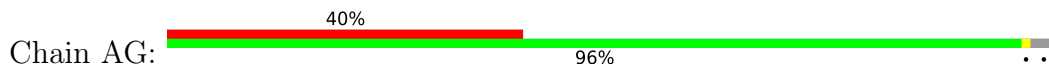


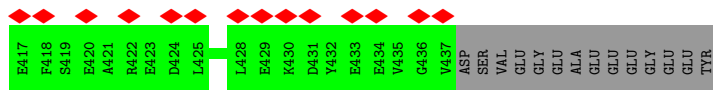


• Molecule 54: Tubulin alpha chain

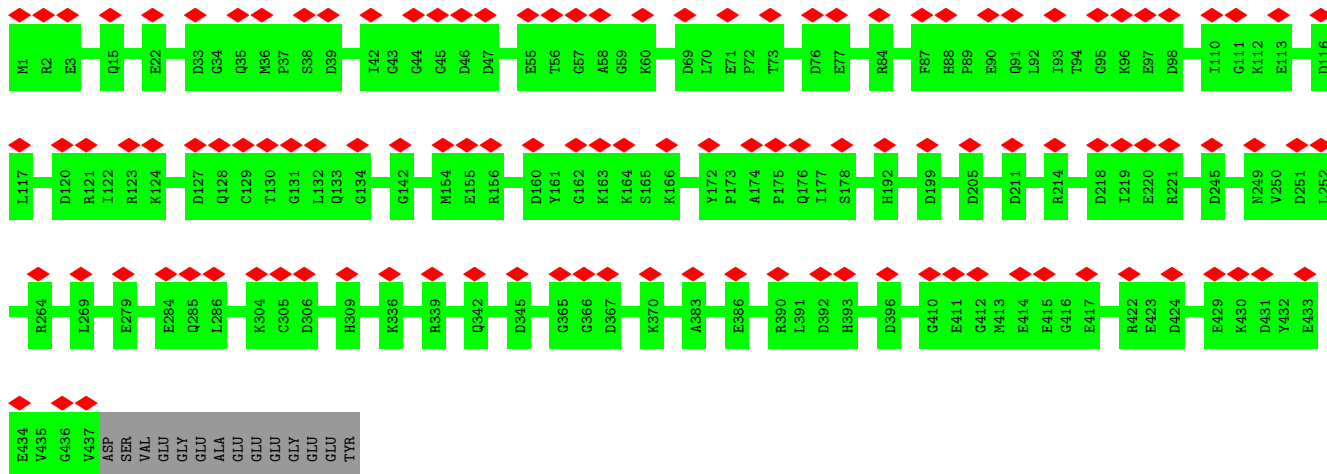


• Molecule 54: Tubulin alpha chain

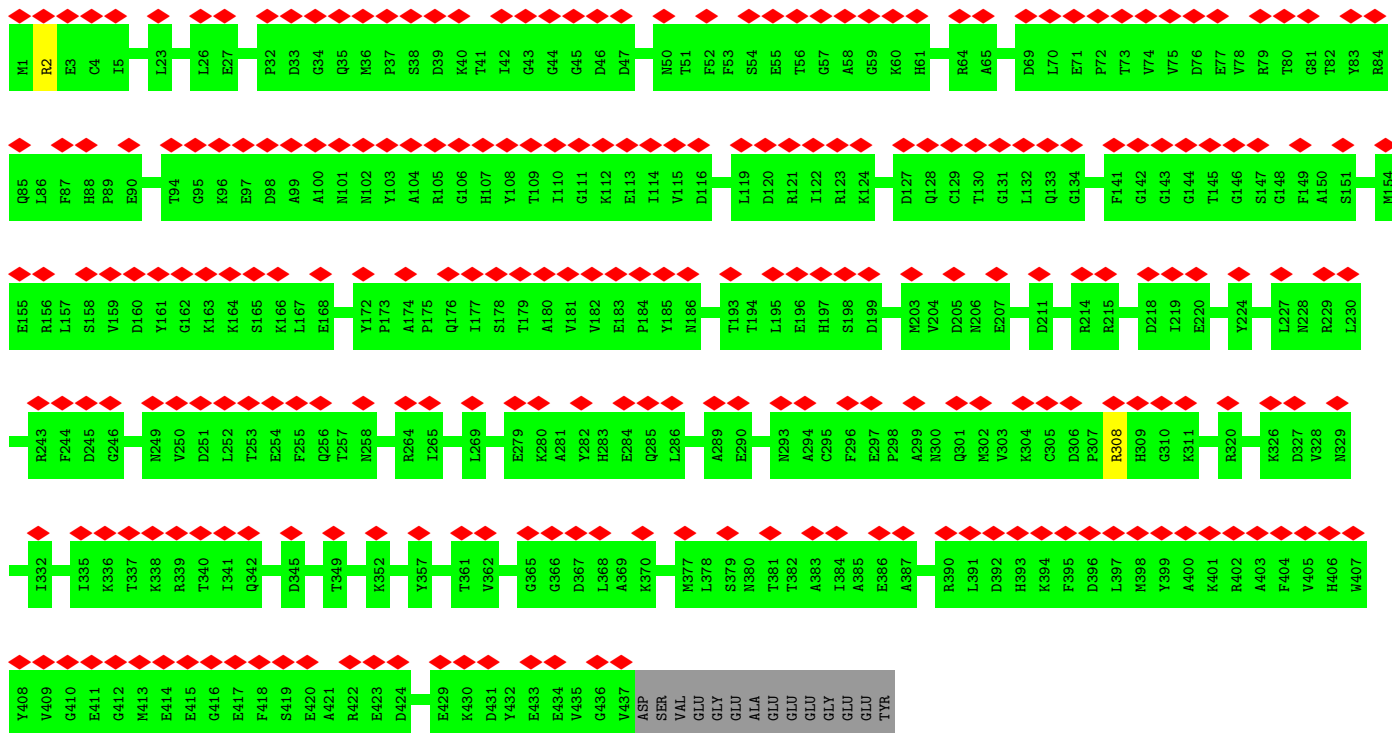




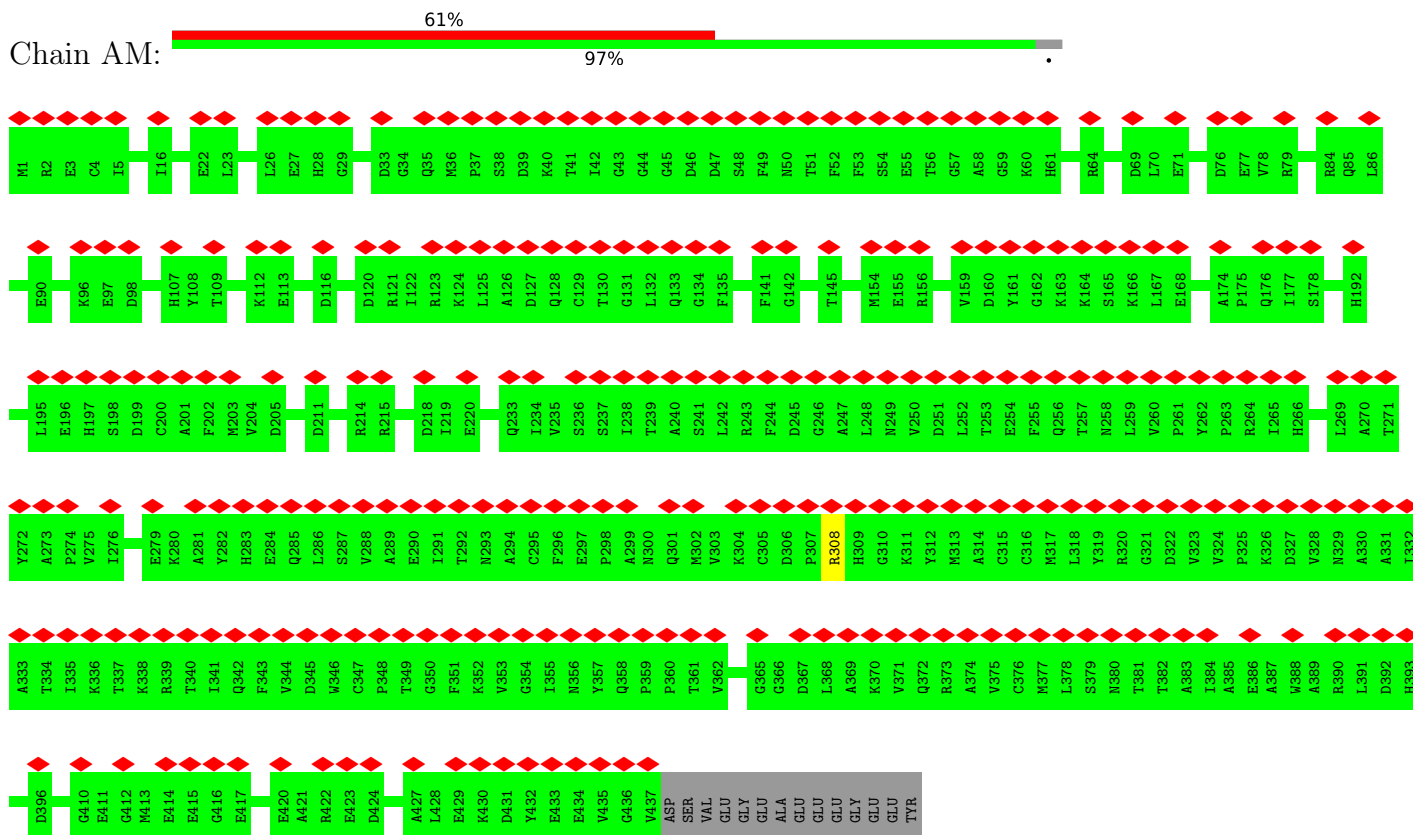
• Molecule 54: Tubulin alpha chain



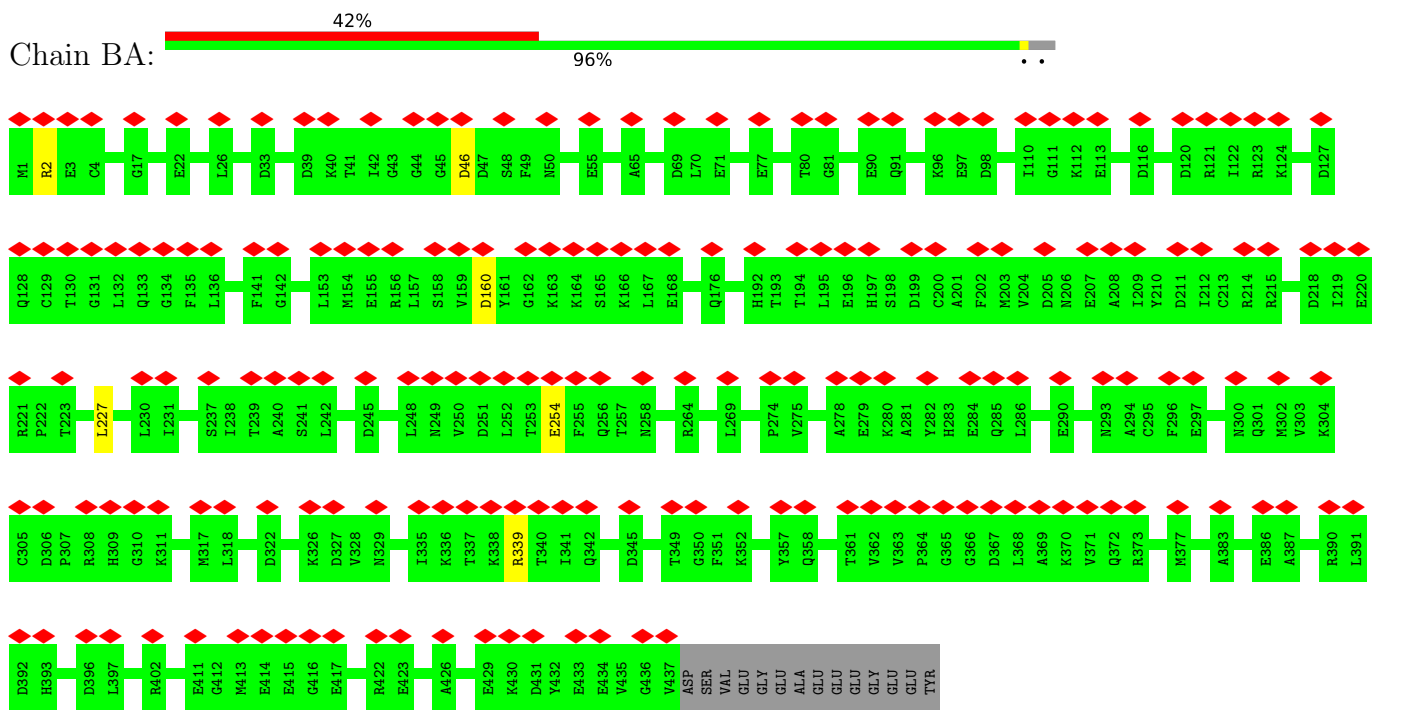
• Molecule 54: Tubulin alpha chain



• Molecule 54: Tubulin alpha chain

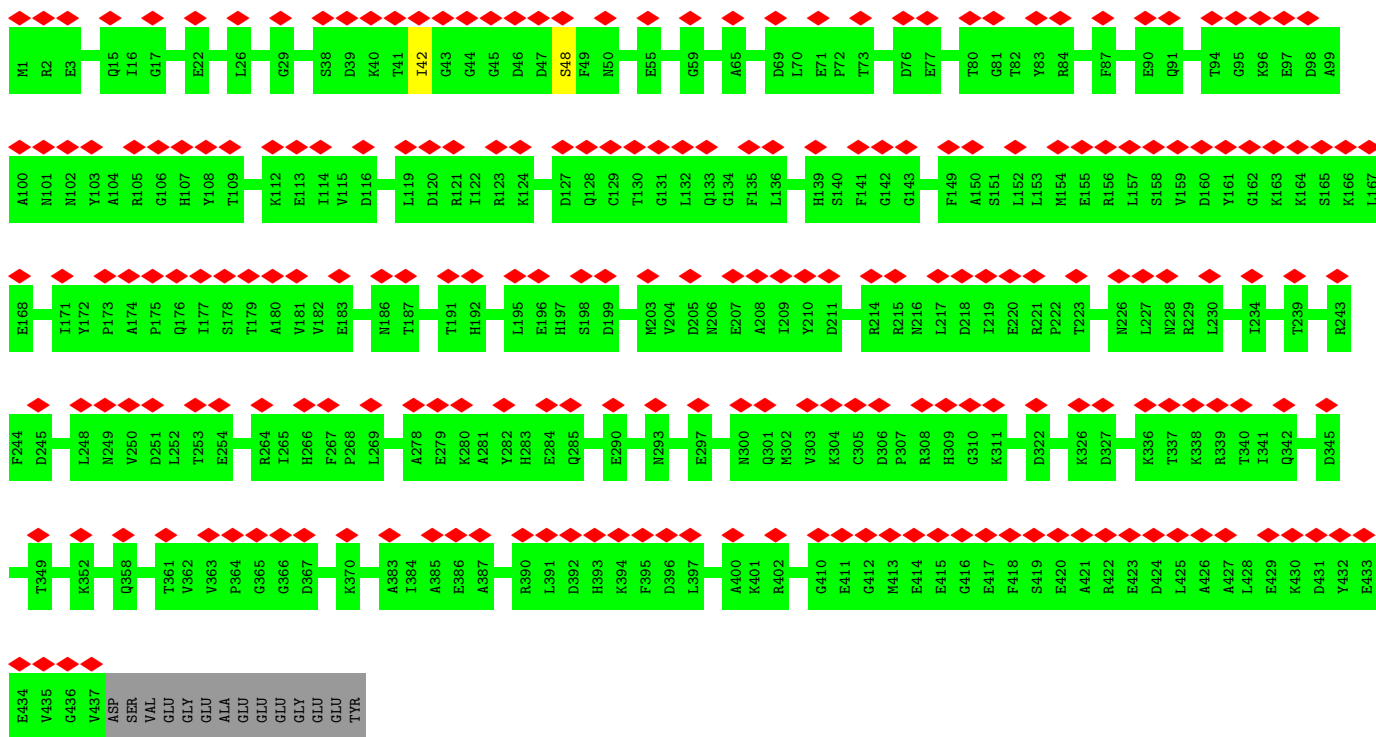


• Molecule 54: Tubulin alpha chain

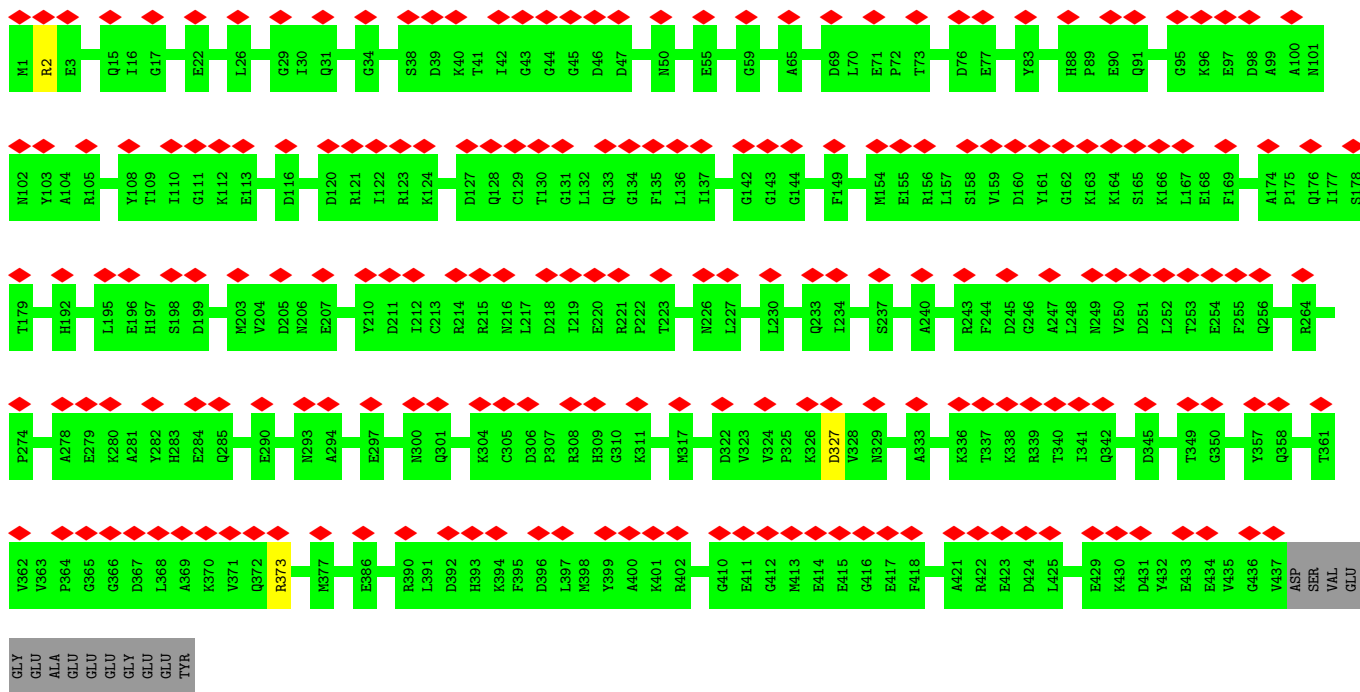


• Molecule 54: Tubulin alpha chain



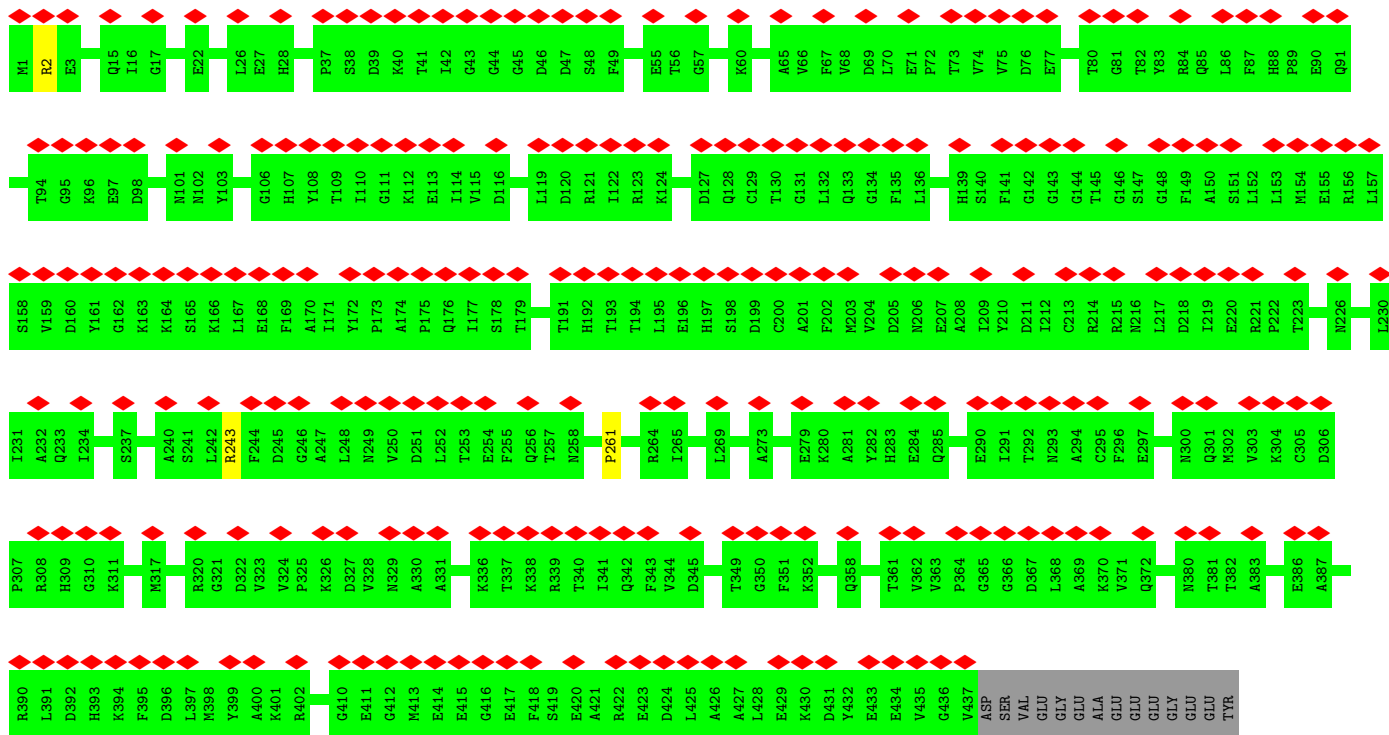


• Molecule 54: Tubulin alpha chain

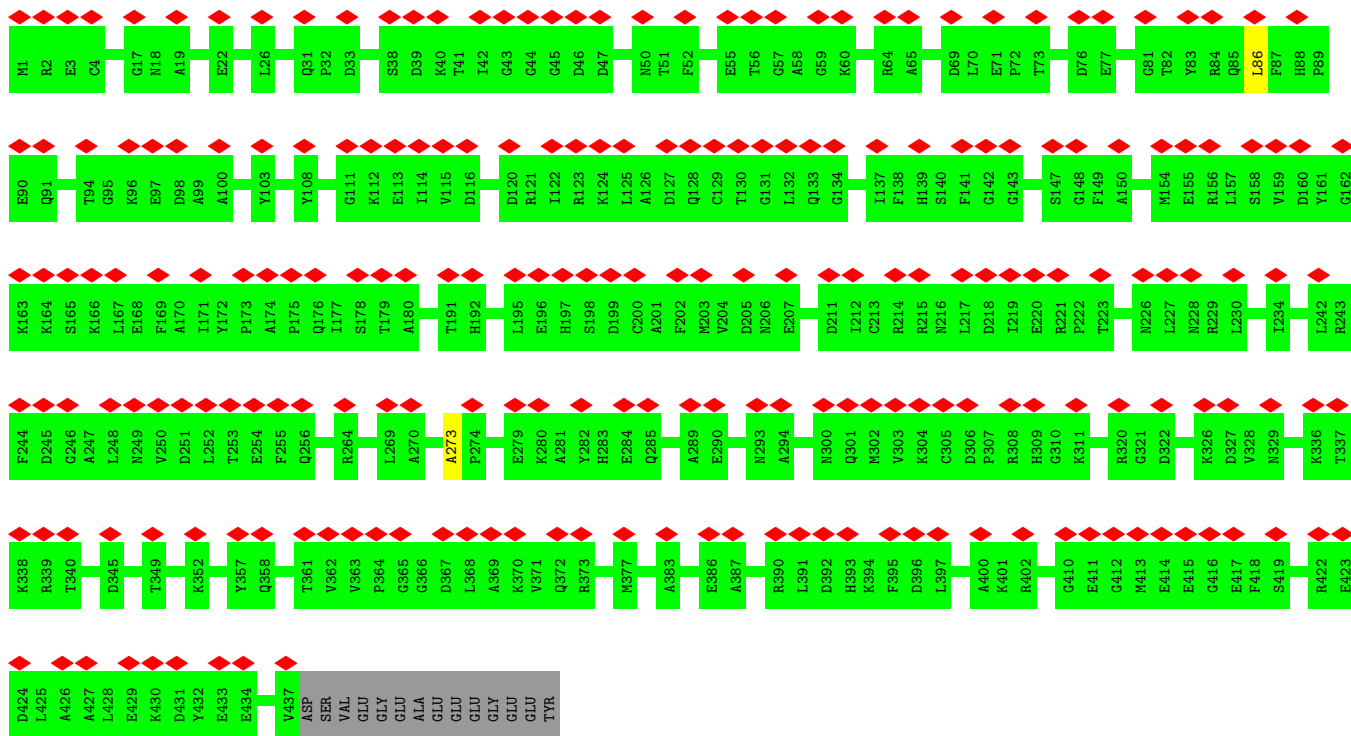


• Molecule 54: Tubulin alpha chain

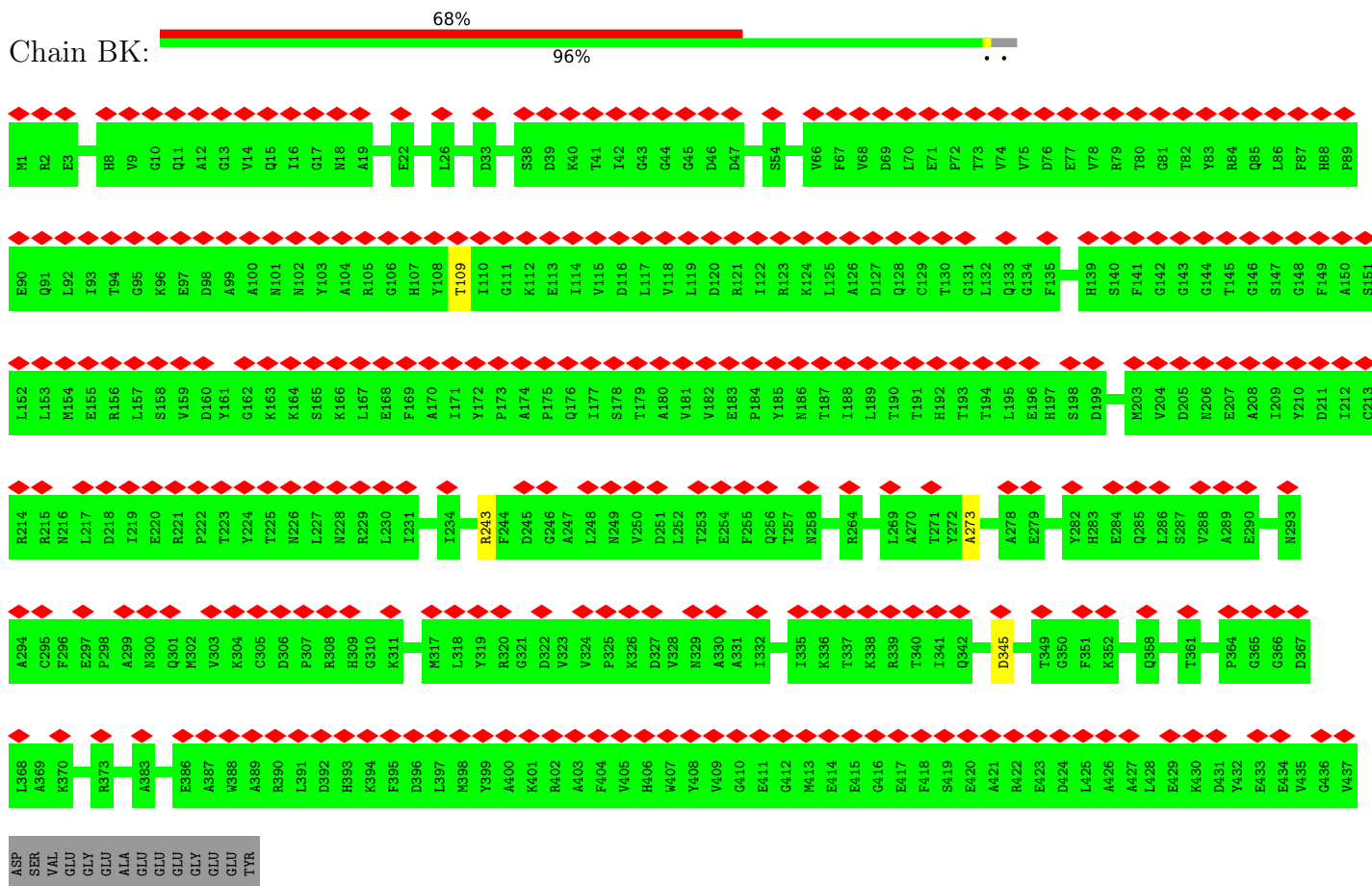




• Molecule 54: Tubulin alpha chain



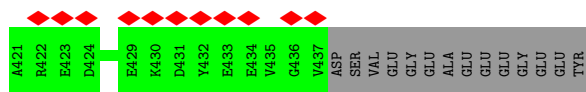
• Molecule 54: Tubulin alpha chain



• Molecule 54: Tubulin alpha chain



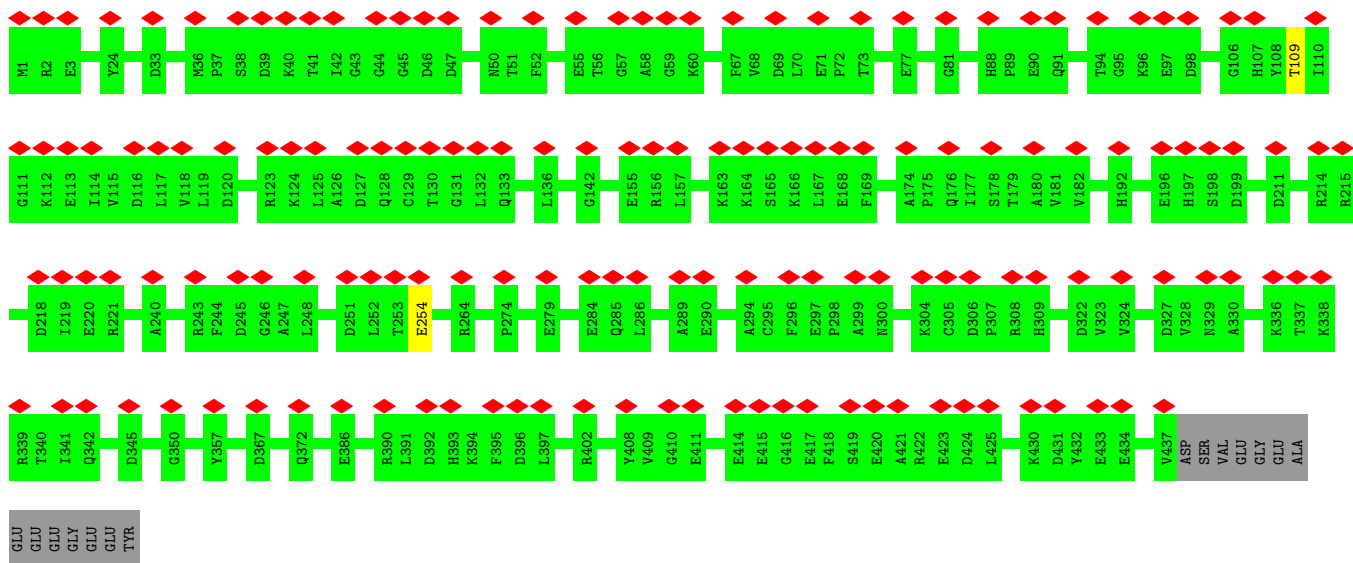




• Molecule 54: Tubulin alpha chain



Chain CA:



• Molecule 54: Tubulin alpha chain



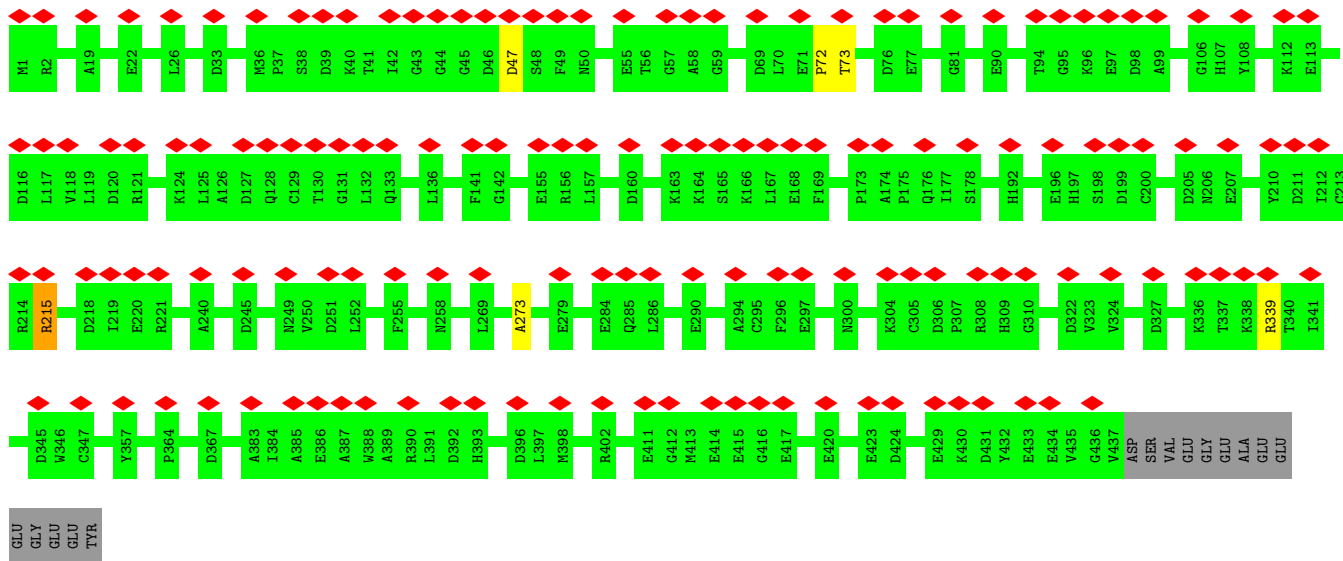
Chain CB:



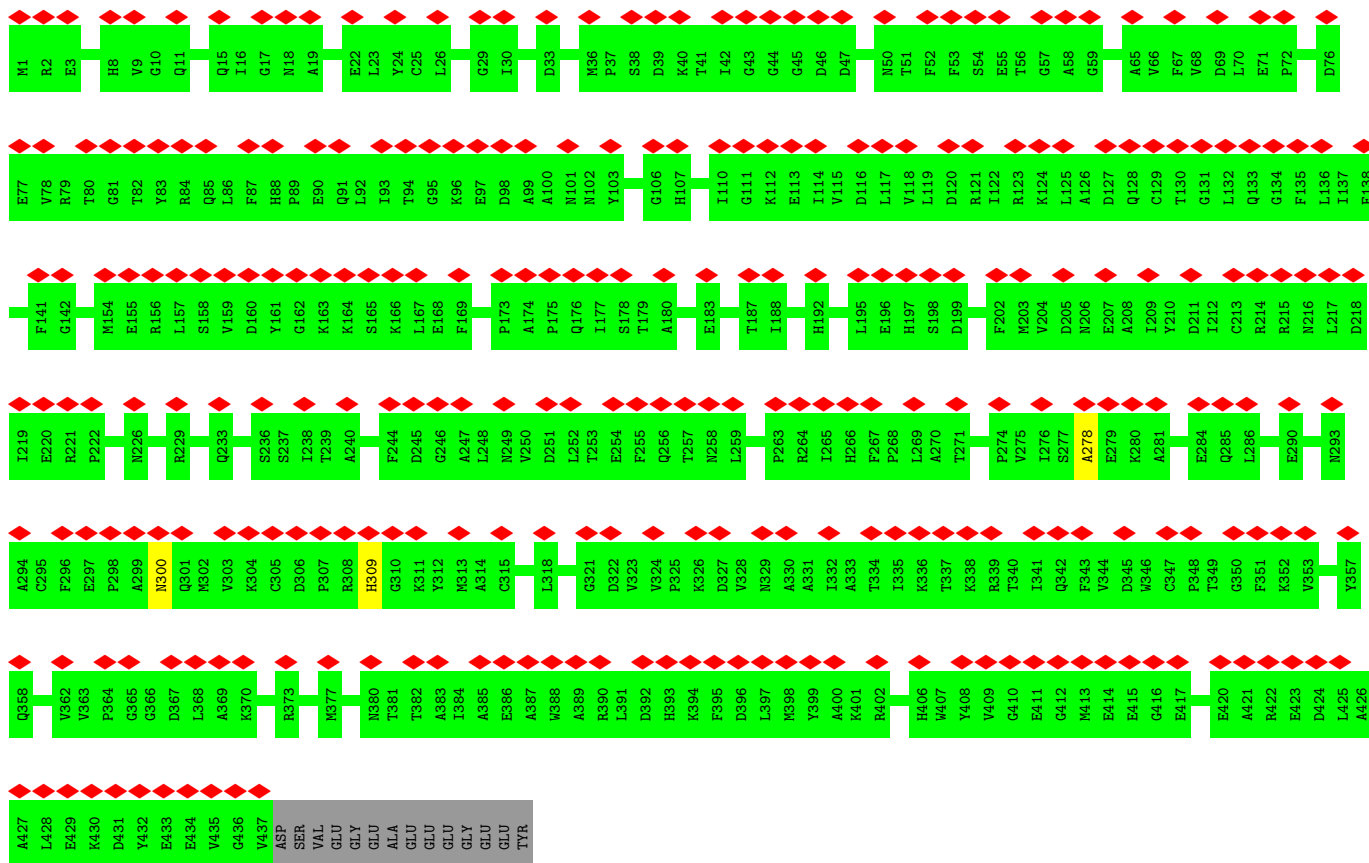
• Molecule 54: Tubulin alpha chain



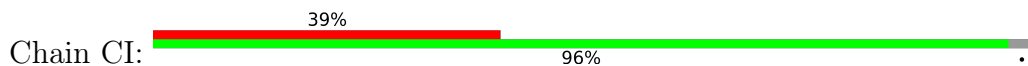
Chain CE:

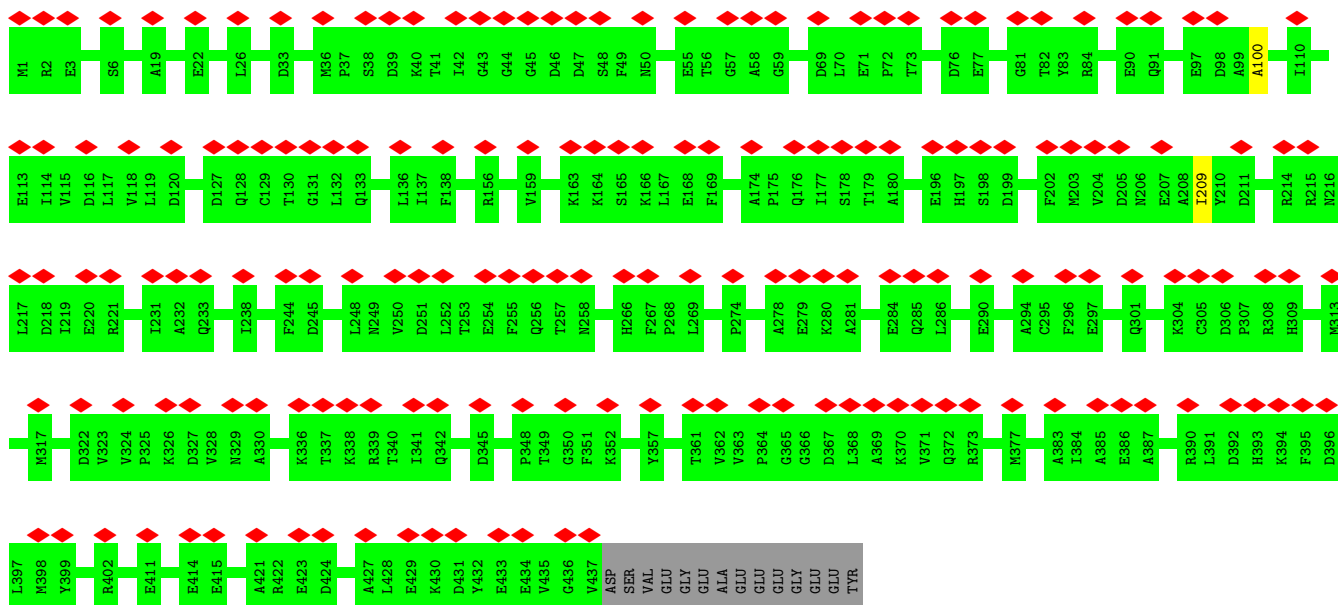


• Molecule 54: Tubulin alpha chain

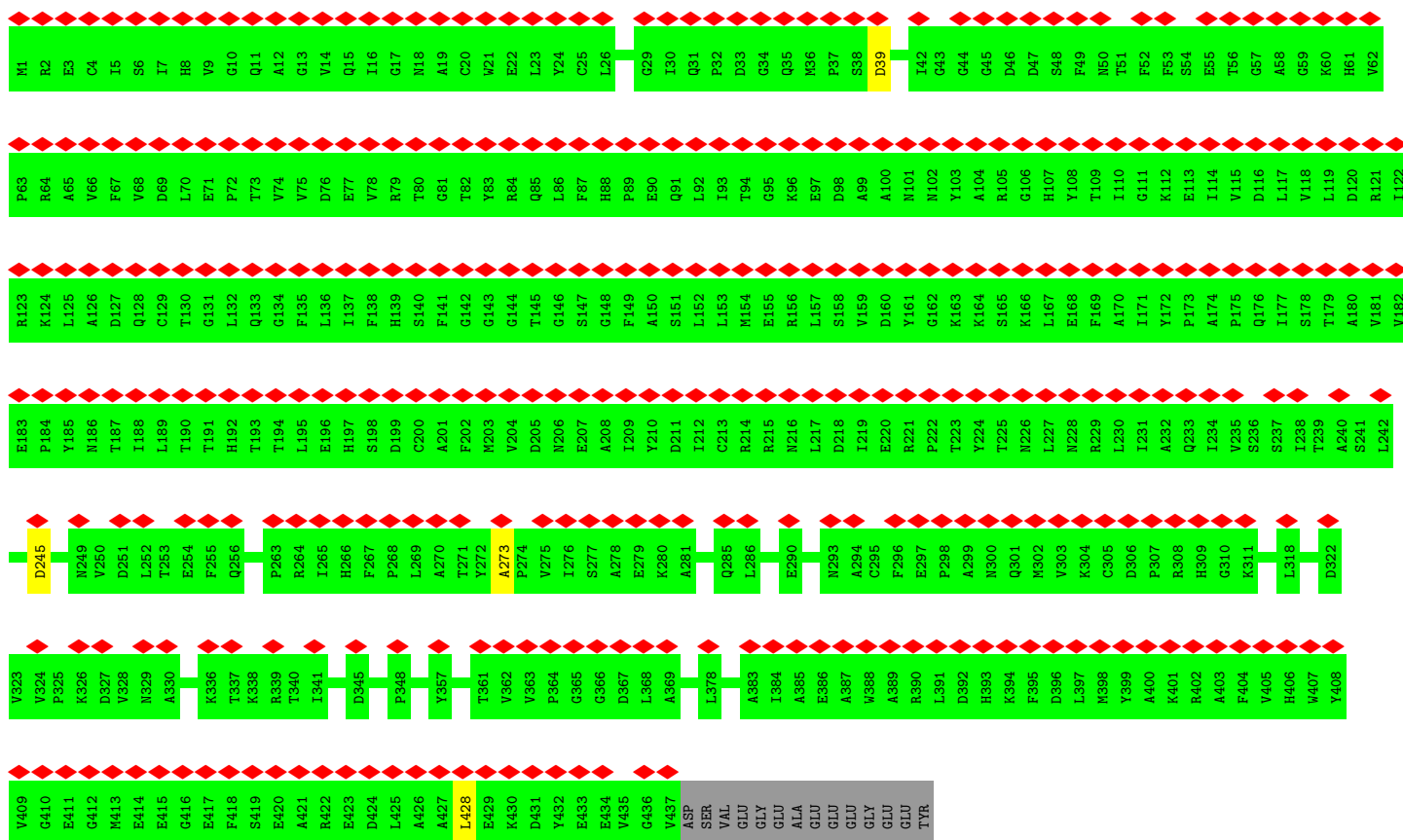
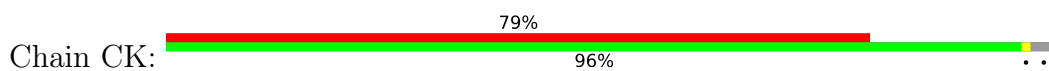


• Molecule 54: Tubulin alpha chain

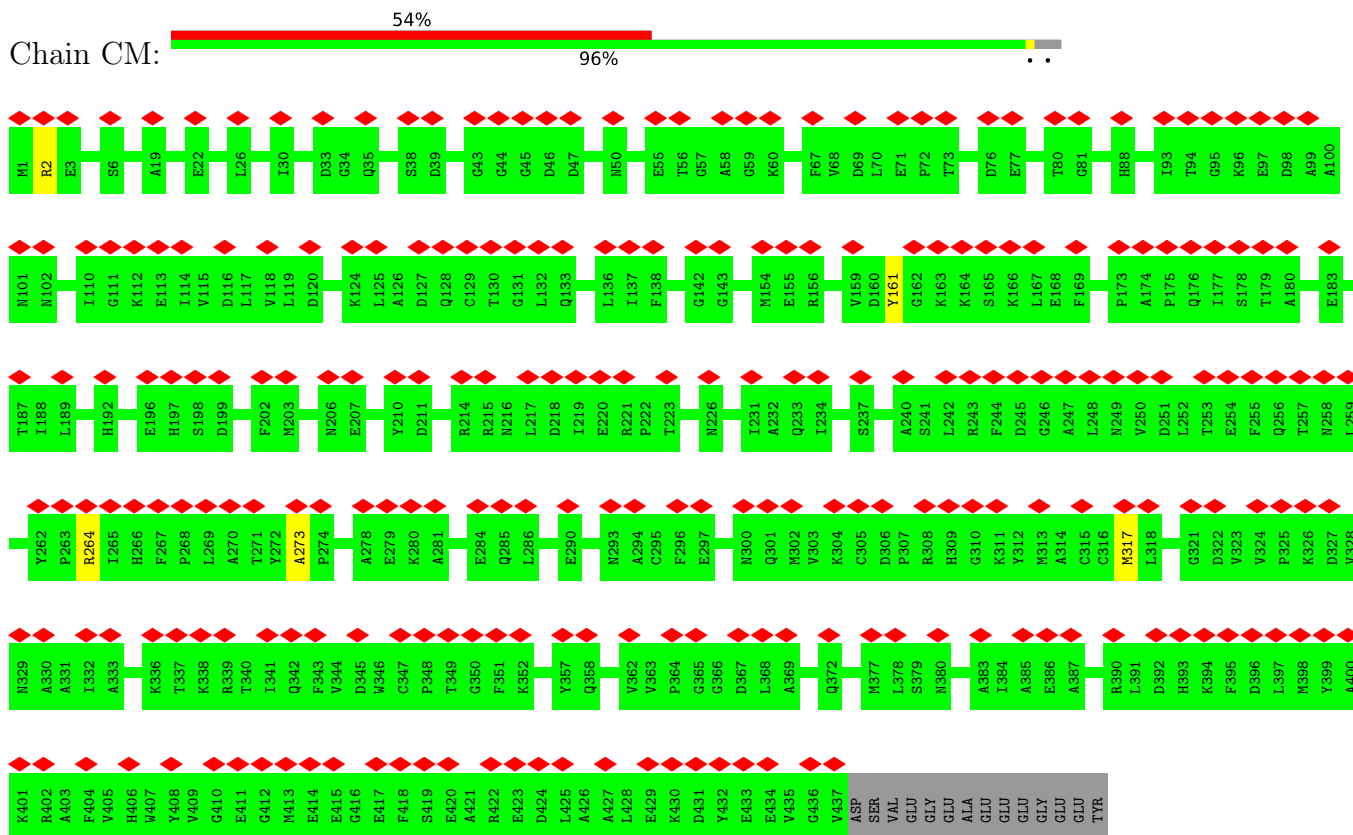




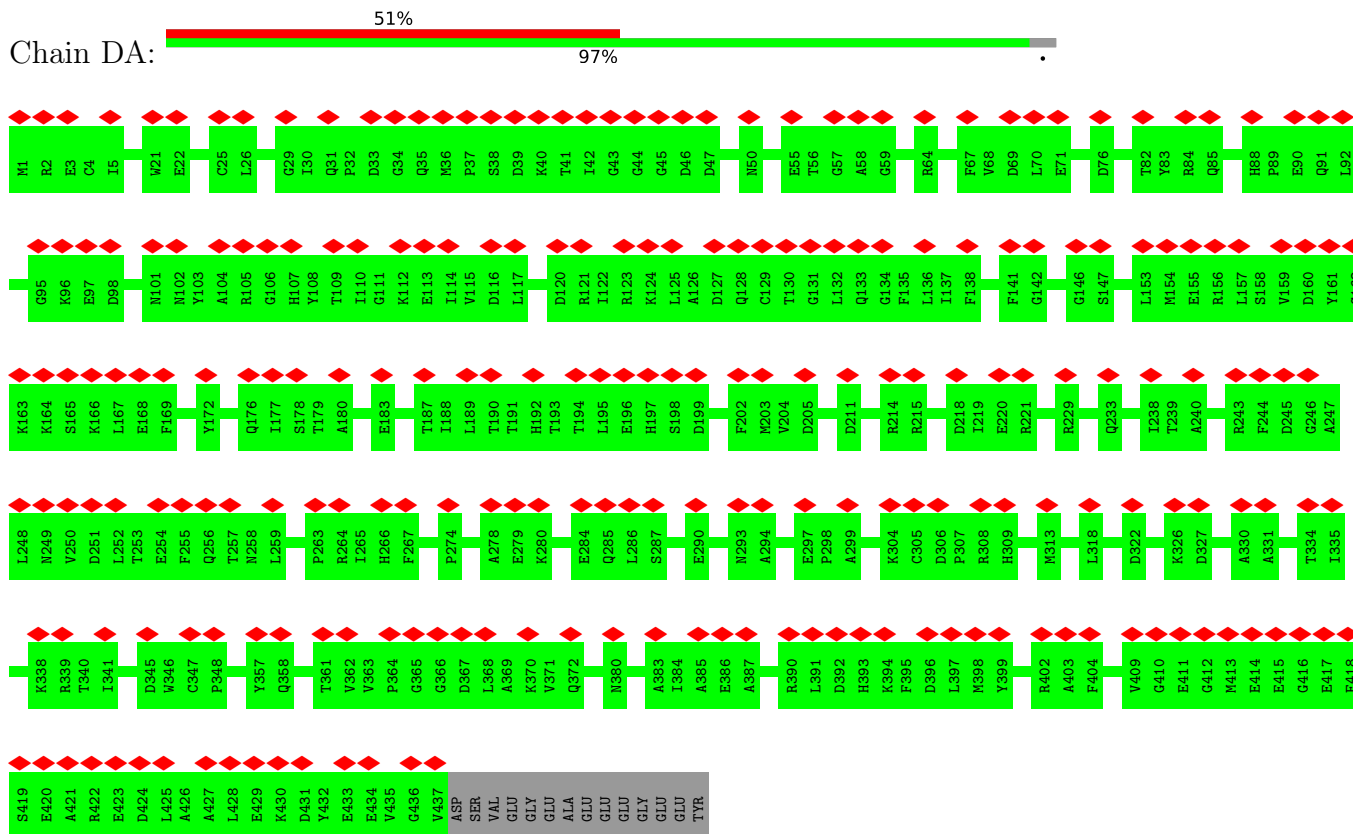
• Molecule 54: Tubulin alpha chain



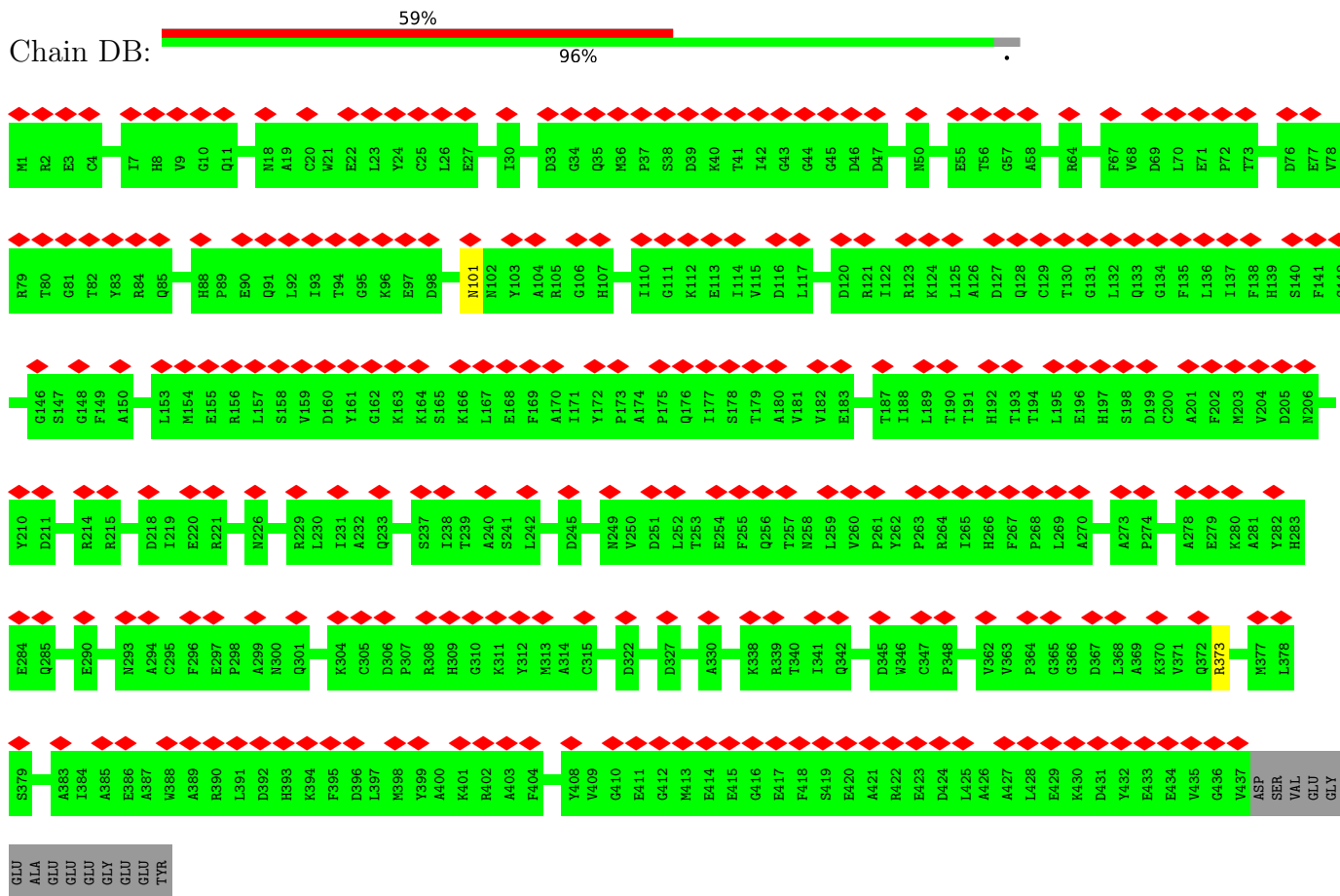
• Molecule 54: Tubulin alpha chain



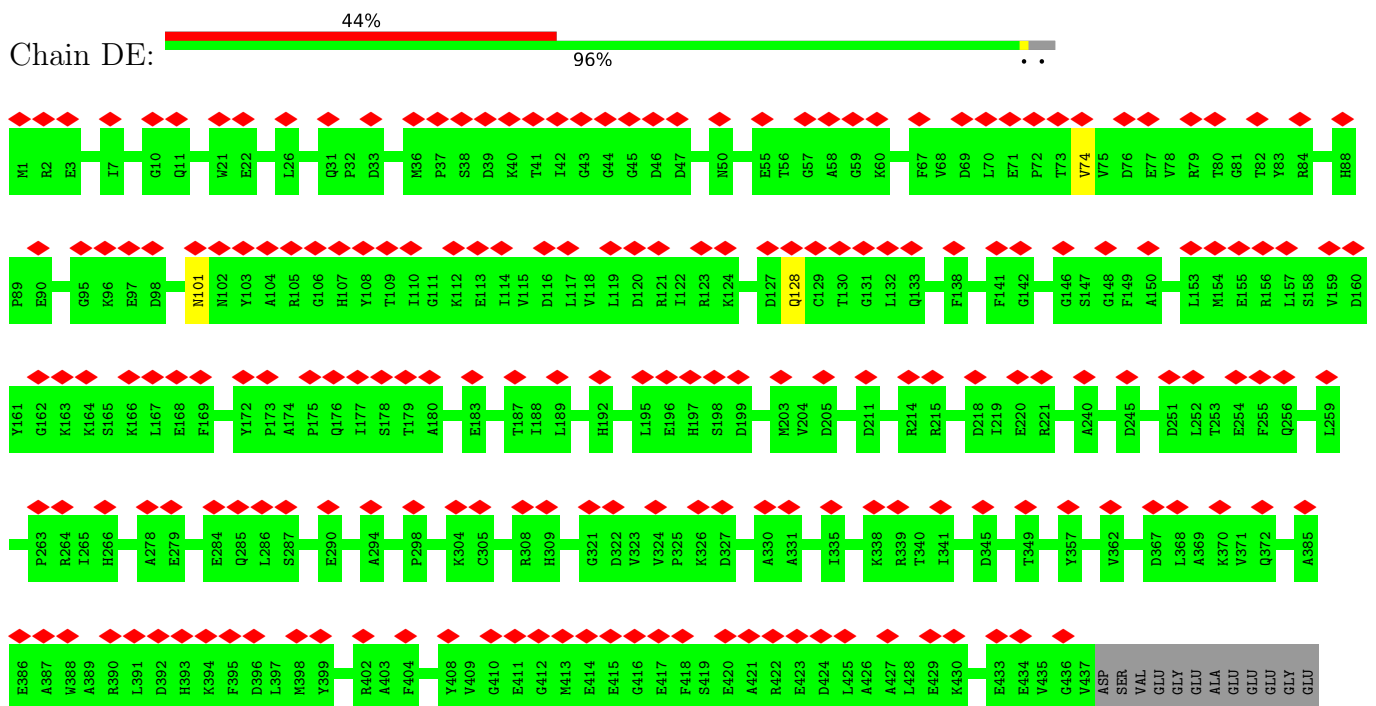
• Molecule 54: Tubulin alpha chain



• Molecule 54: Tubulin alpha chain



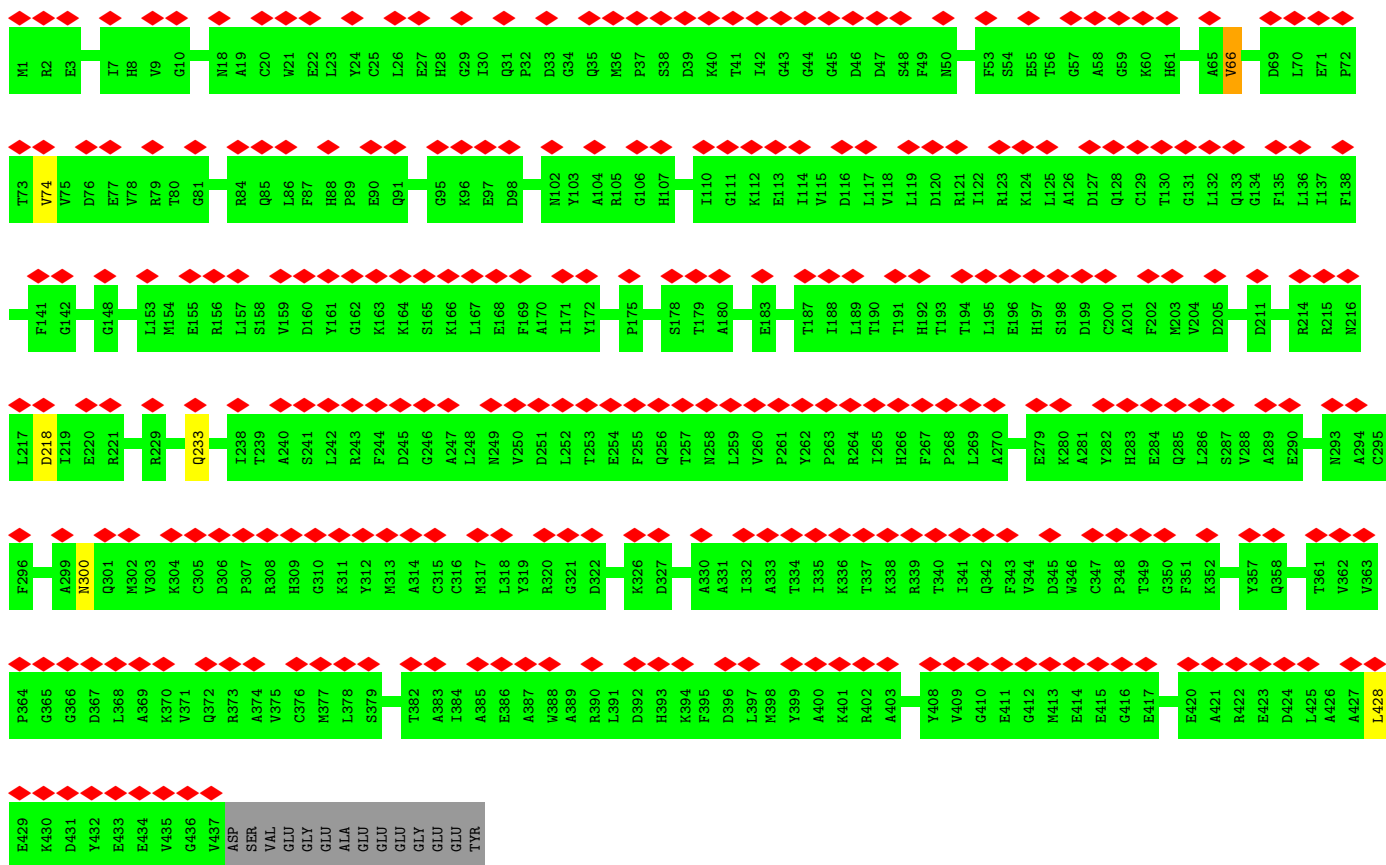
• Molecule 54: Tubulin alpha chain



GLU  
TYR

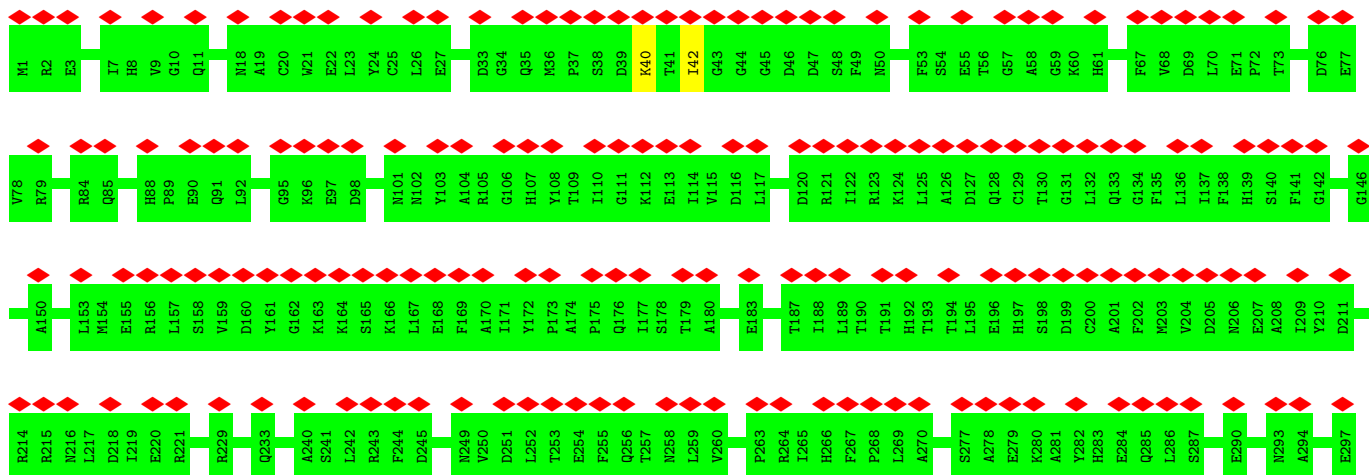
- Molecule 54: Tubulin alpha chain

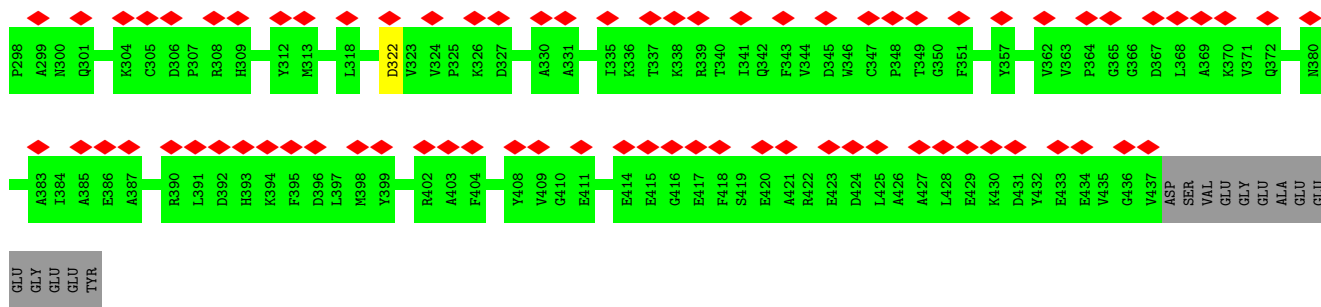
Chain DG:  63%  
96%



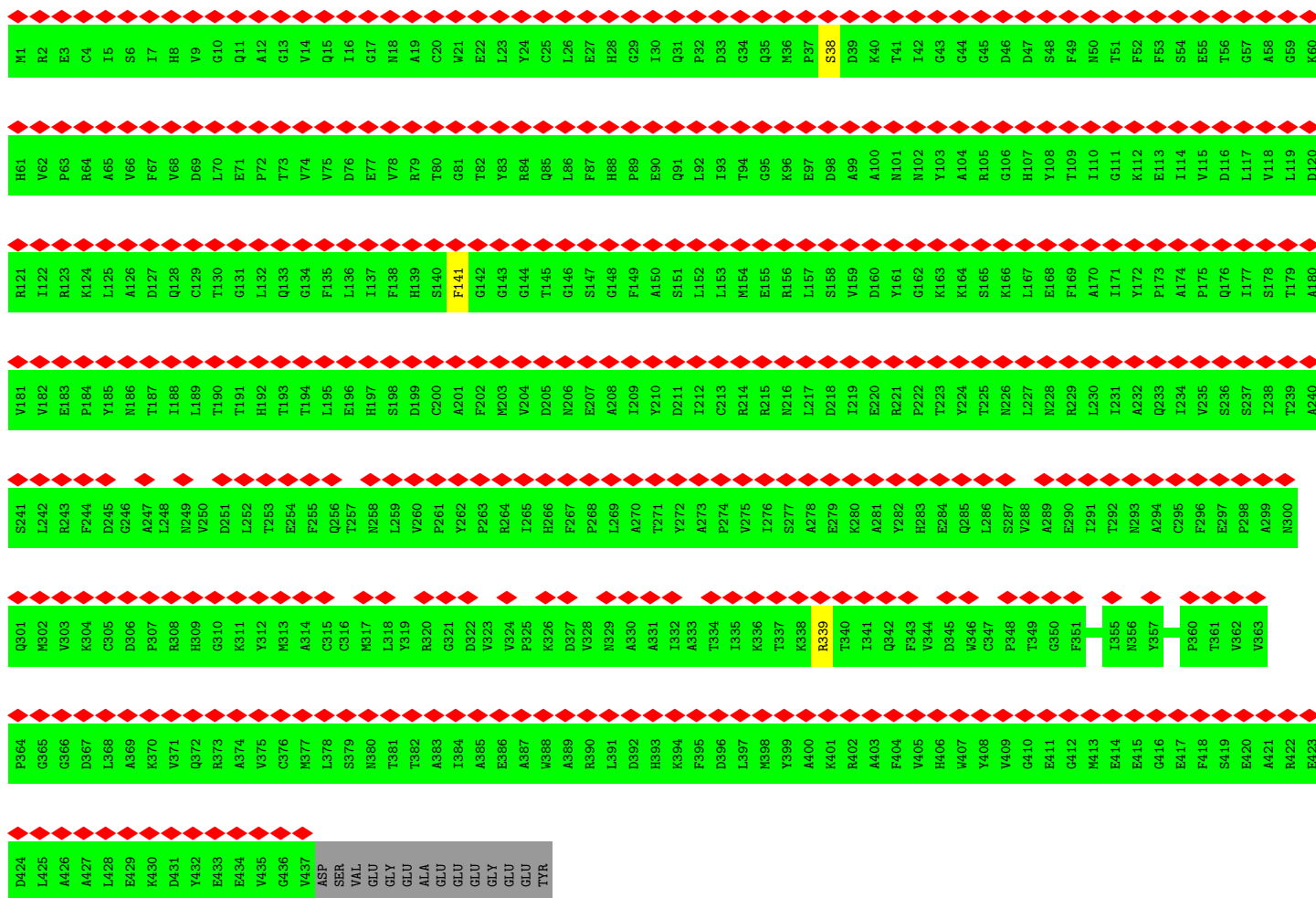
- Molecule 54: Tubulin alpha chain

Chain DI:  56%  
96%

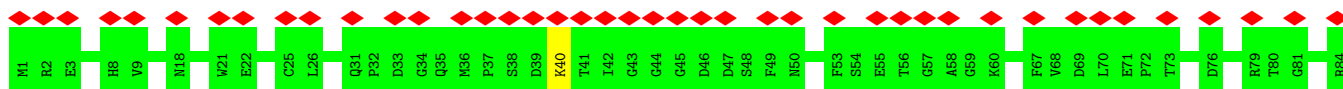


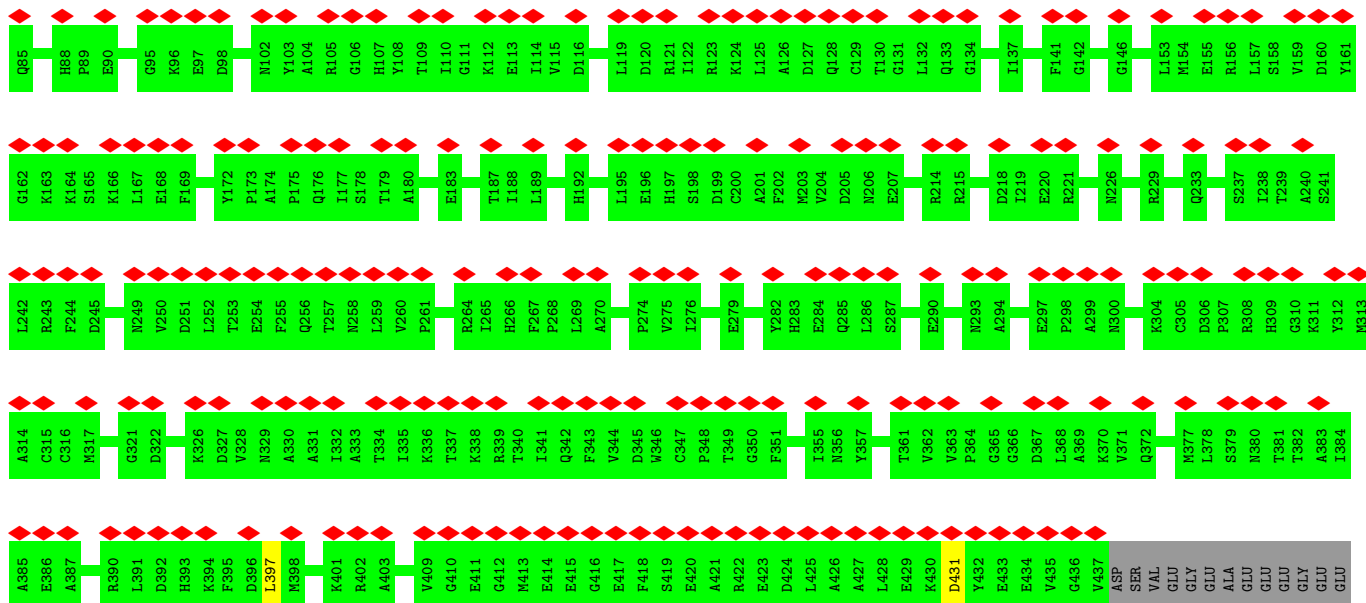


• Molecule 54: Tubulin alpha chain



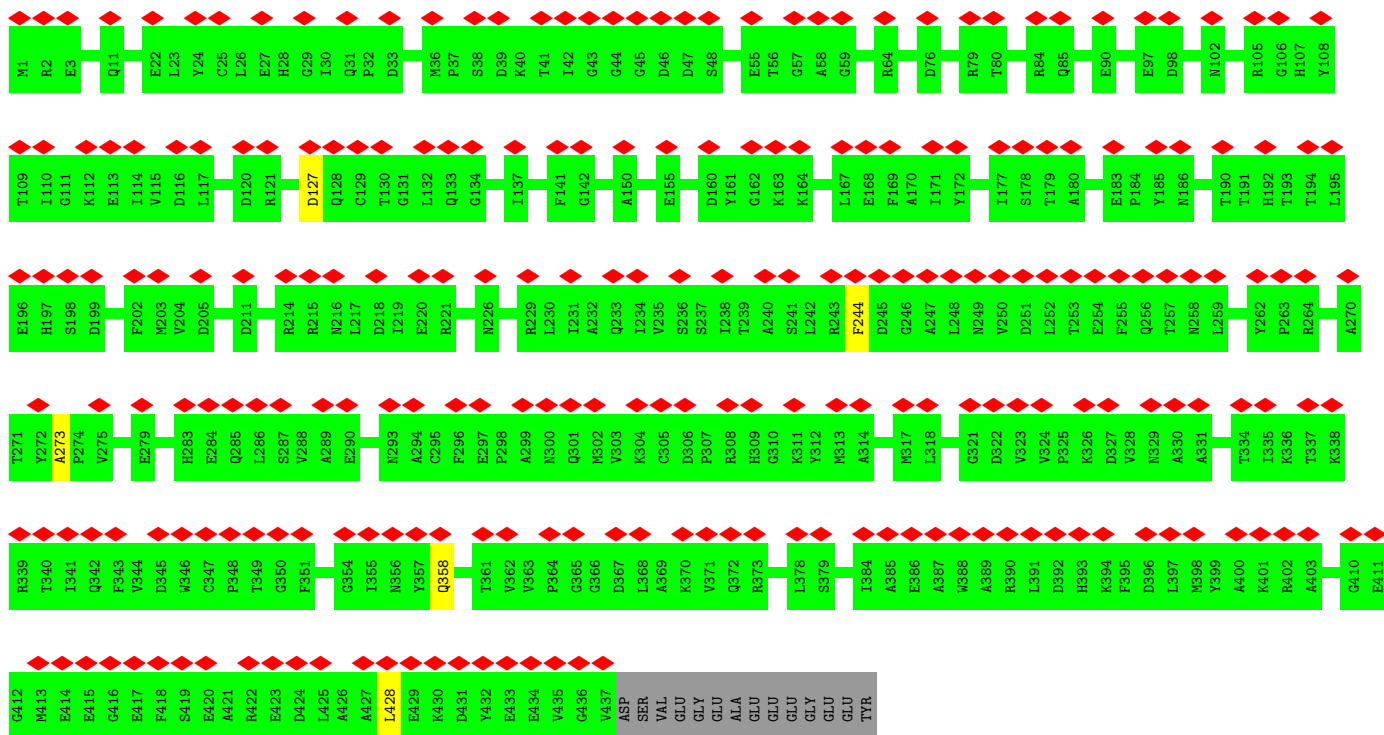
• Molecule 54: Tubulin alpha chain





TYR

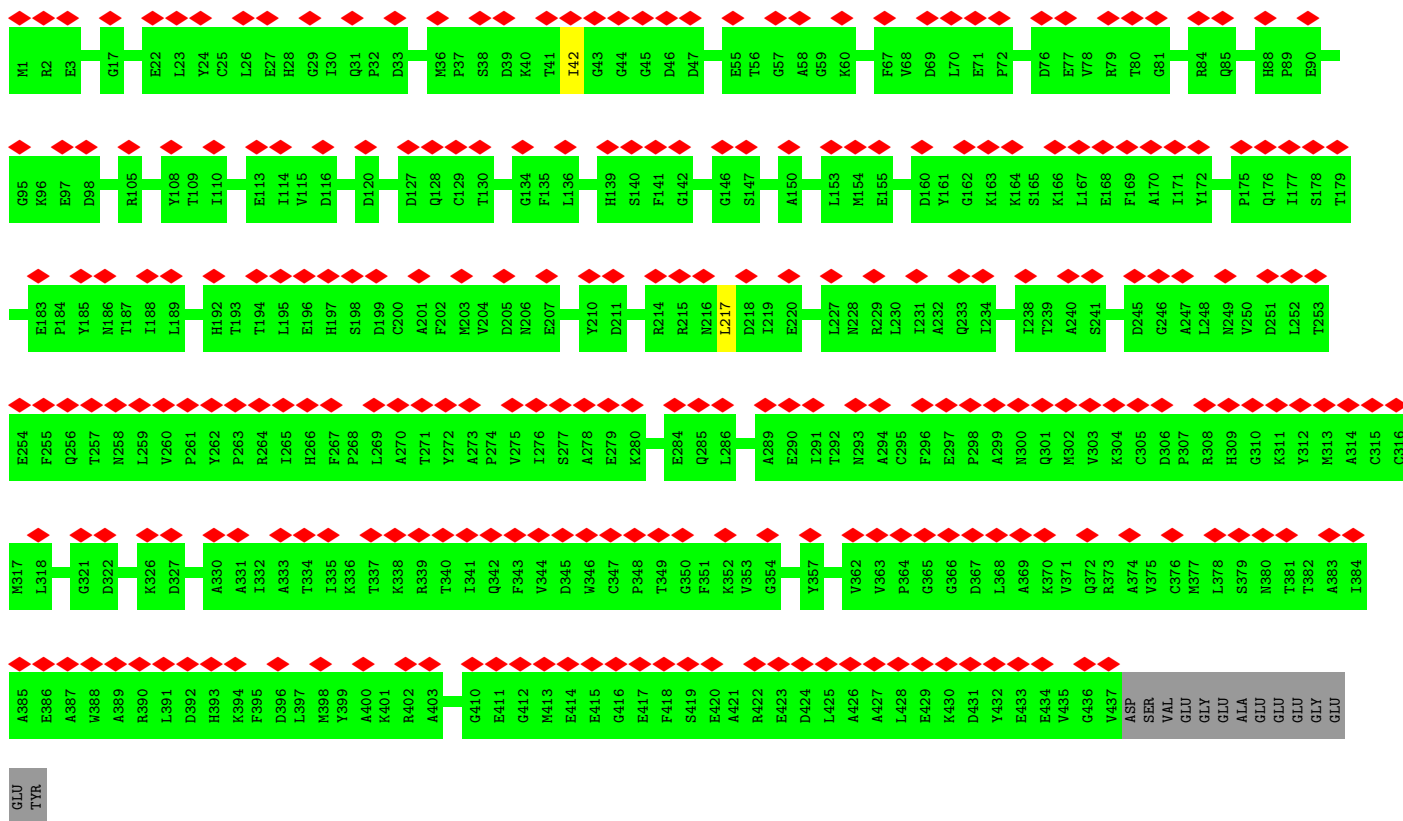
• Molecule 54: Tubulin alpha chain



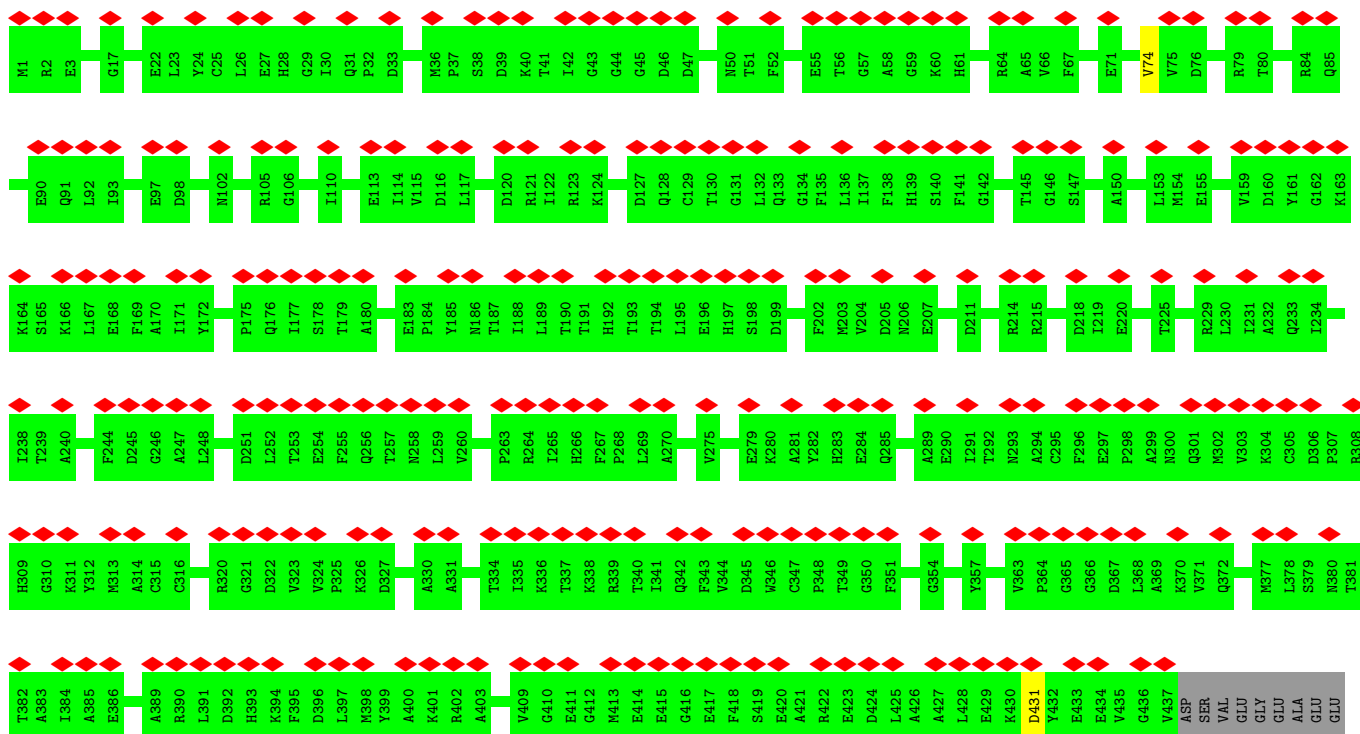
• Molecule 54: Tubulin alpha chain





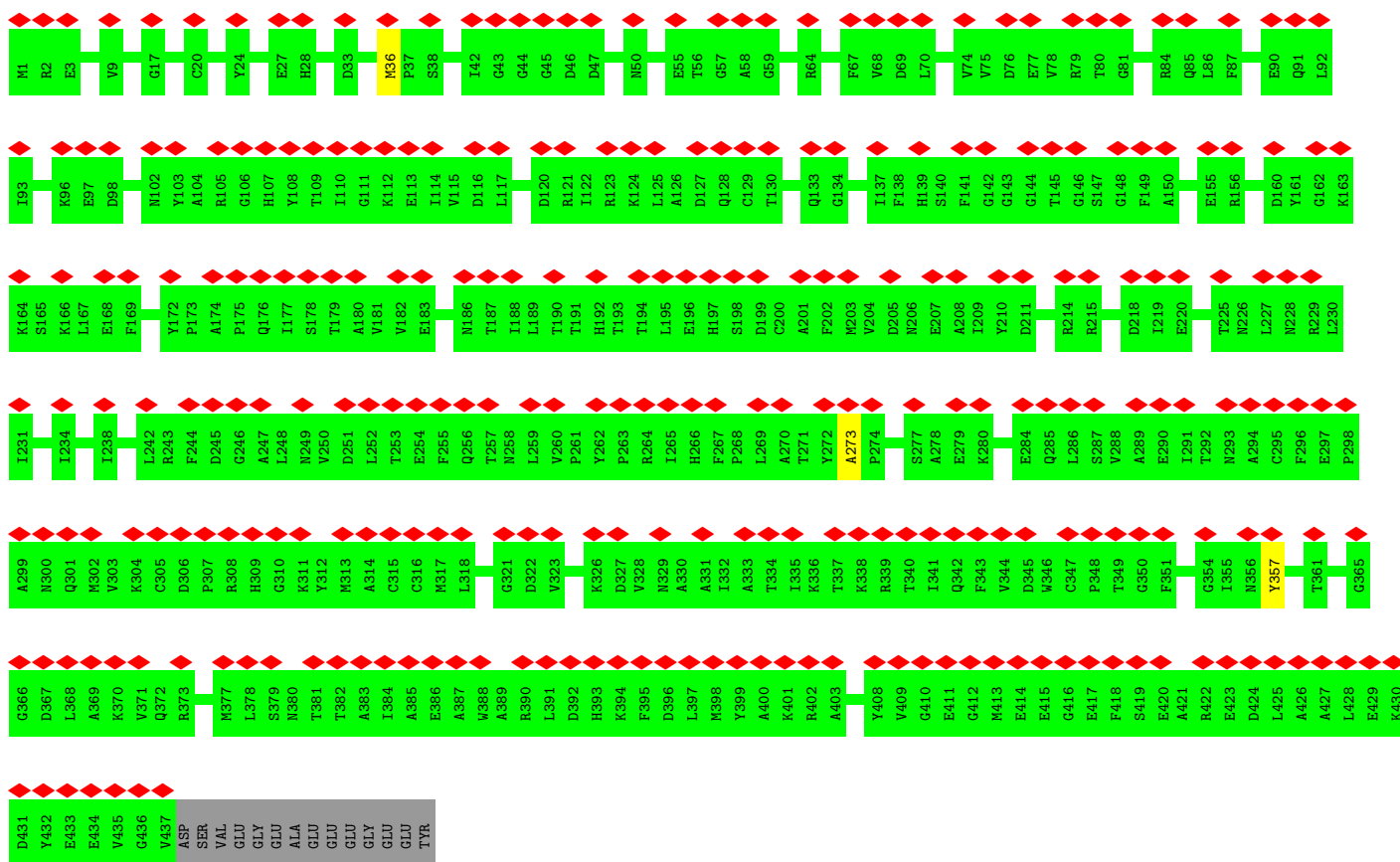


• Molecule 54: Tubulin alpha chain

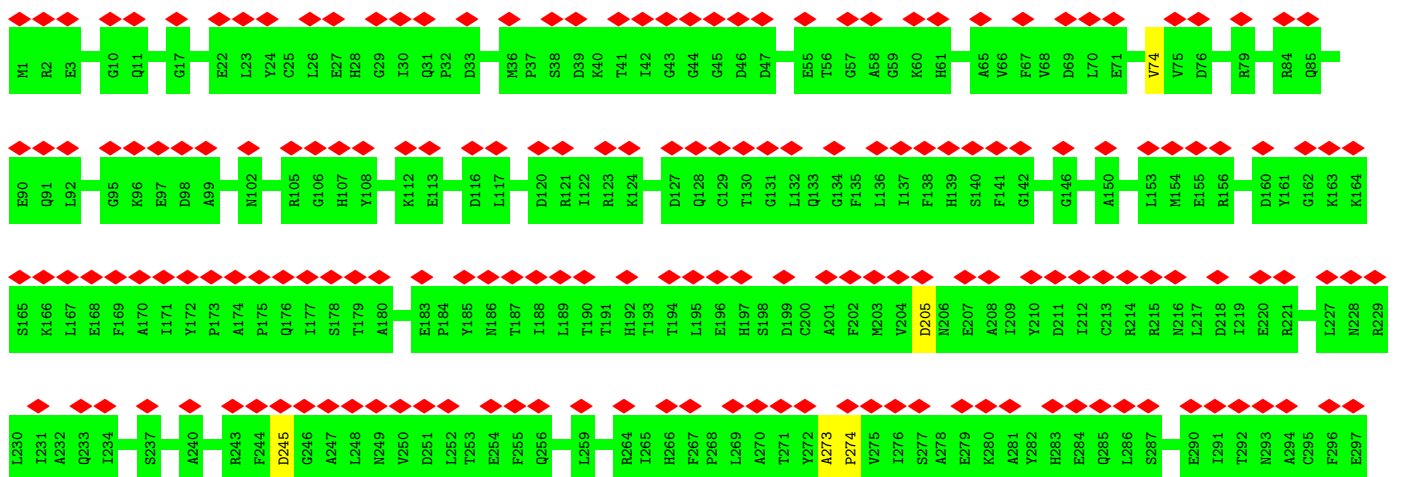


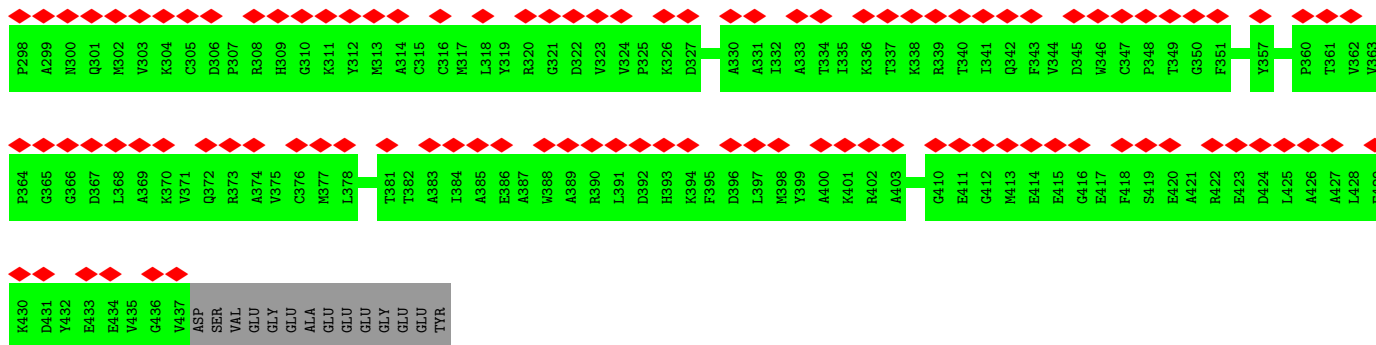
GLU  
GLY  
GLU  
TYR

• Molecule 54: Tubulin alpha chain

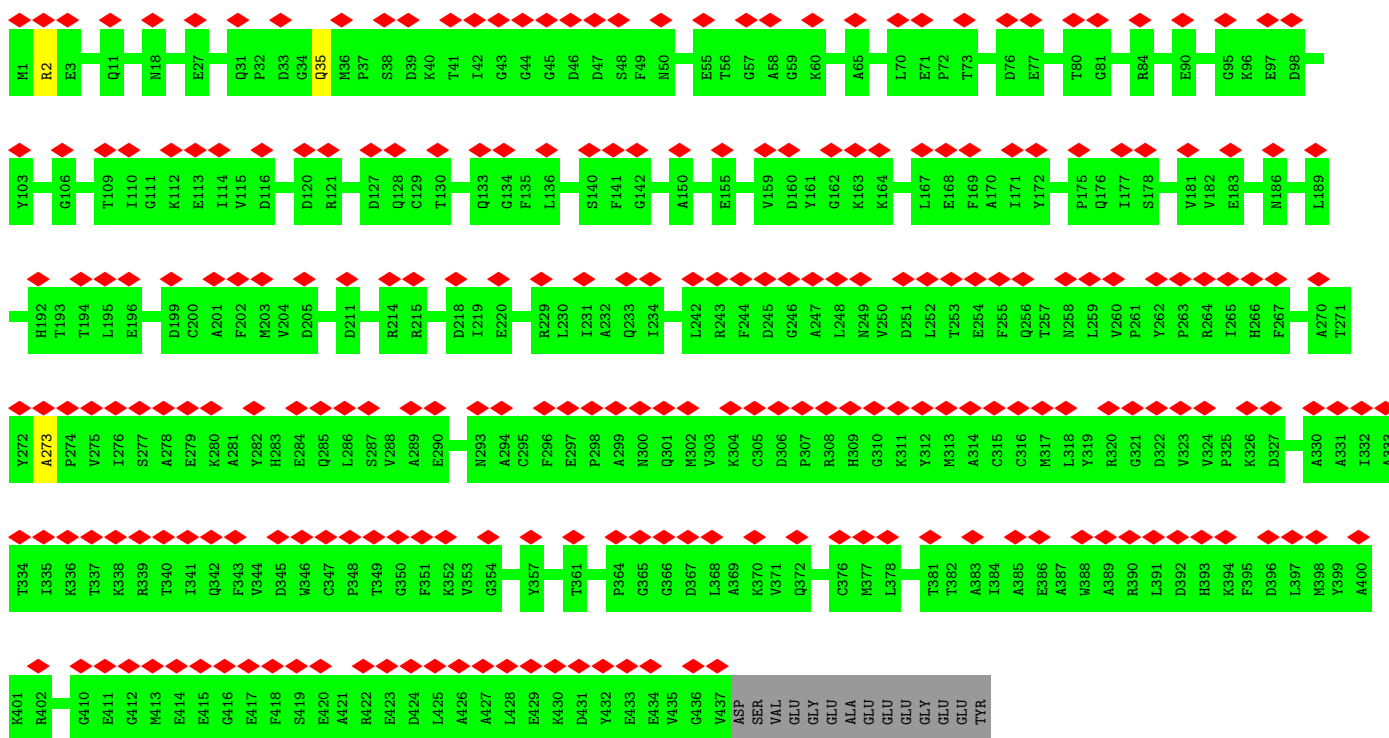


• Molecule 54: Tubulin alpha chain

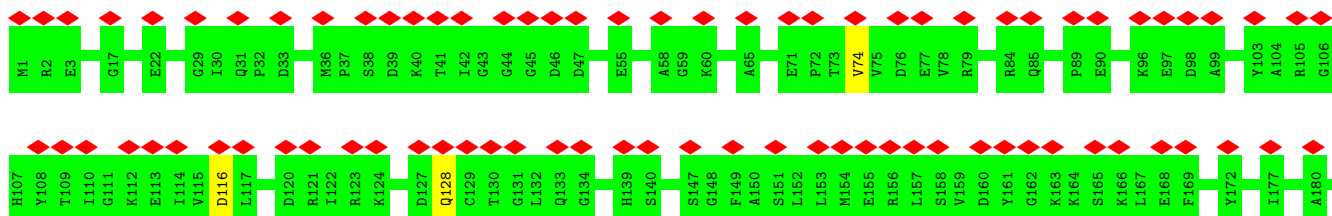


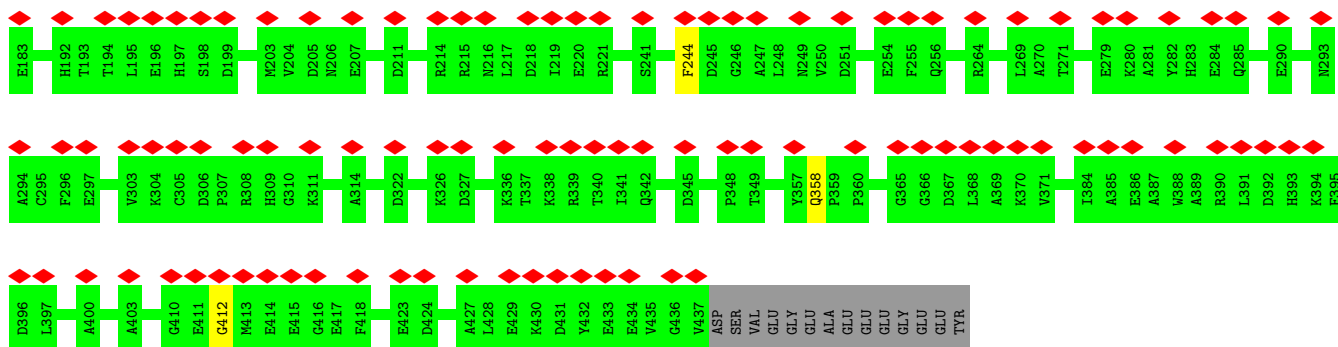


• Molecule 54: Tubulin alpha chain

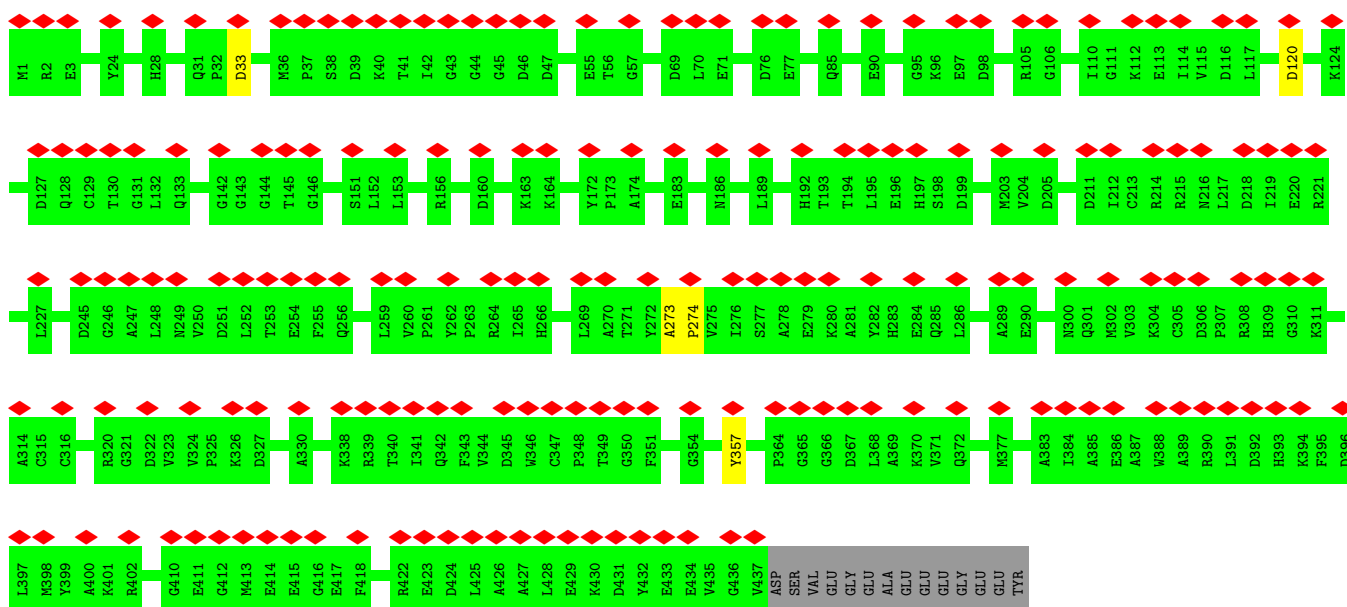


• Molecule 54: Tubulin alpha chain

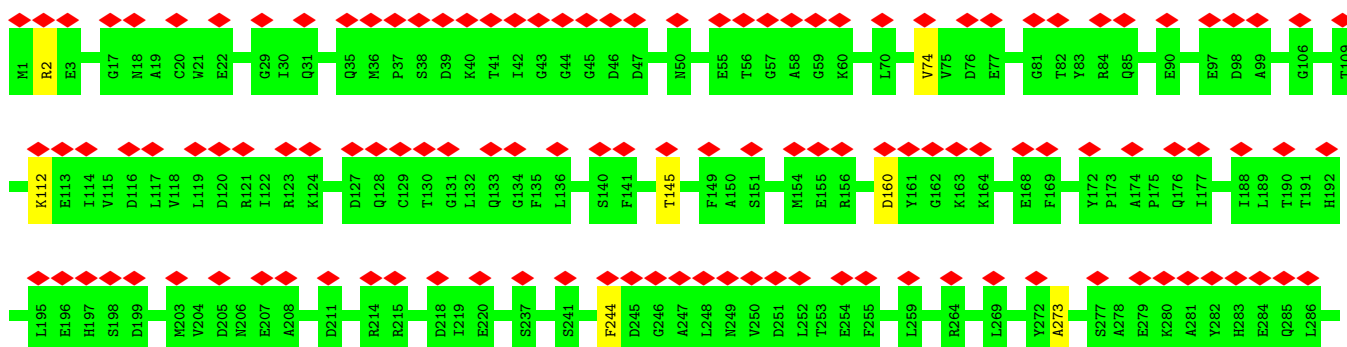


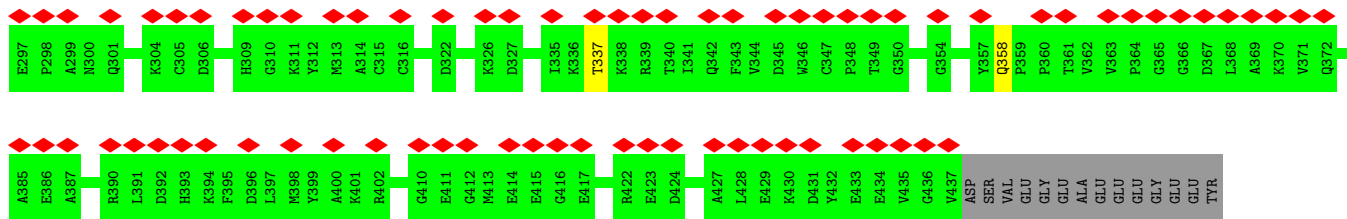


• Molecule 54: Tubulin alpha chain

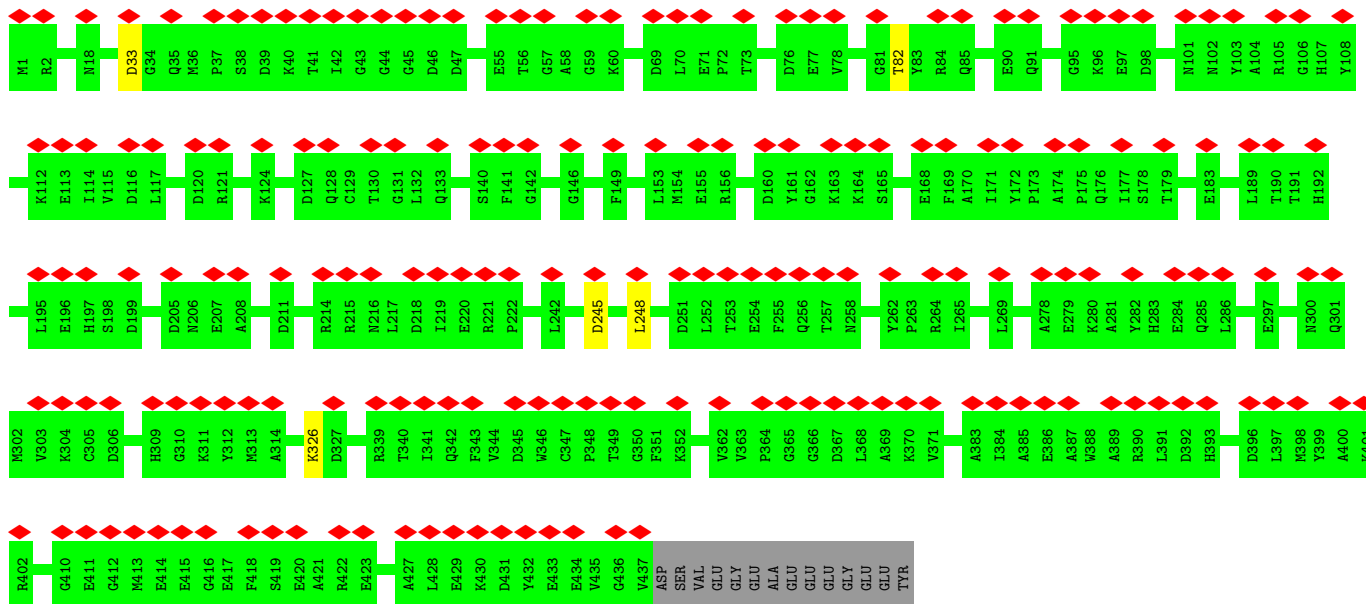
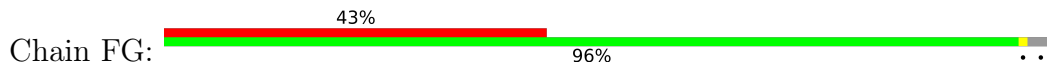


• Molecule 54: Tubulin alpha chain

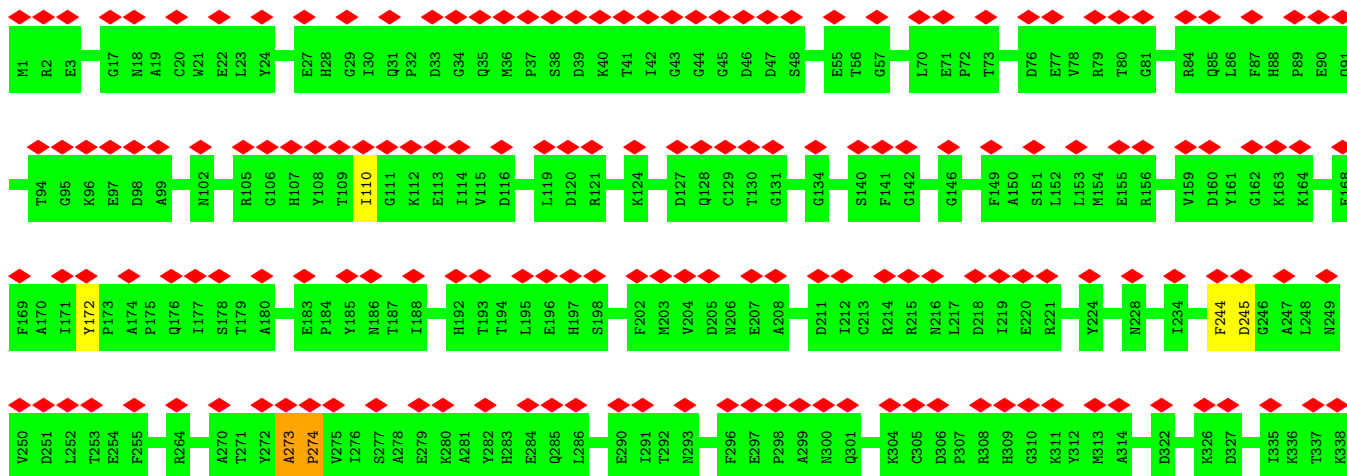


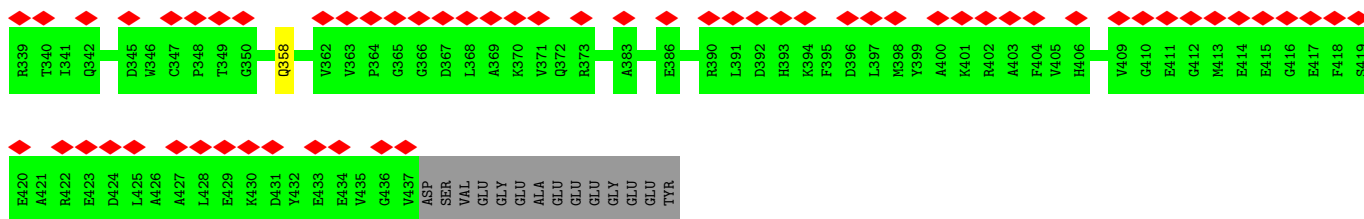


• Molecule 54: Tubulin alpha chain

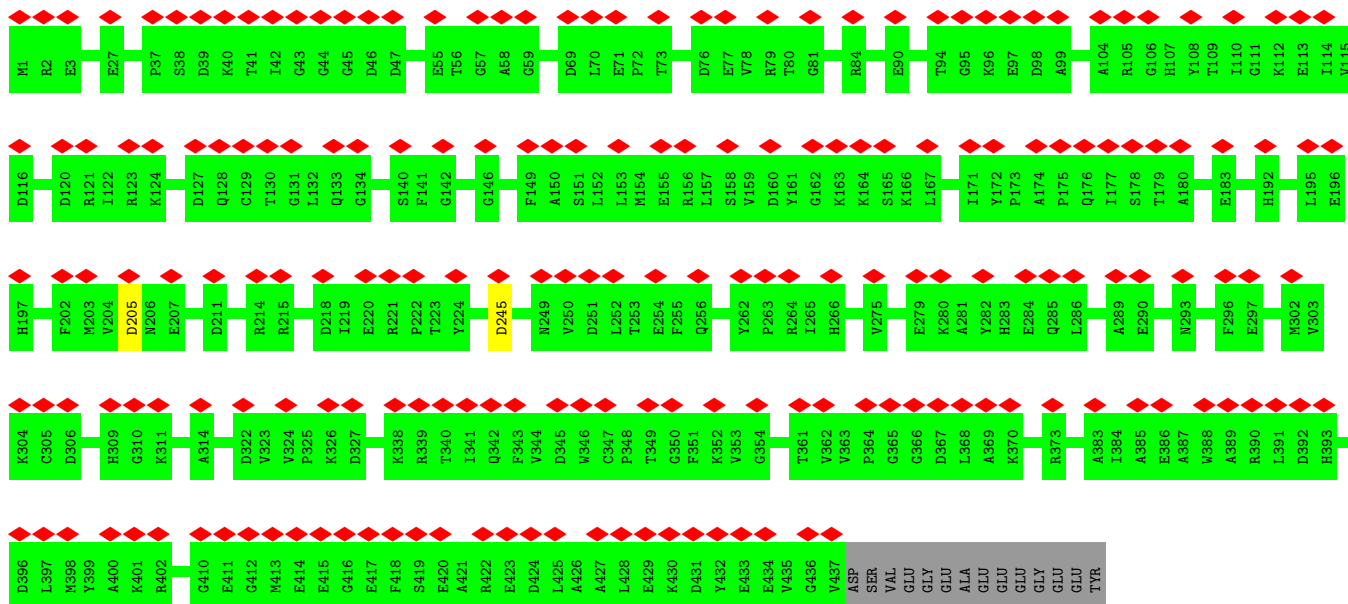
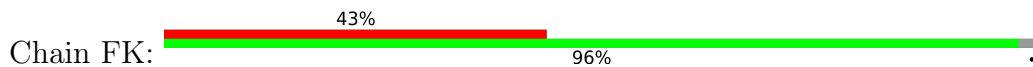


• Molecule 54: Tubulin alpha chain

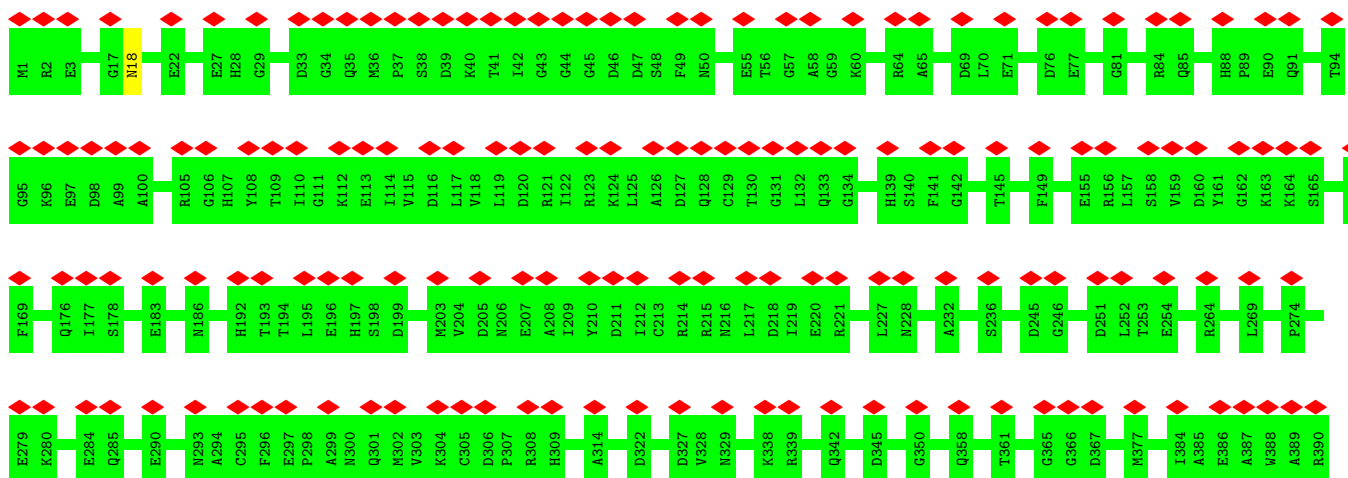
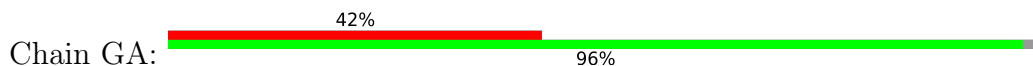


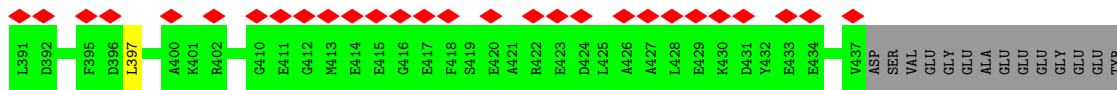


• Molecule 54: Tubulin alpha chain

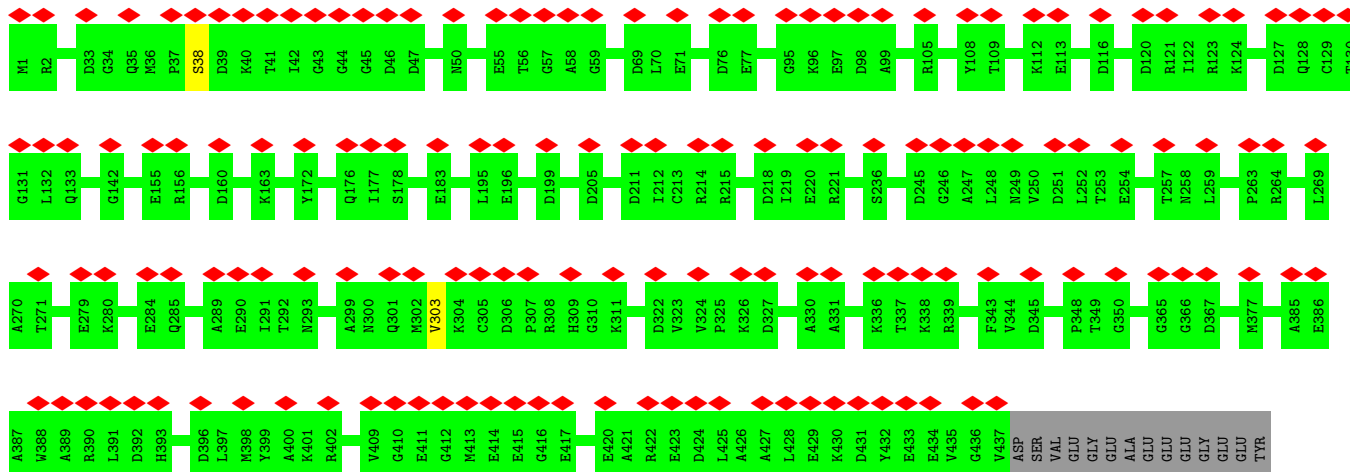


• Molecule 54: Tubulin alpha chain





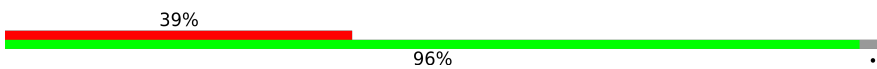
• Molecule 54: Tubulin alpha chain

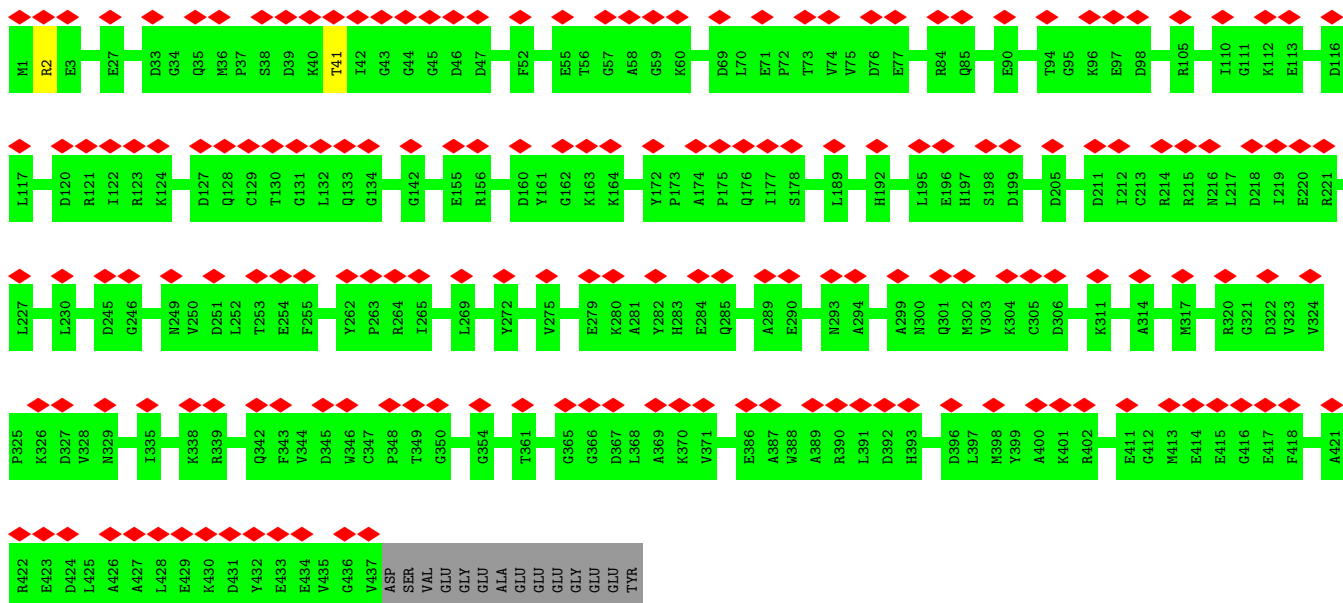


• Molecule 54: Tubulin alpha chain



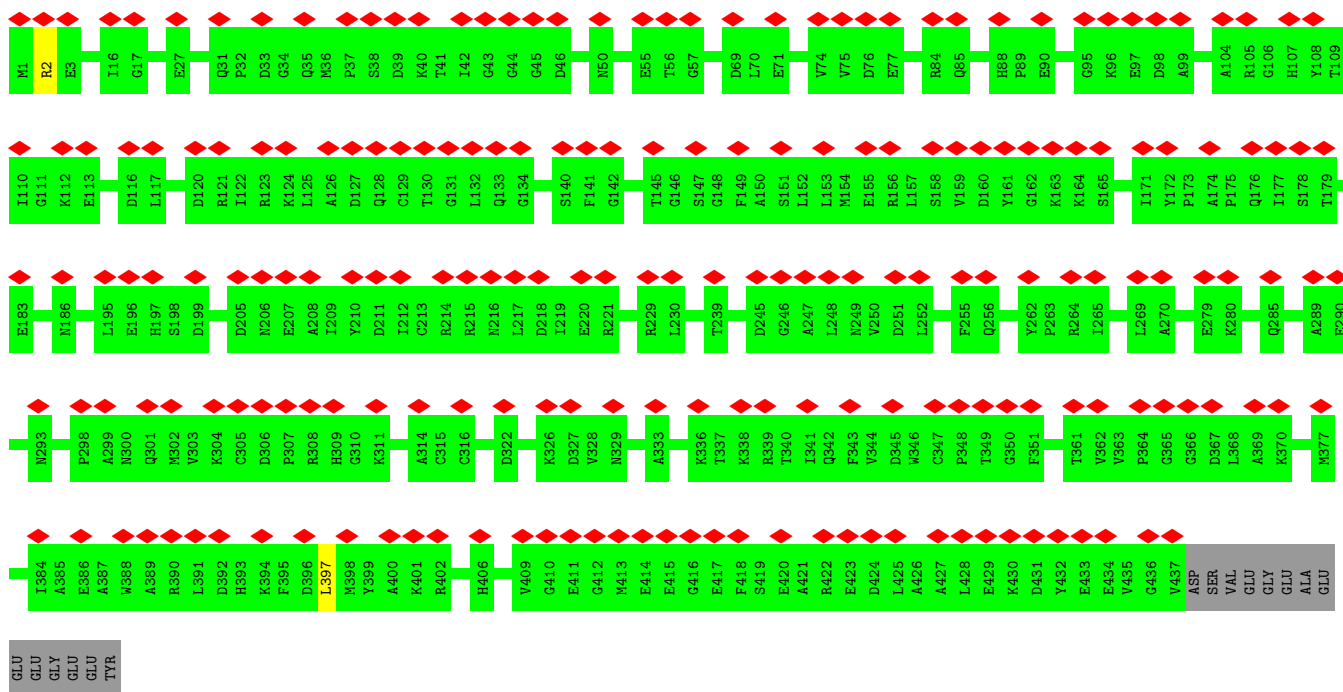
• Molecule 54: Tubulin alpha chain

Chain GG: 

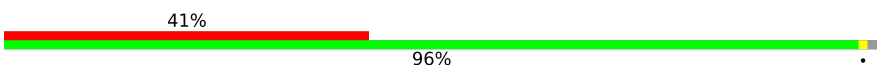


• Molecule 54: Tubulin alpha chain

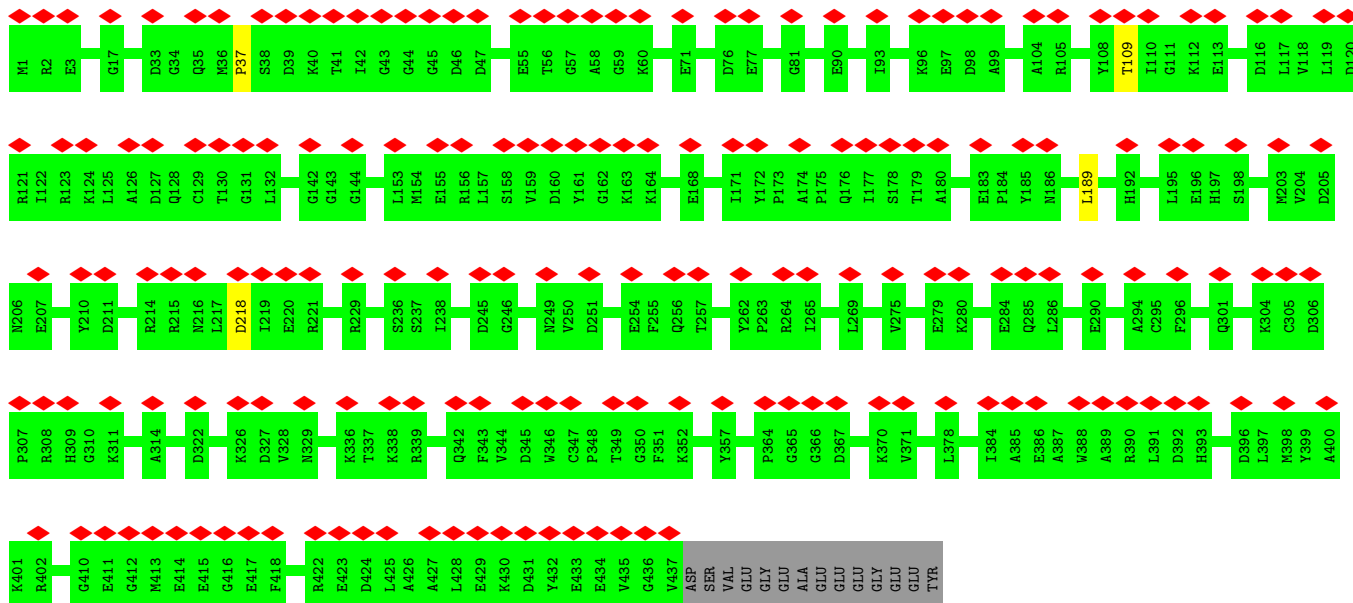
Chain GI: 



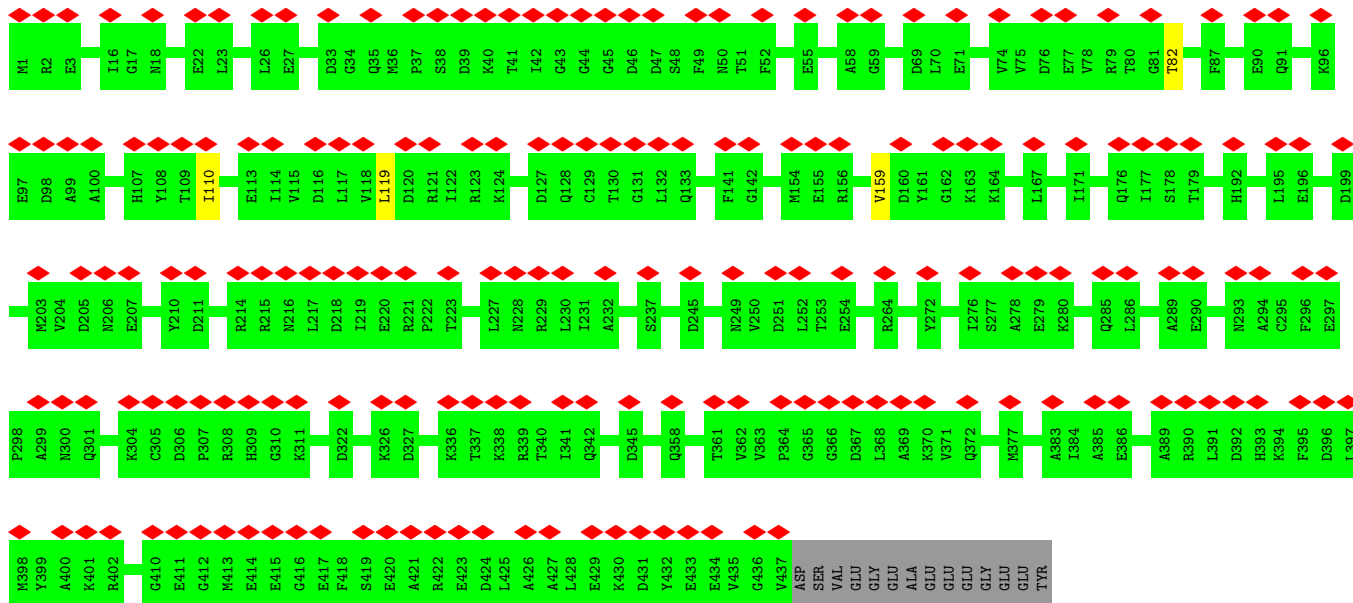
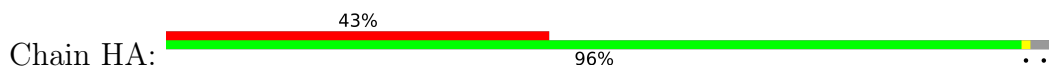
• Molecule 54: Tubulin alpha chain

Chain GK: 

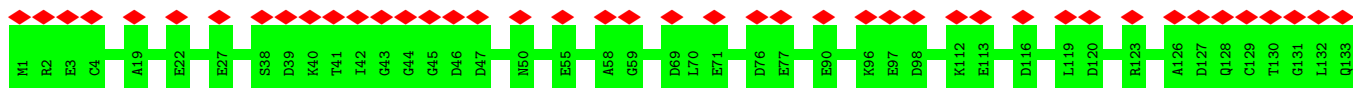


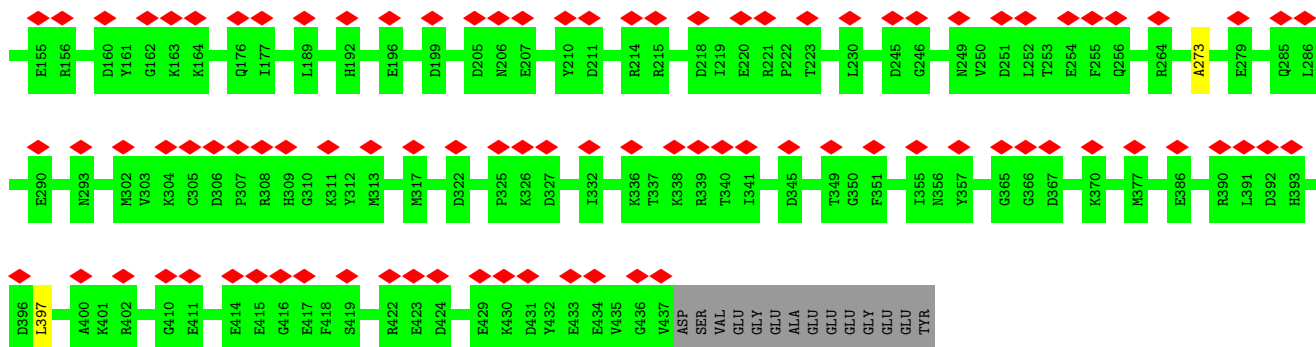


• Molecule 54: Tubulin alpha chain

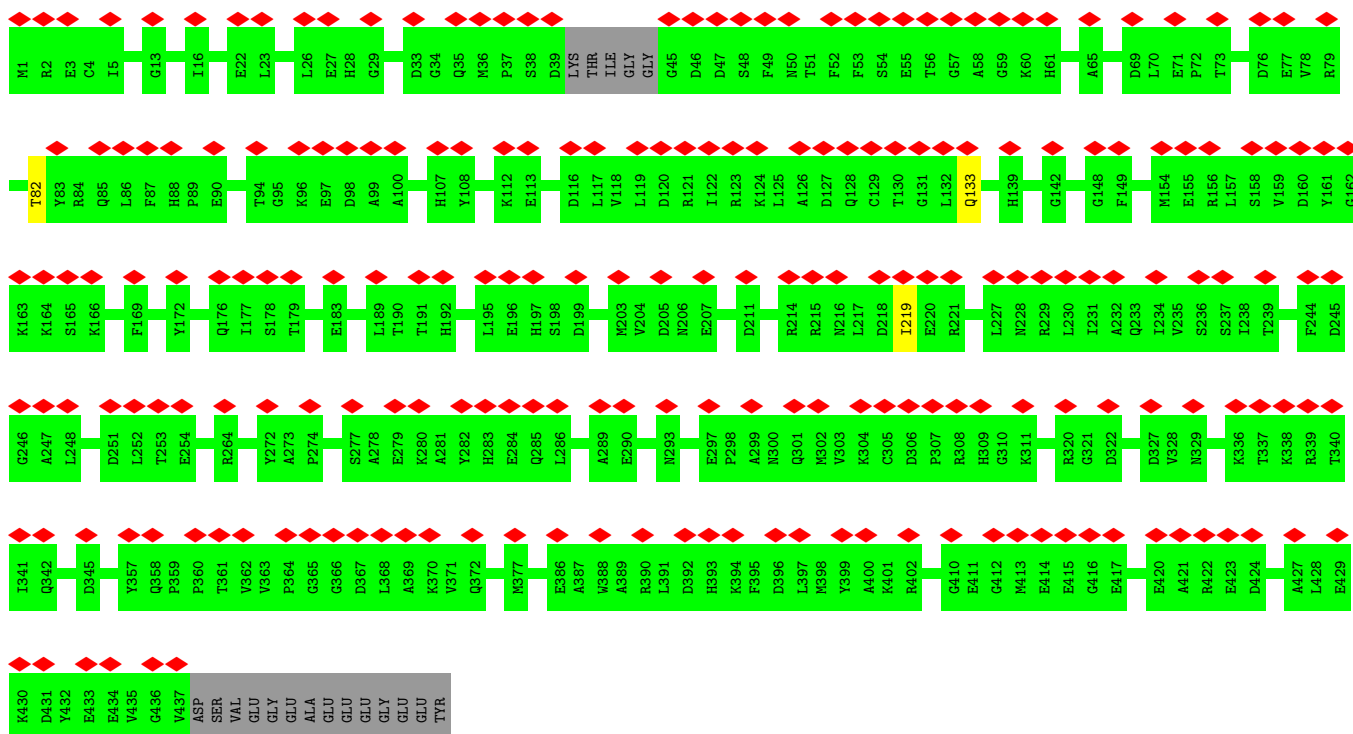


• Molecule 54: Tubulin alpha chain

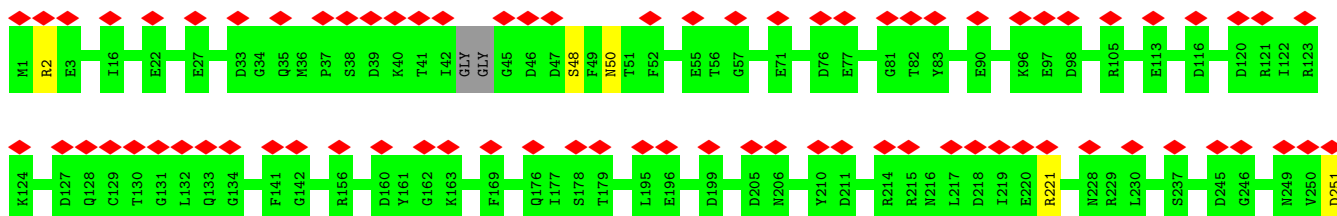


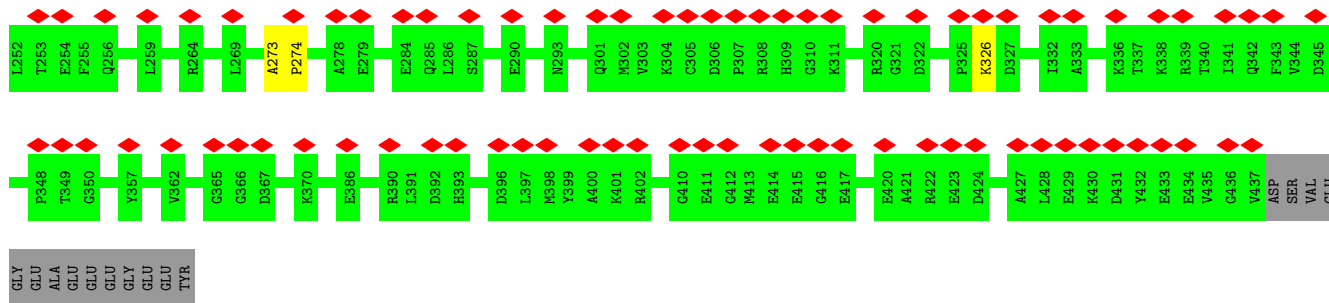


• Molecule 54: Tubulin alpha chain

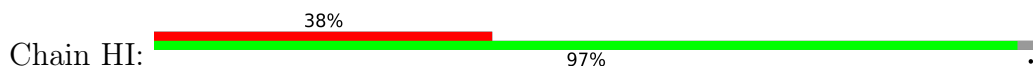


• Molecule 54: Tubulin alpha chain

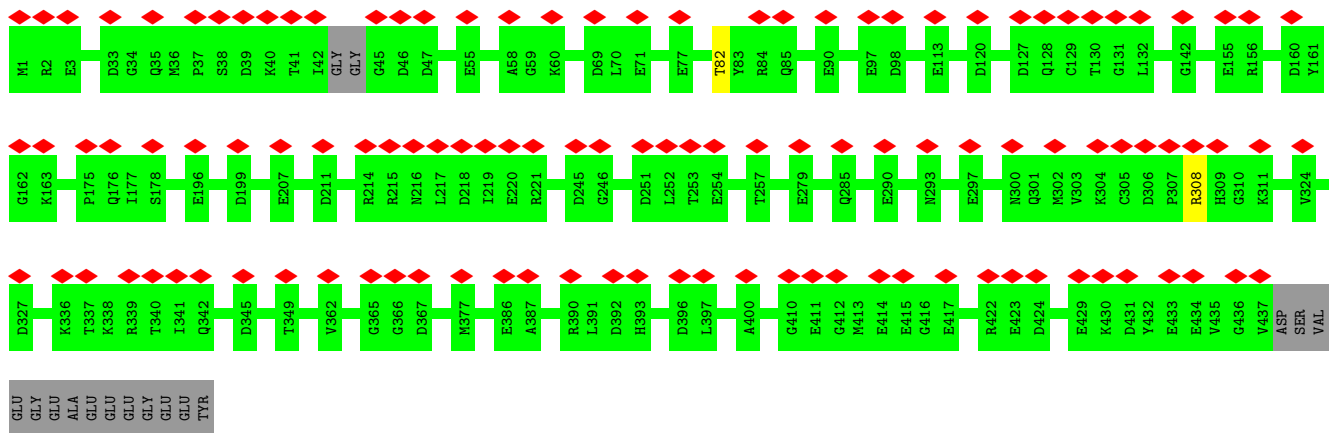




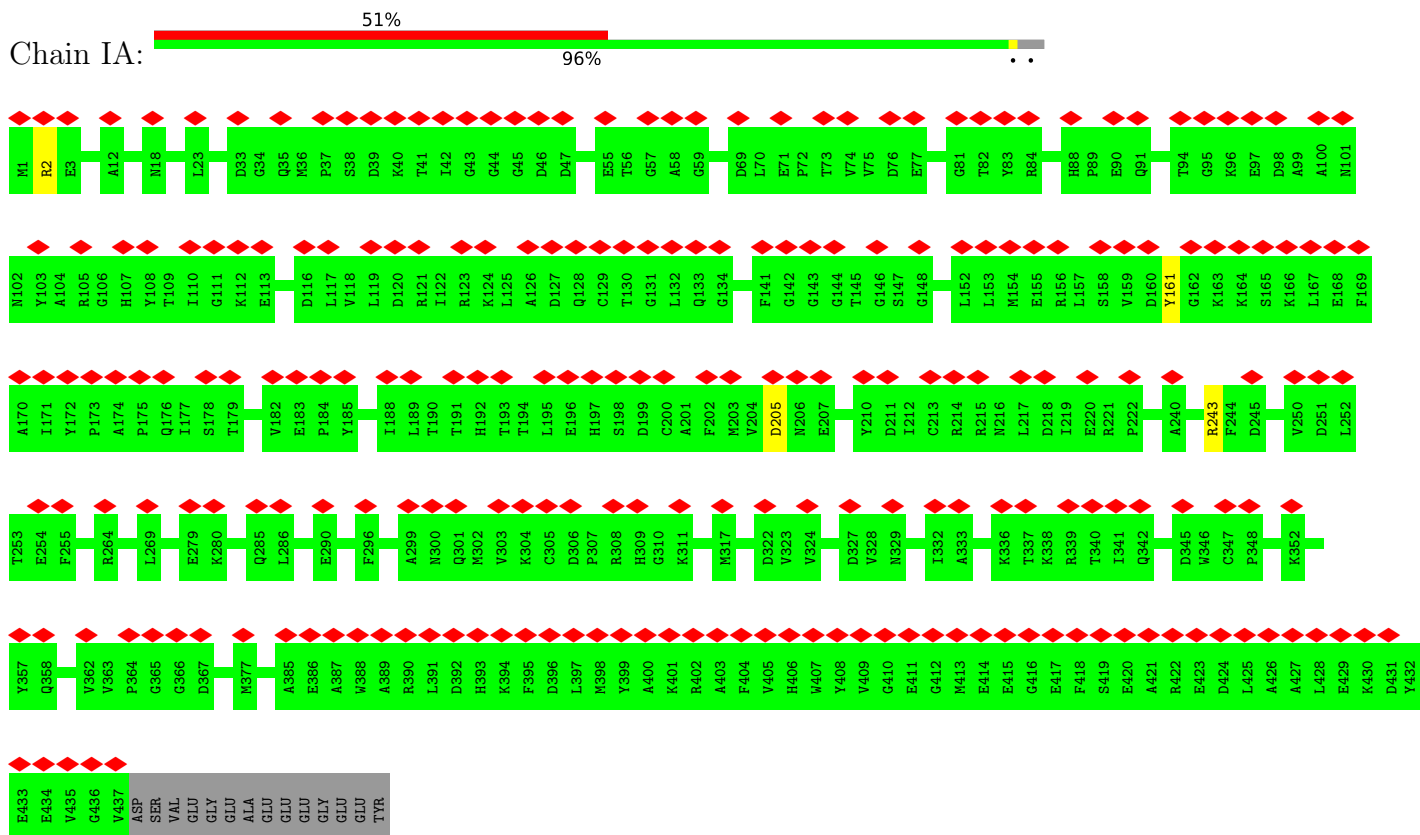
• Molecule 54: Tubulin alpha chain



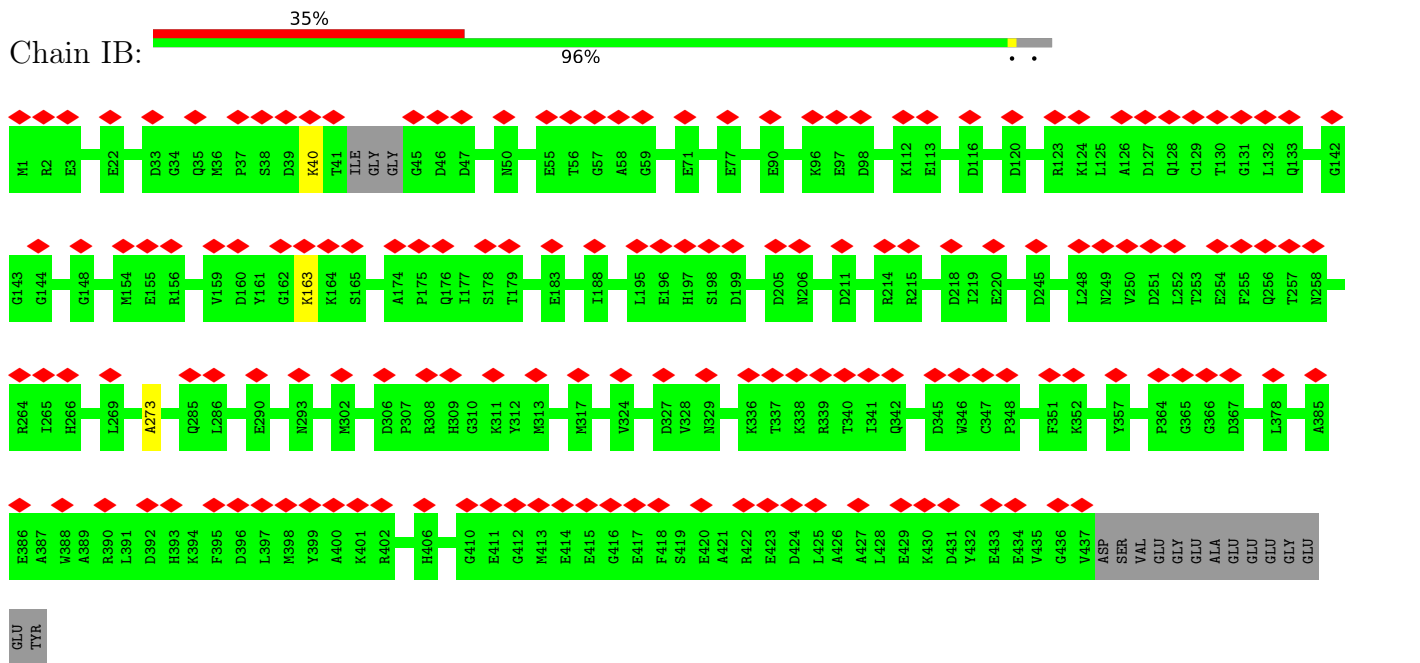
• Molecule 54: Tubulin alpha chain



• Molecule 54: Tubulin alpha chain

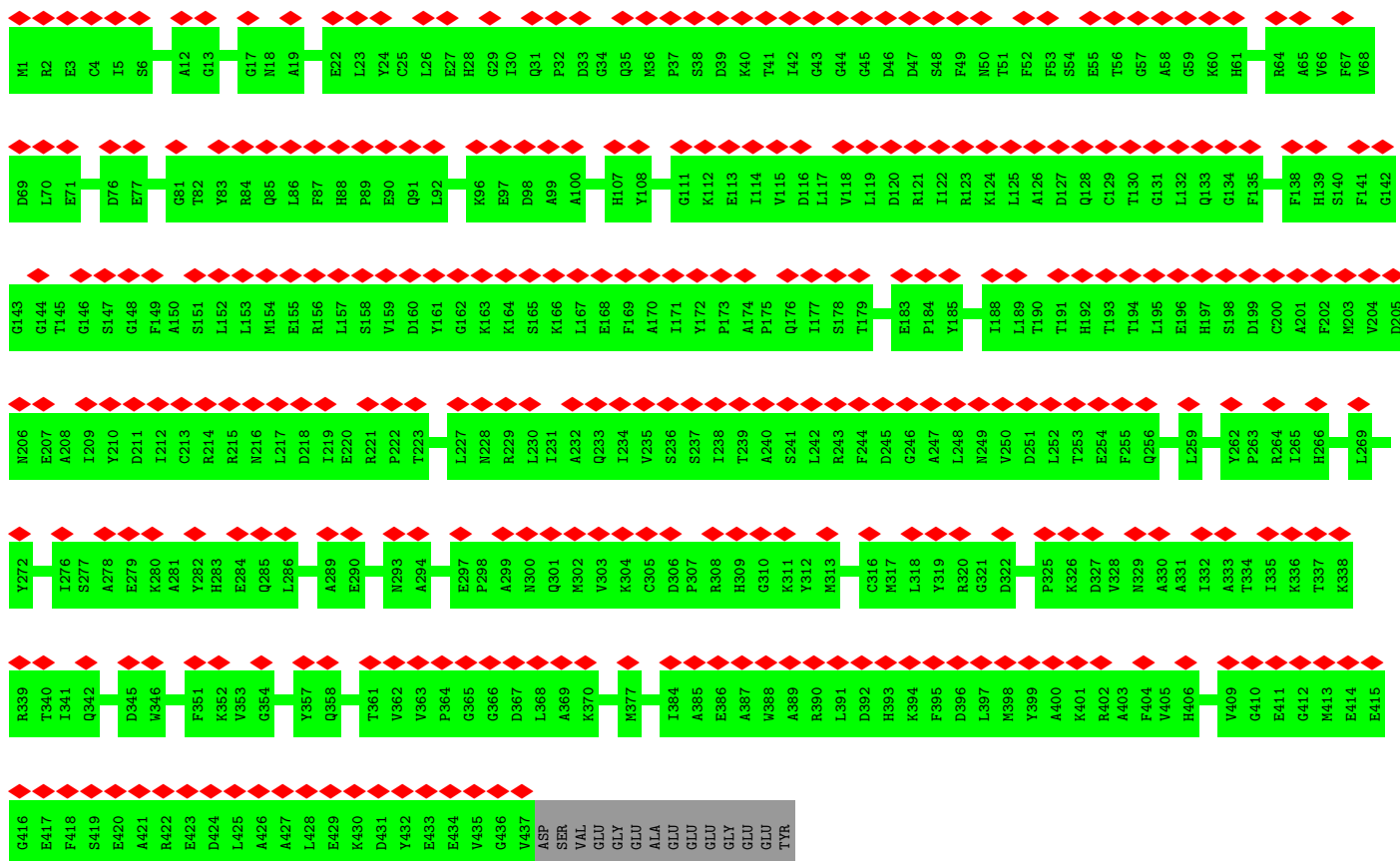


• Molecule 54: Tubulin alpha chain

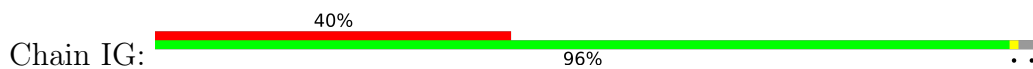


• Molecule 54: Tubulin alpha chain

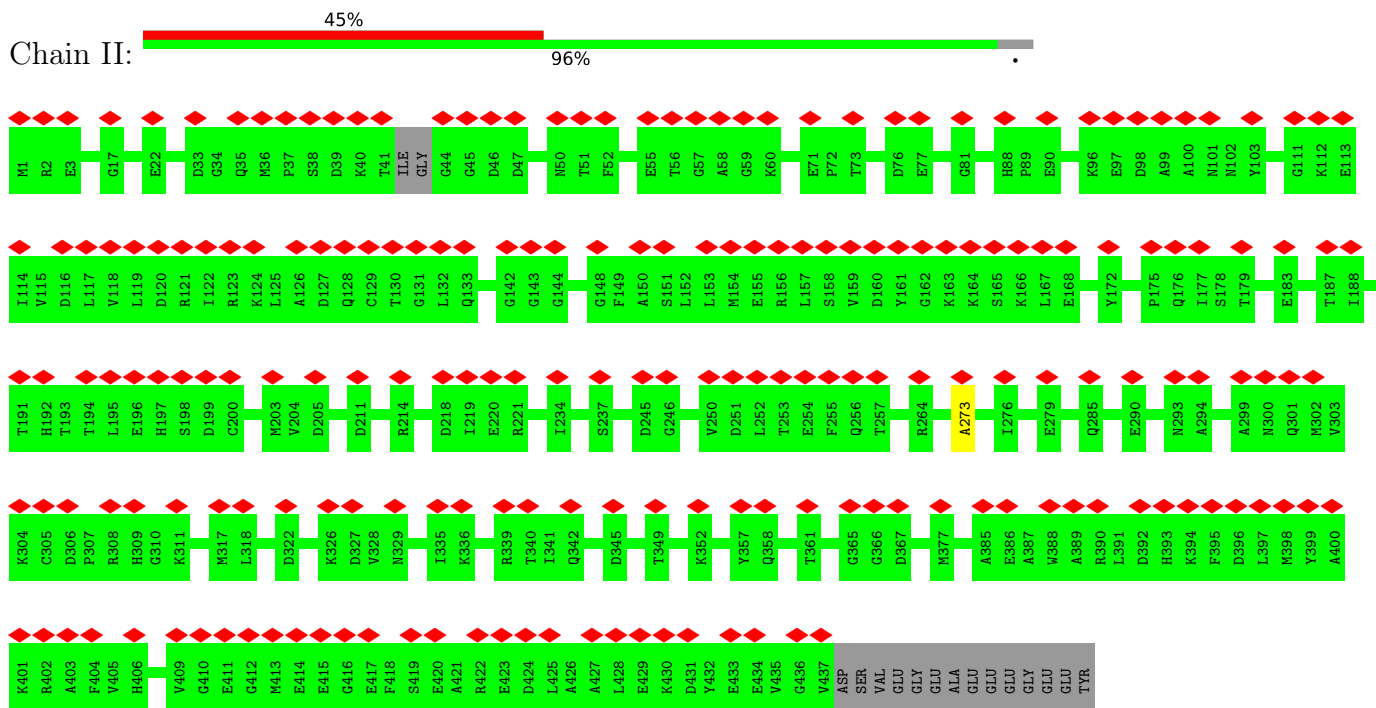




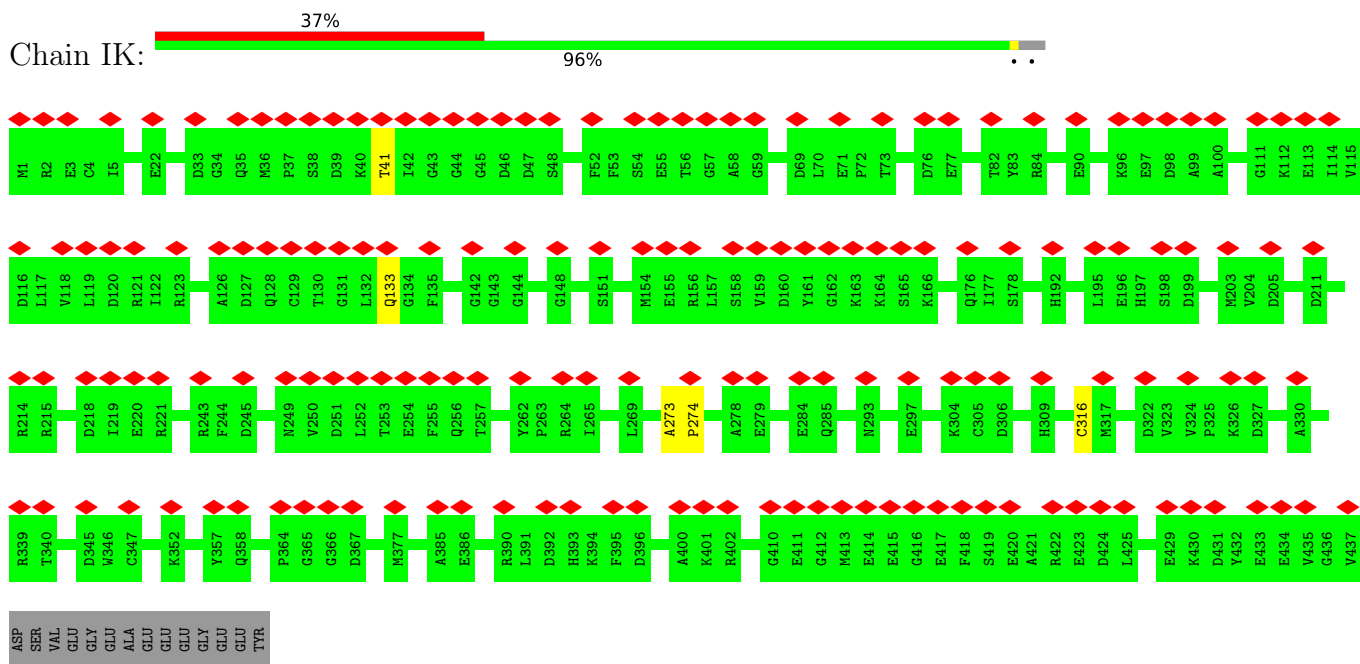
• Molecule 54: Tubulin alpha chain



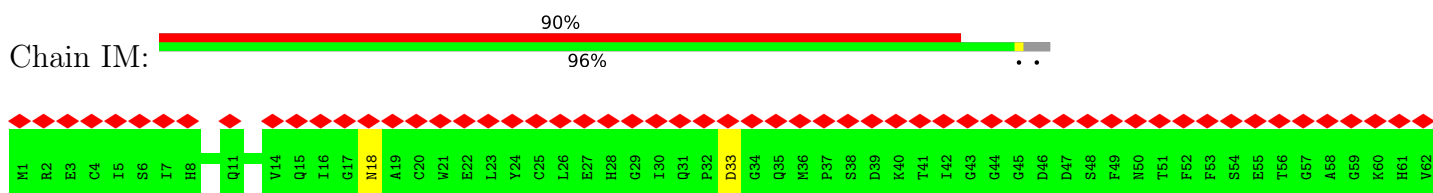
• Molecule 54: Tubulin alpha chain

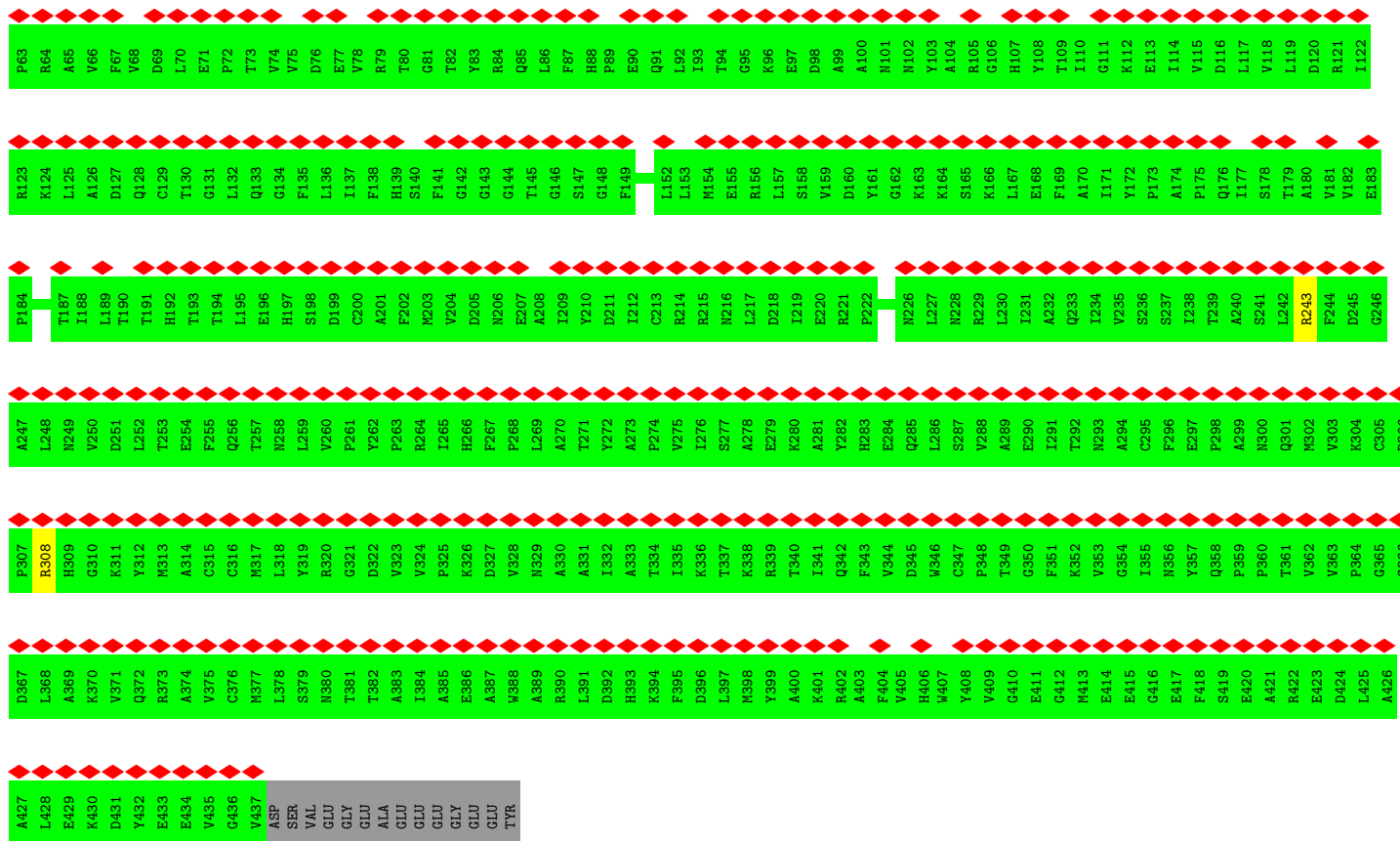


• Molecule 54: Tubulin alpha chain

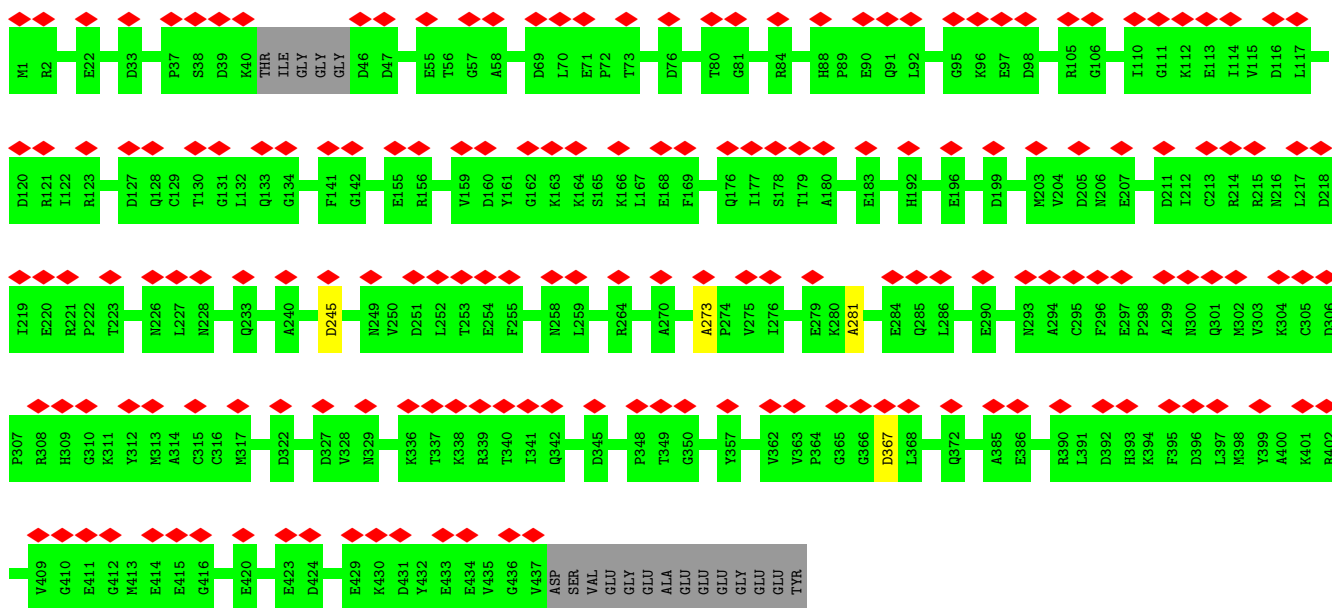


• Molecule 54: Tubulin alpha chain

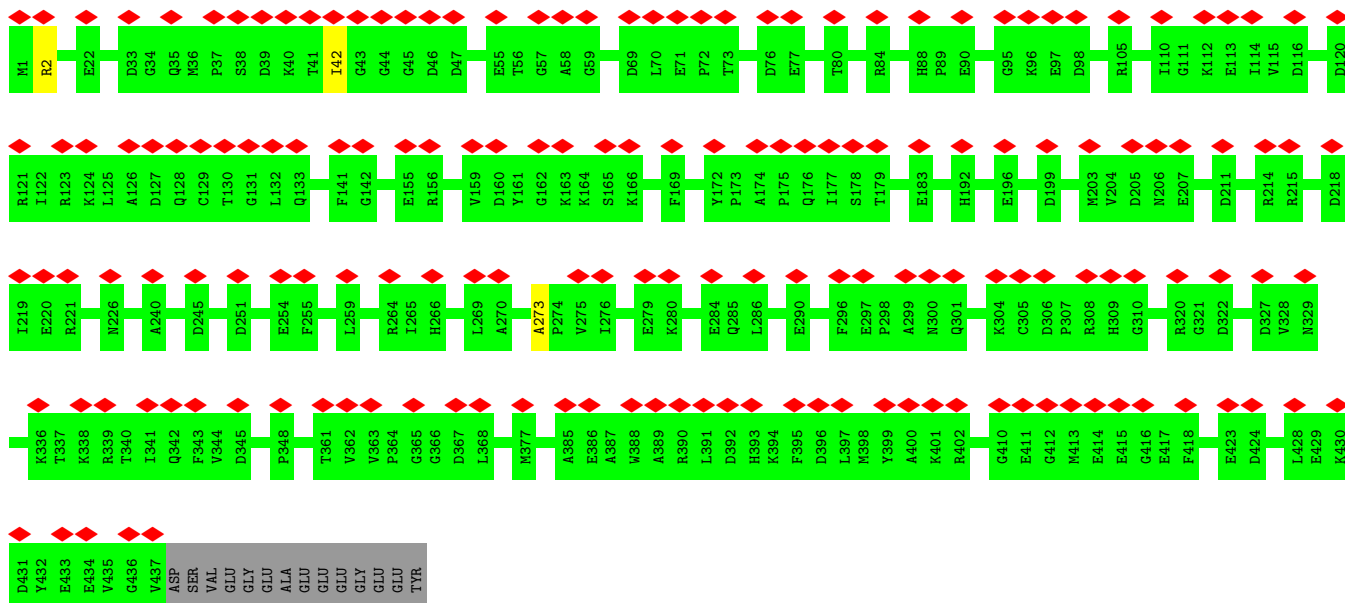




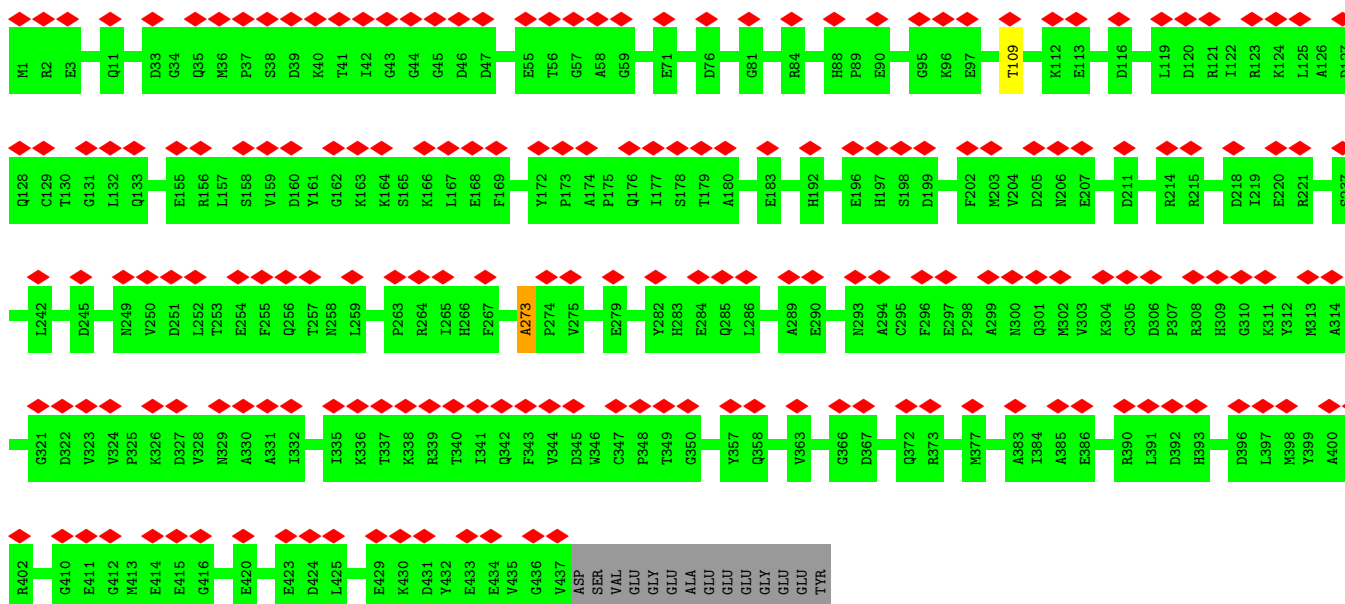
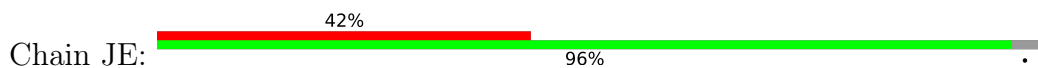
• Molecule 54: Tubulin alpha chain



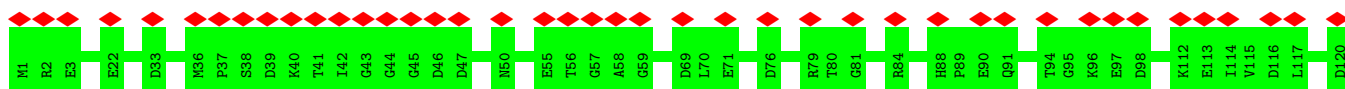
• Molecule 54: Tubulin alpha chain



• Molecule 54: Tubulin alpha chain



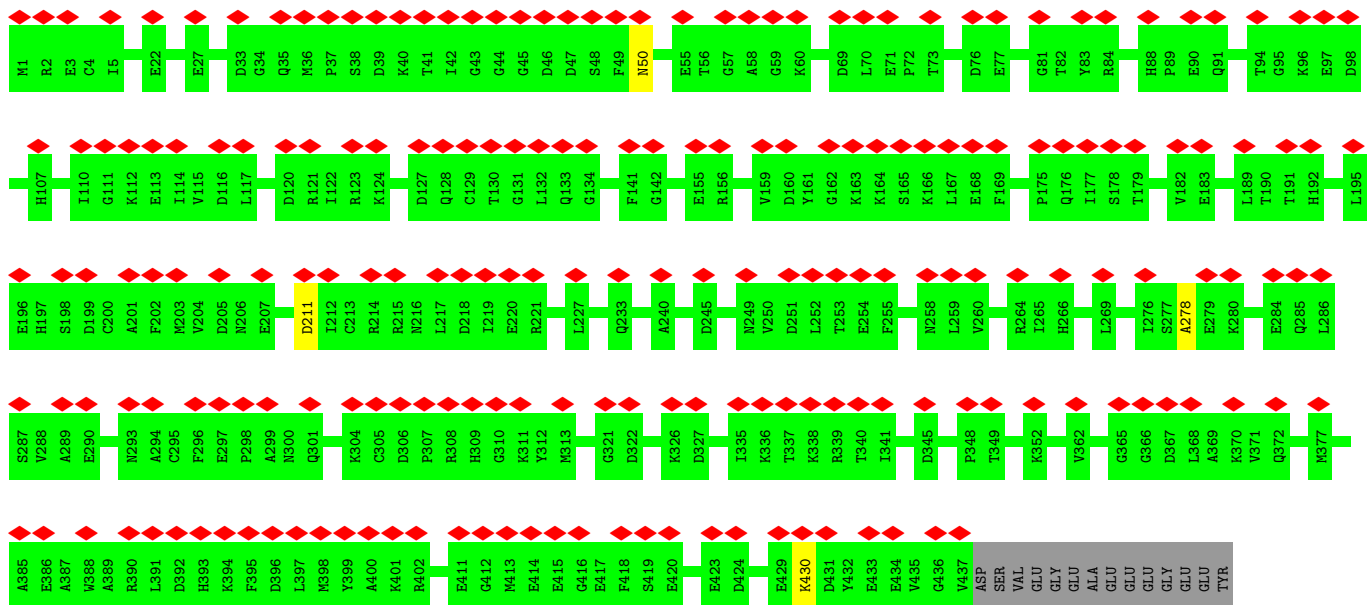
• Molecule 54: Tubulin alpha chain



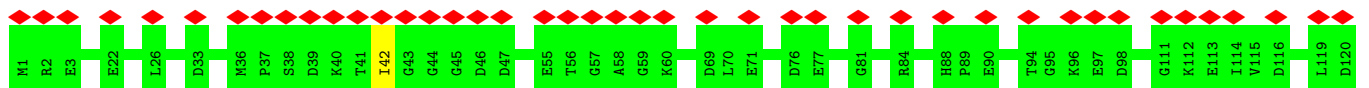


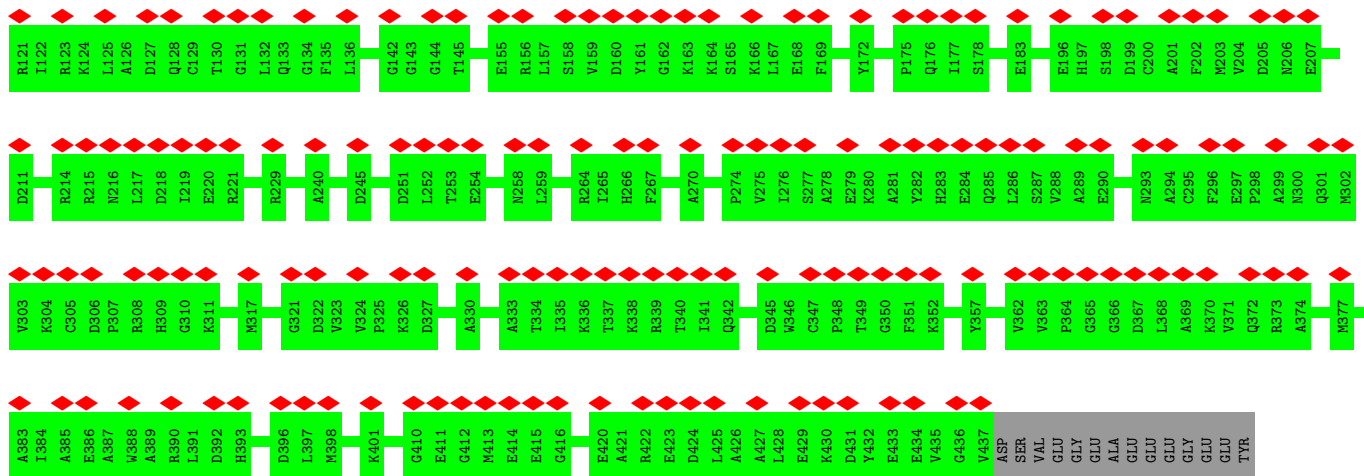


• Molecule 54: Tubulin alpha chain

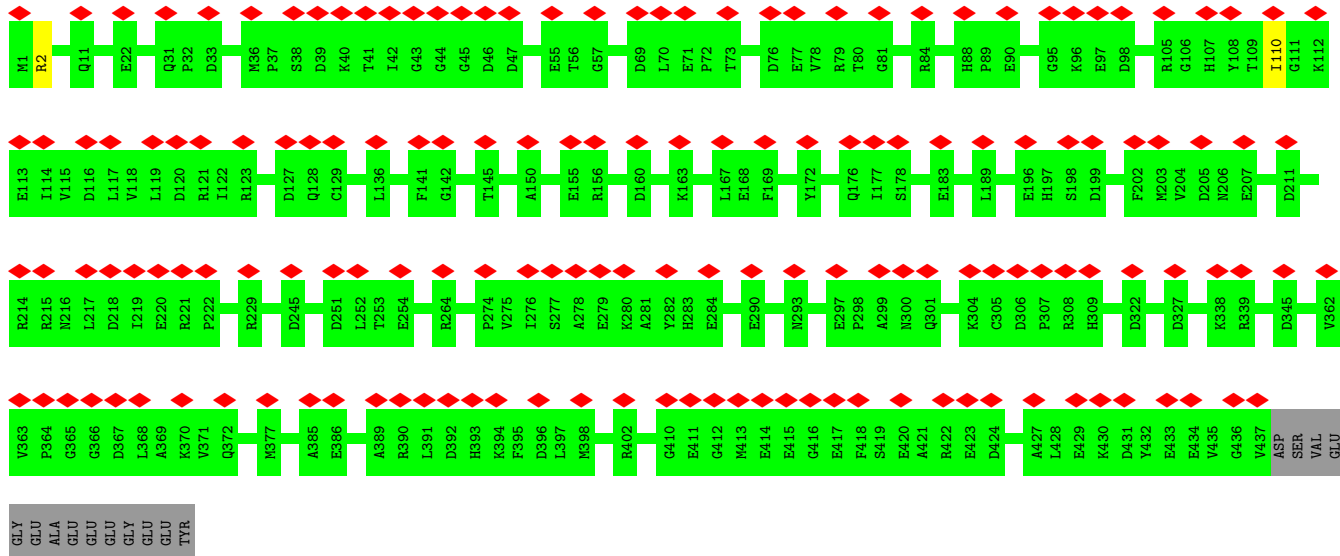


• Molecule 54: Tubulin alpha chain

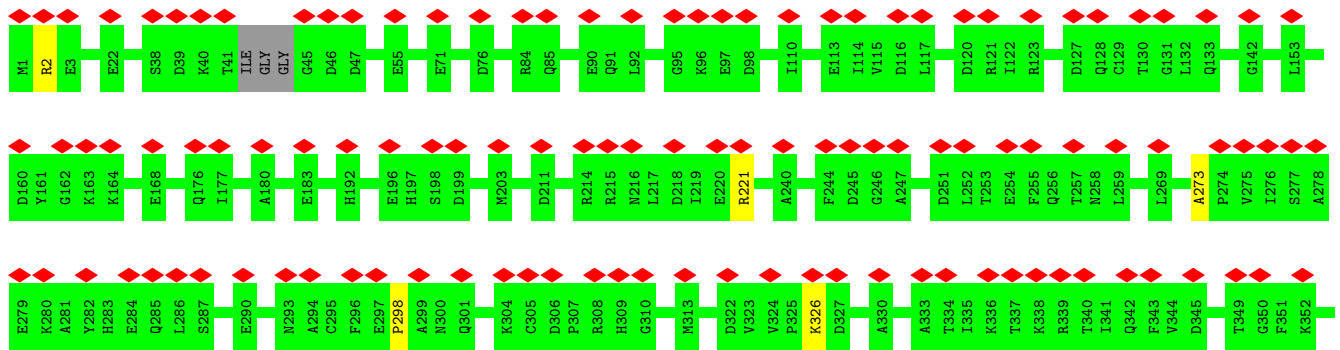


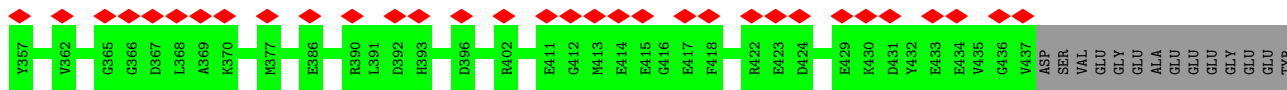


• Molecule 54: Tubulin alpha chain

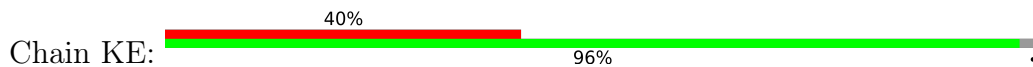


• Molecule 54: Tubulin alpha chain

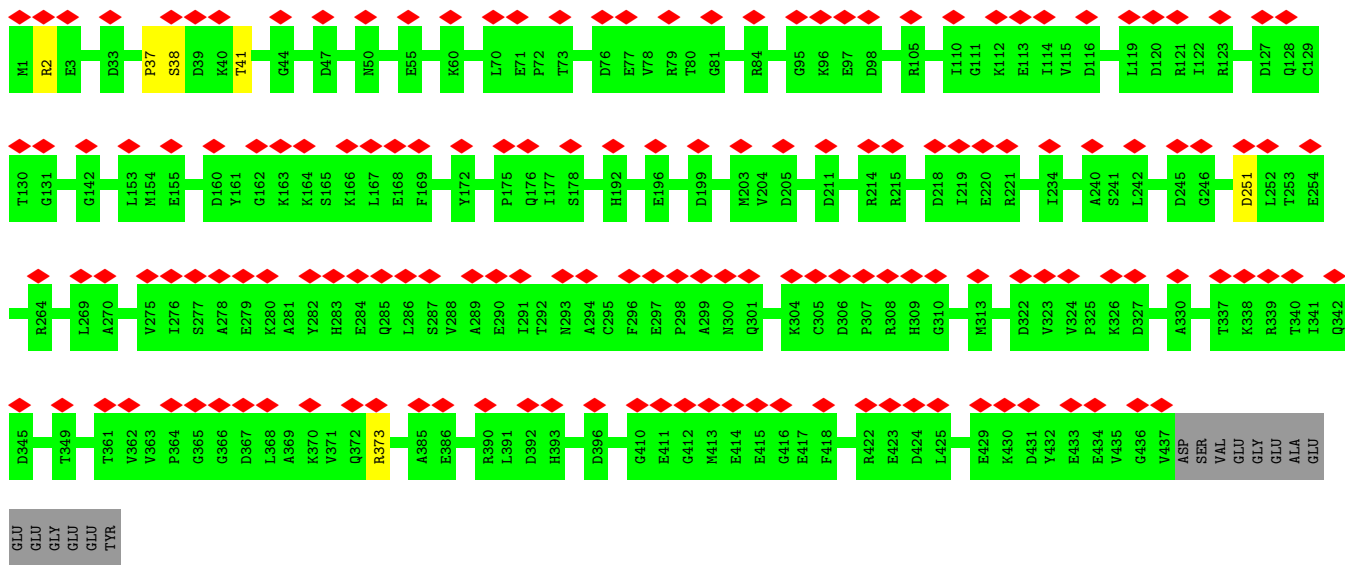




• Molecule 54: Tubulin alpha chain

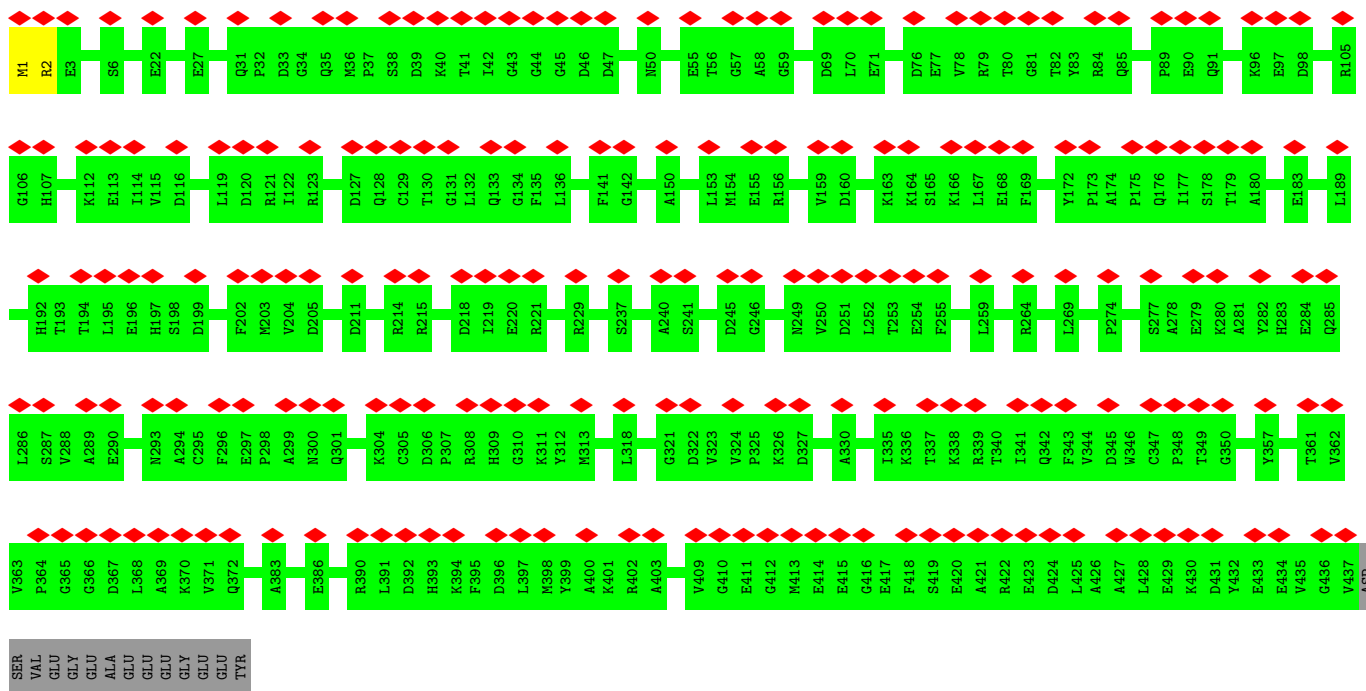


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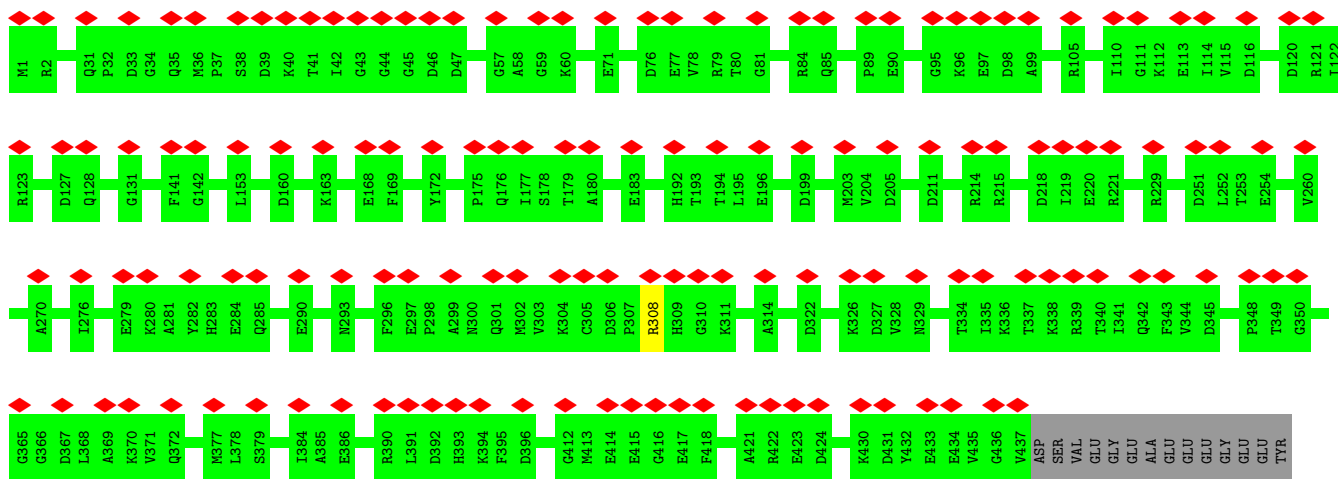


• Molecule 54: Tubulin alpha chain

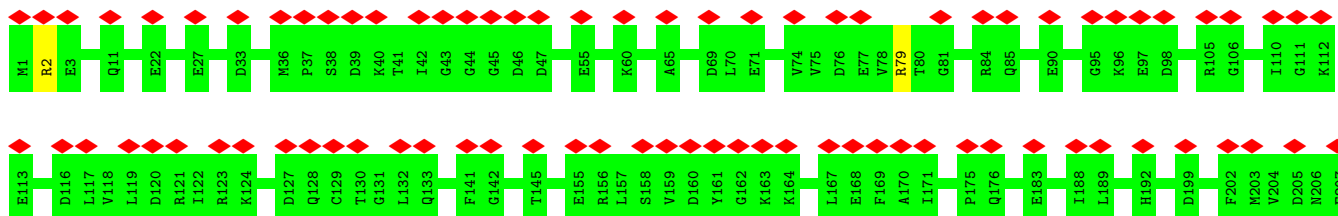


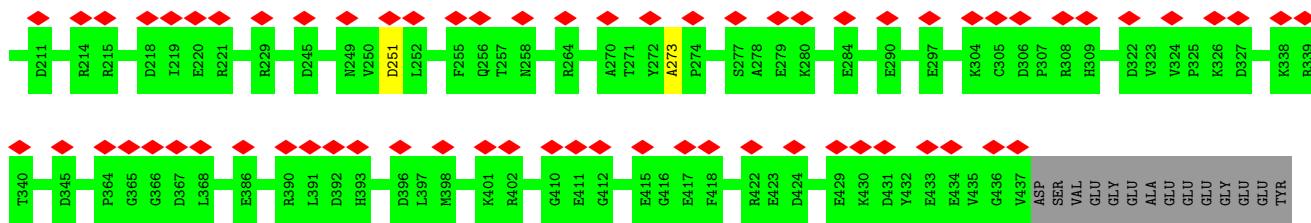


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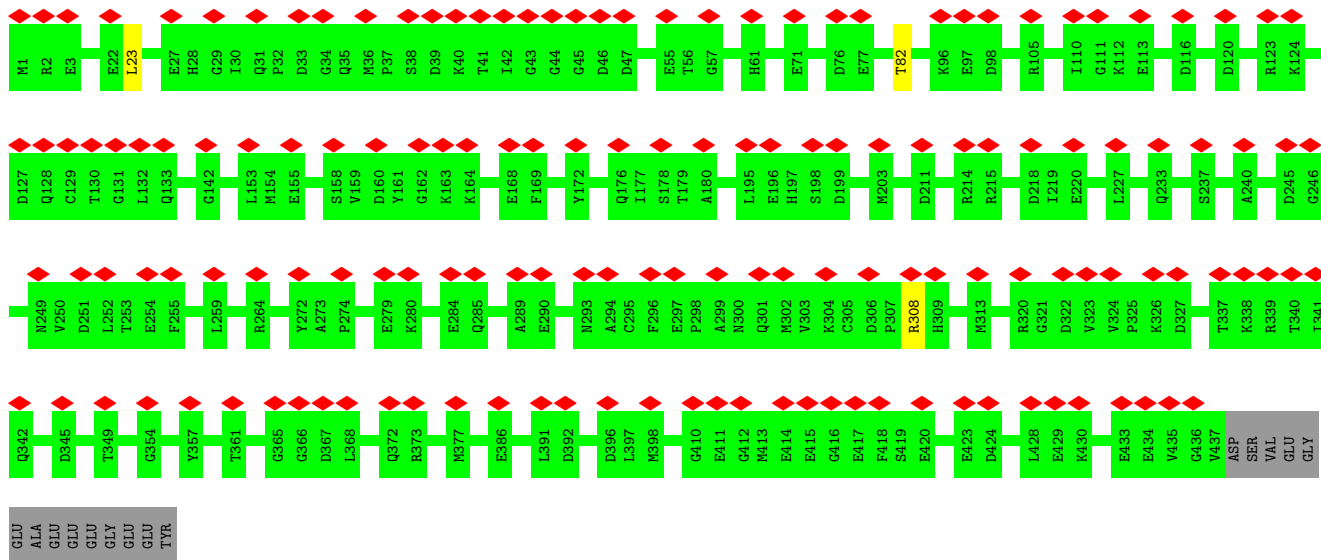


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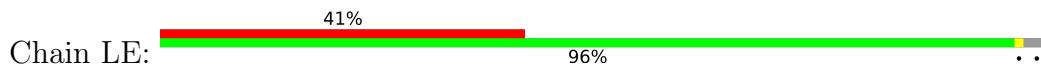




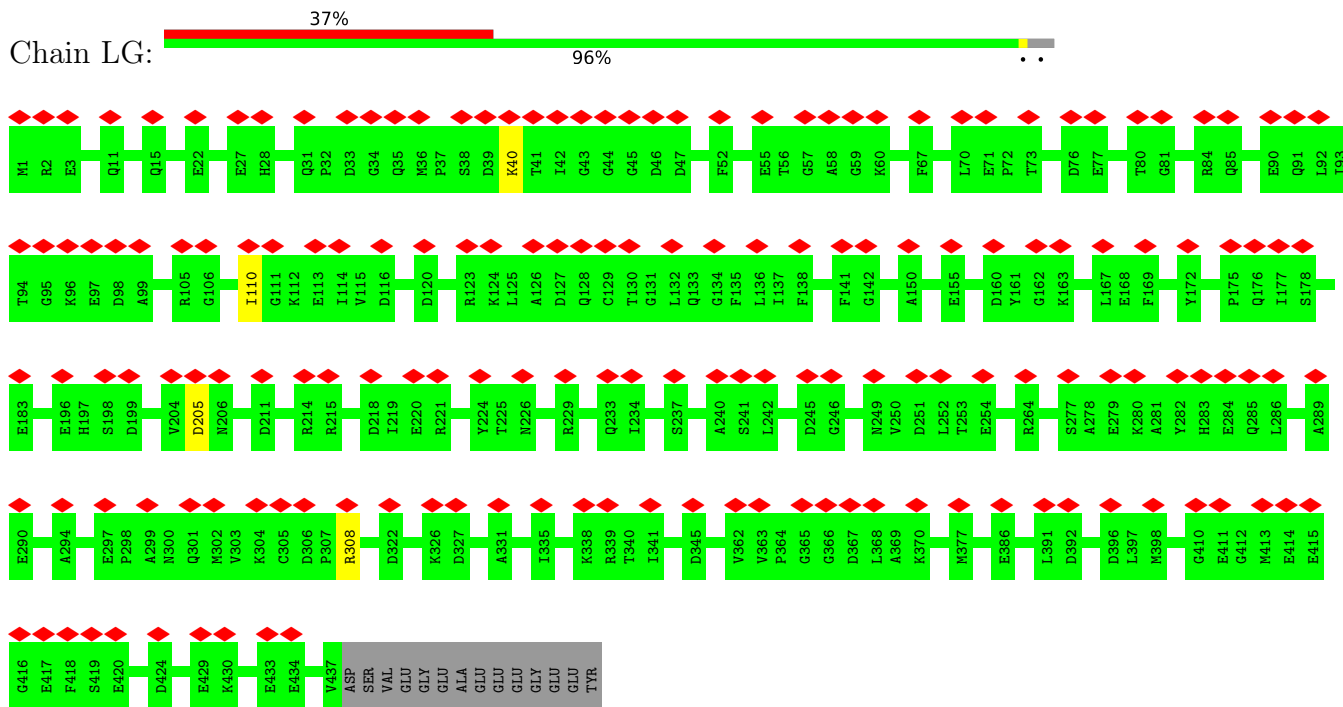
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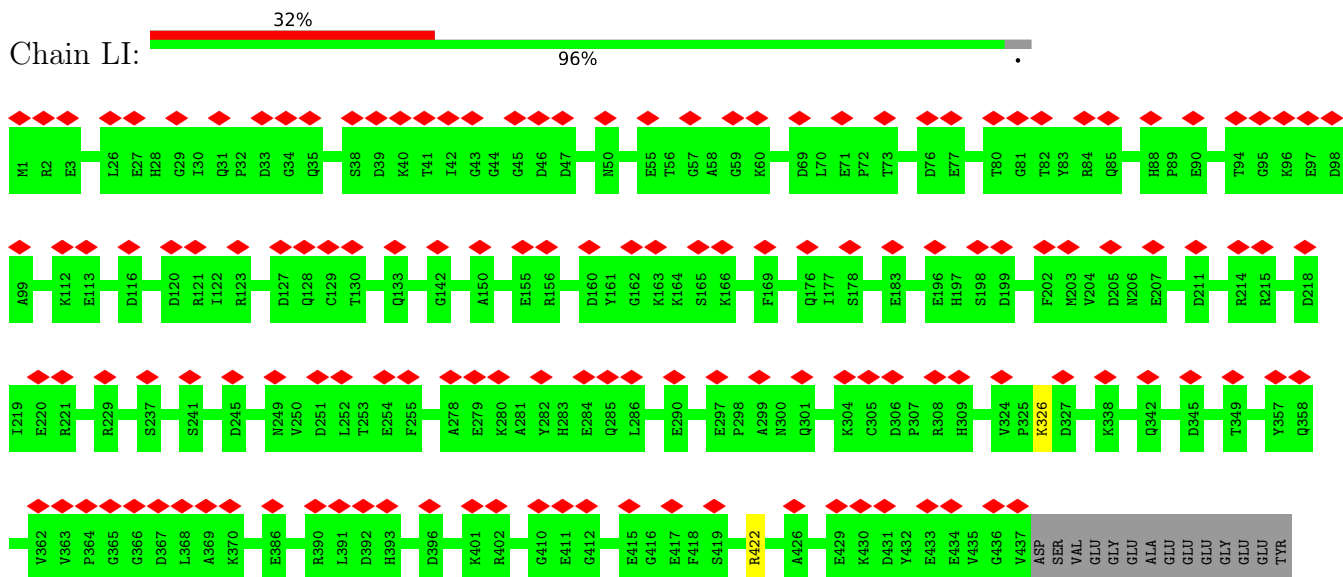
• Molecule 54: Tubulin alpha chain



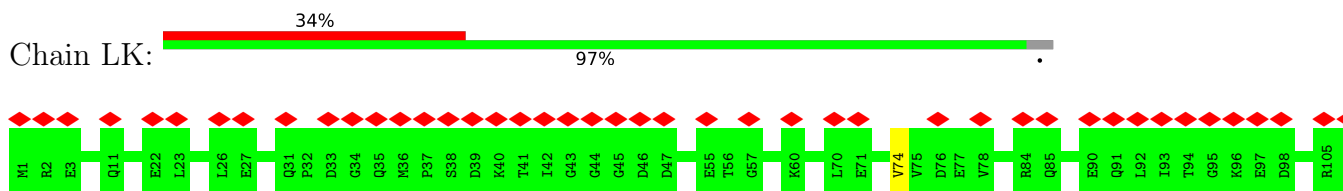
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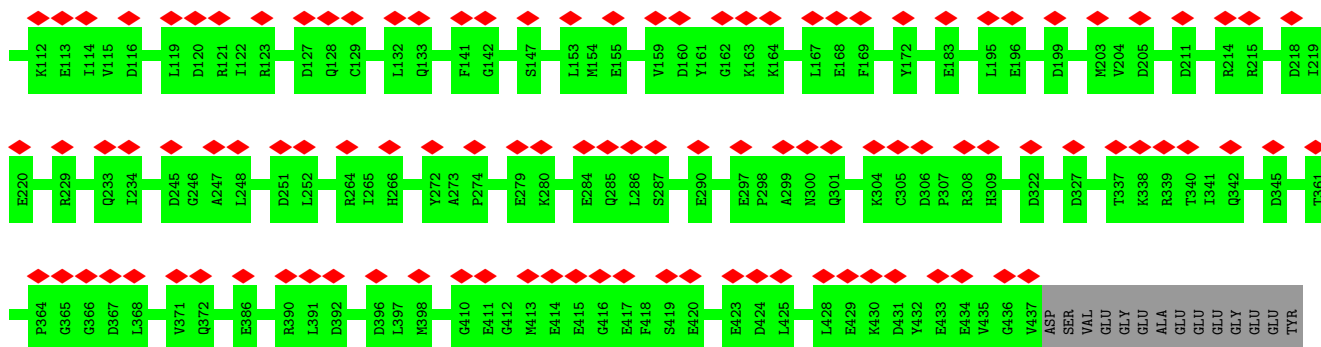


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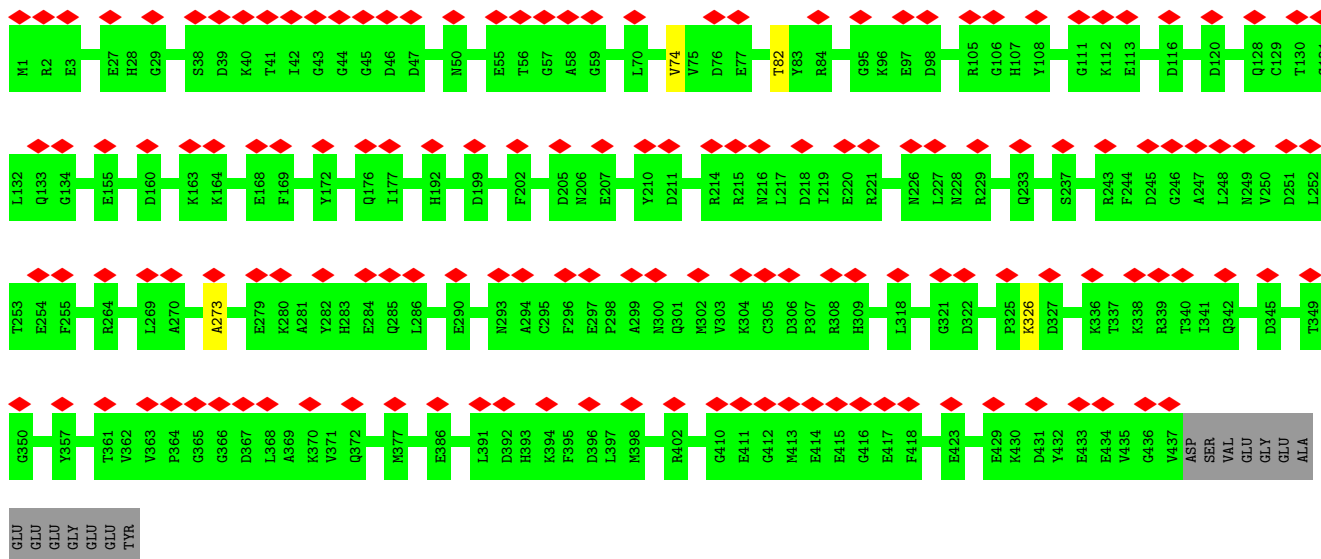


• Molecule 54: Tubulin alpha chain

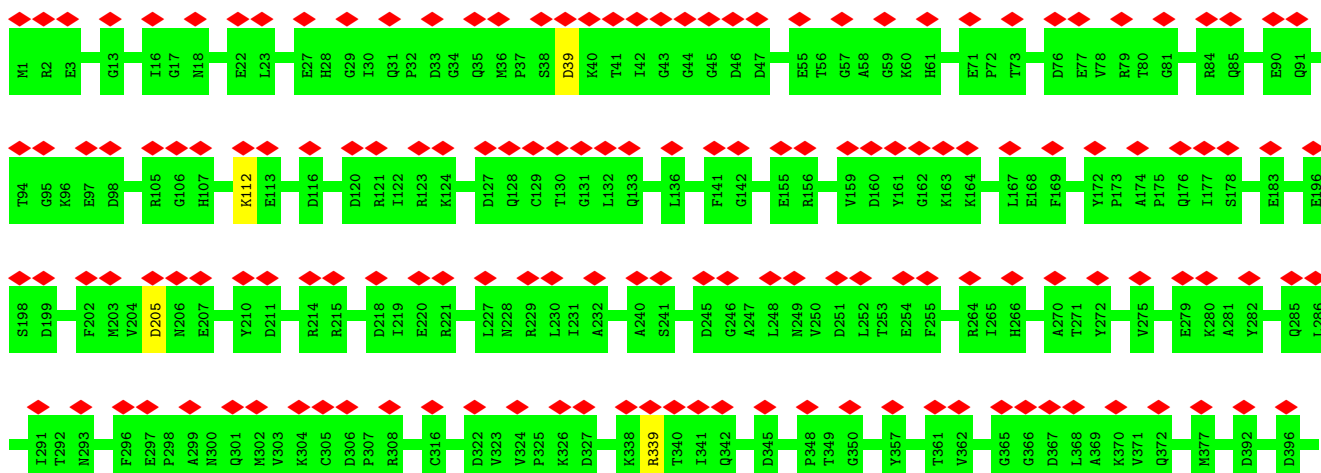
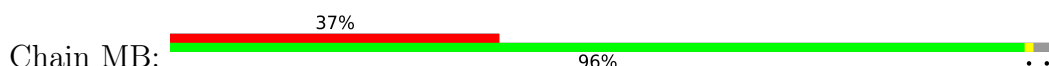


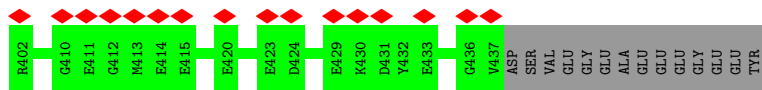


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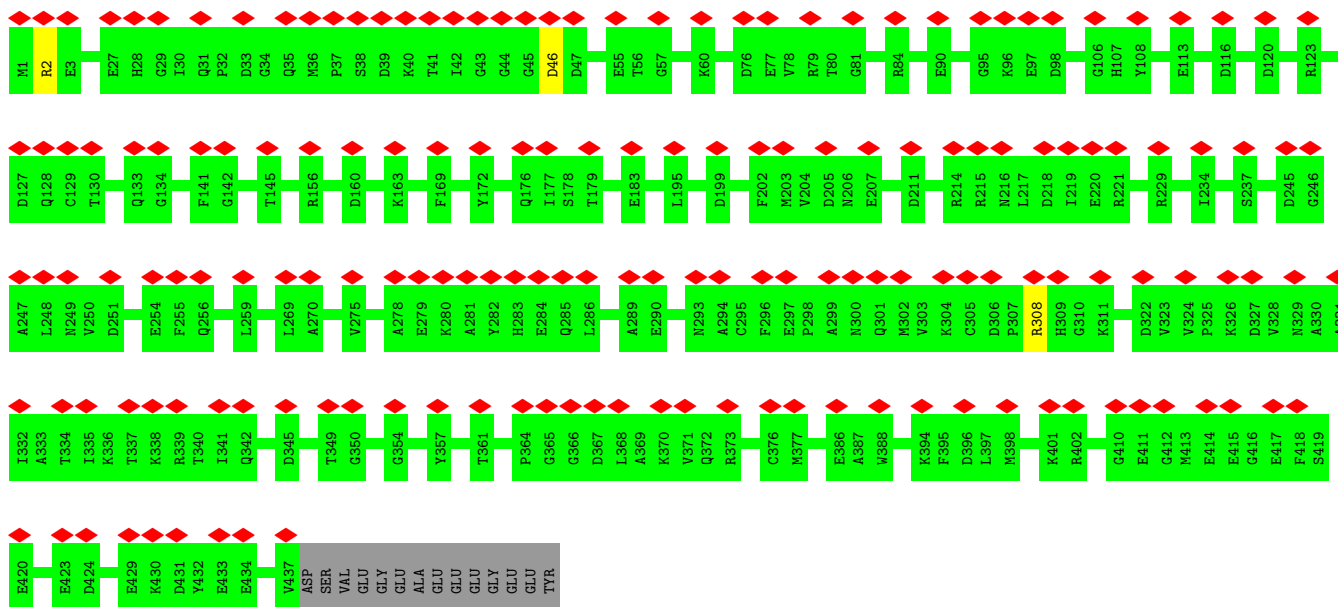
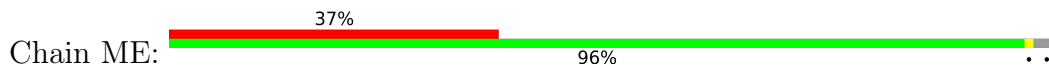


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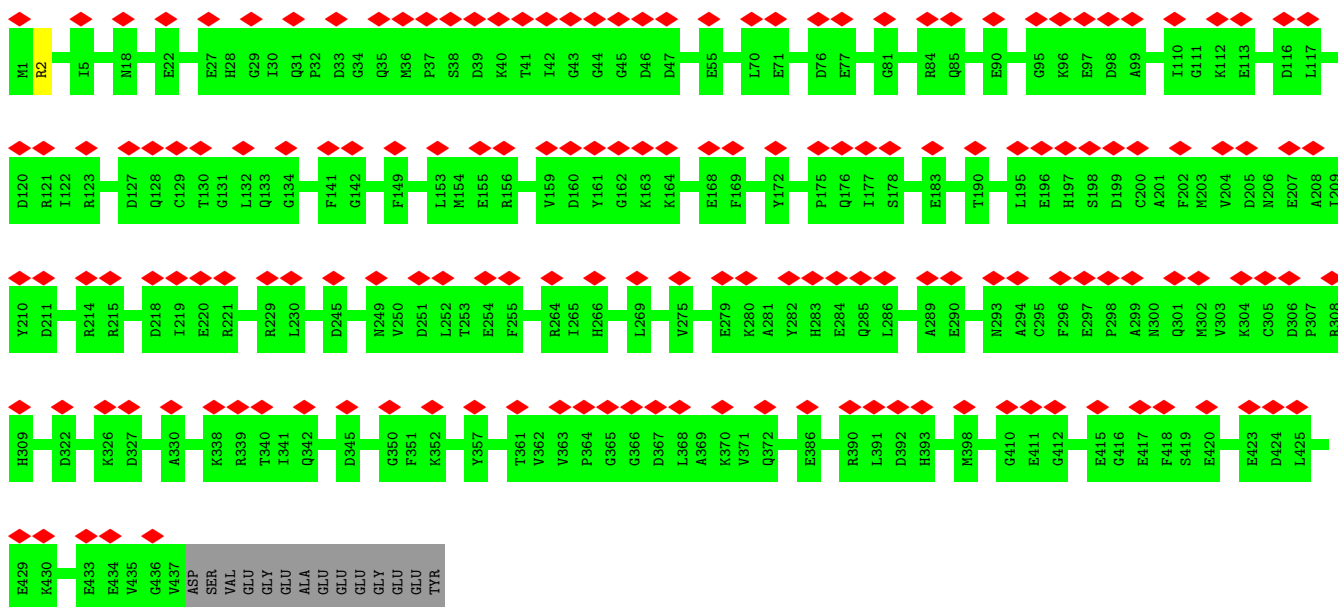
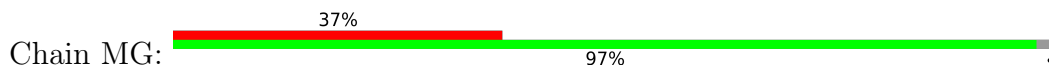




• Molecule 54: Tubulin alpha chain

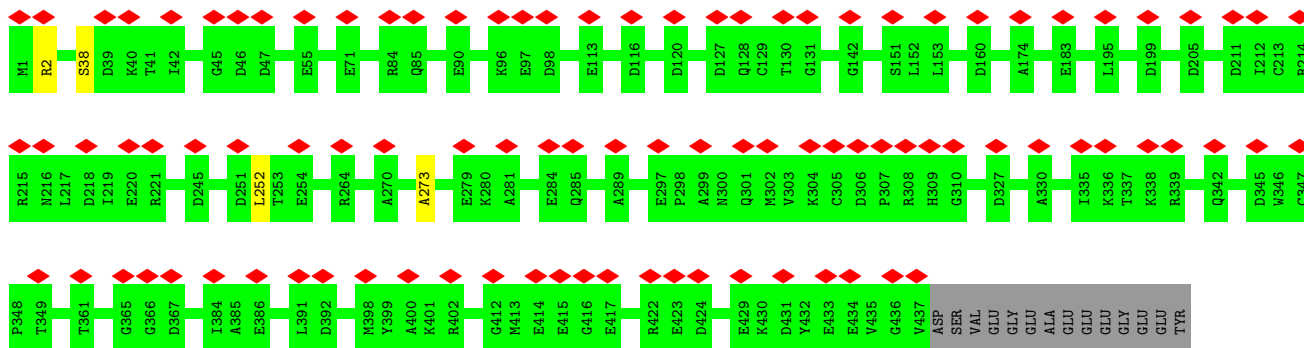


• Molecule 54: Tubulin alpha chain

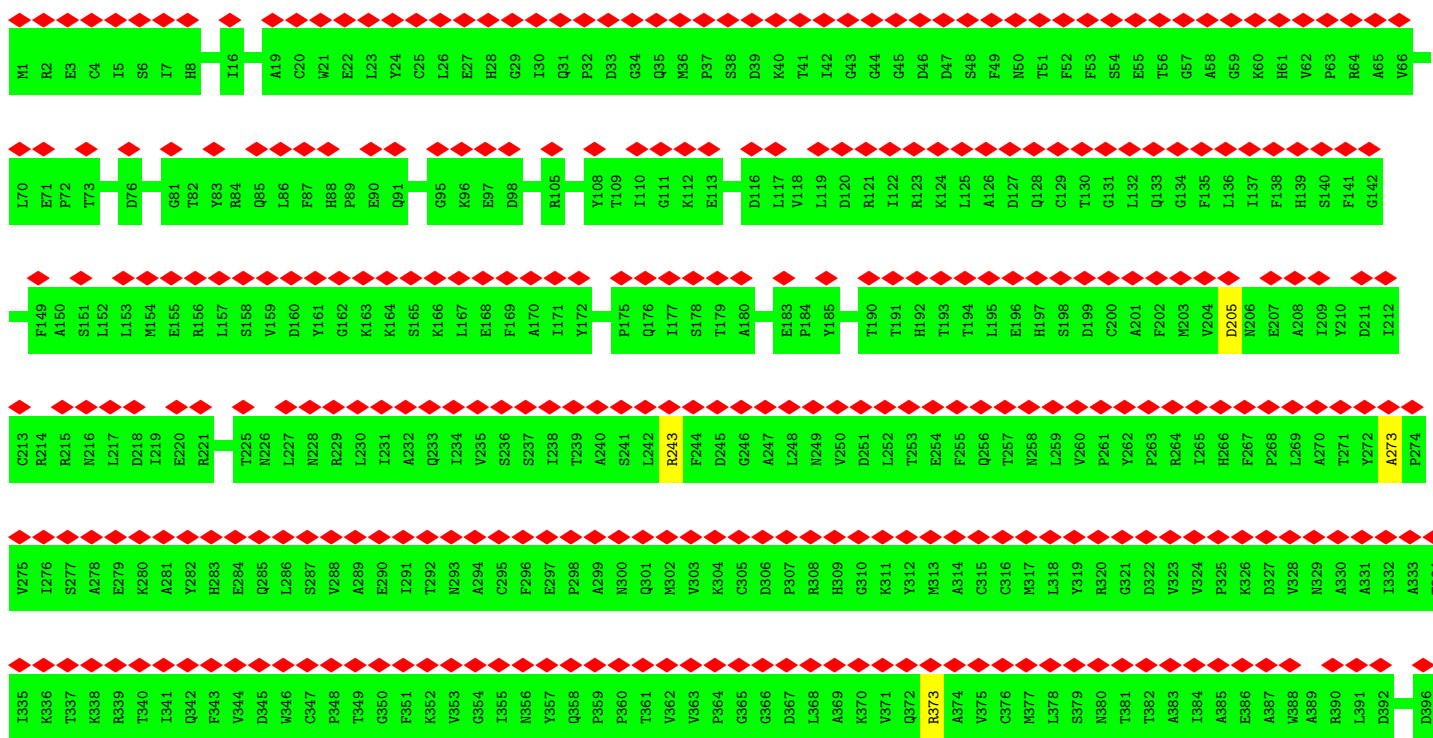
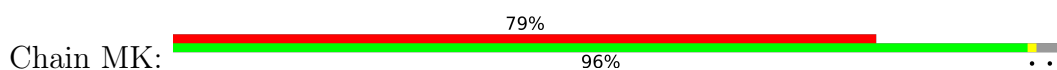


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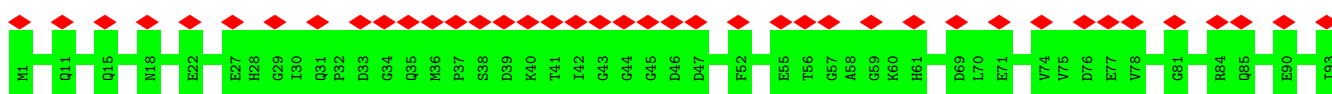


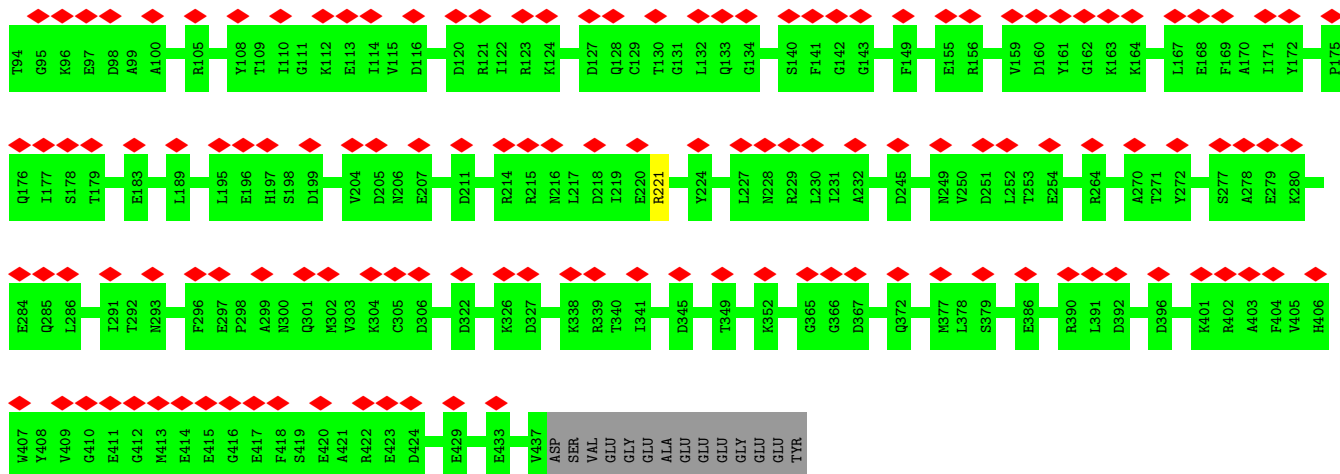


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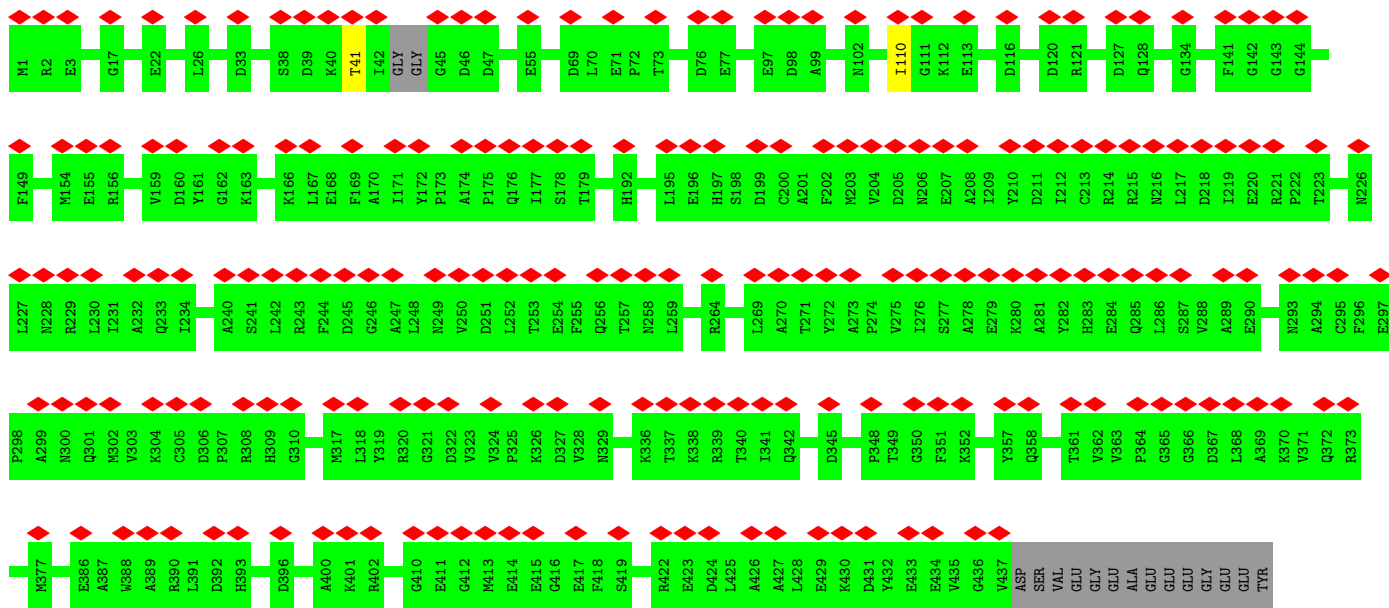


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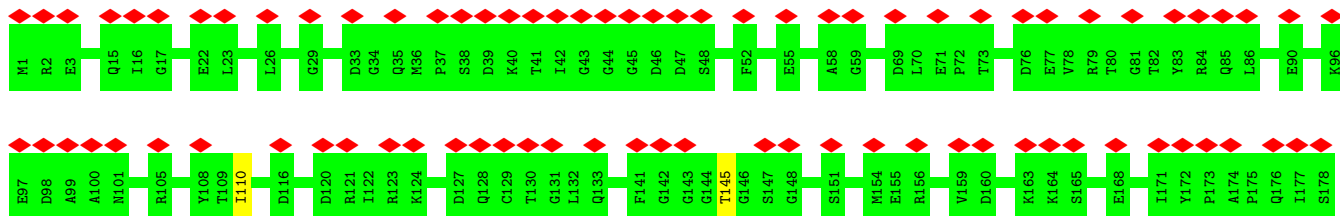


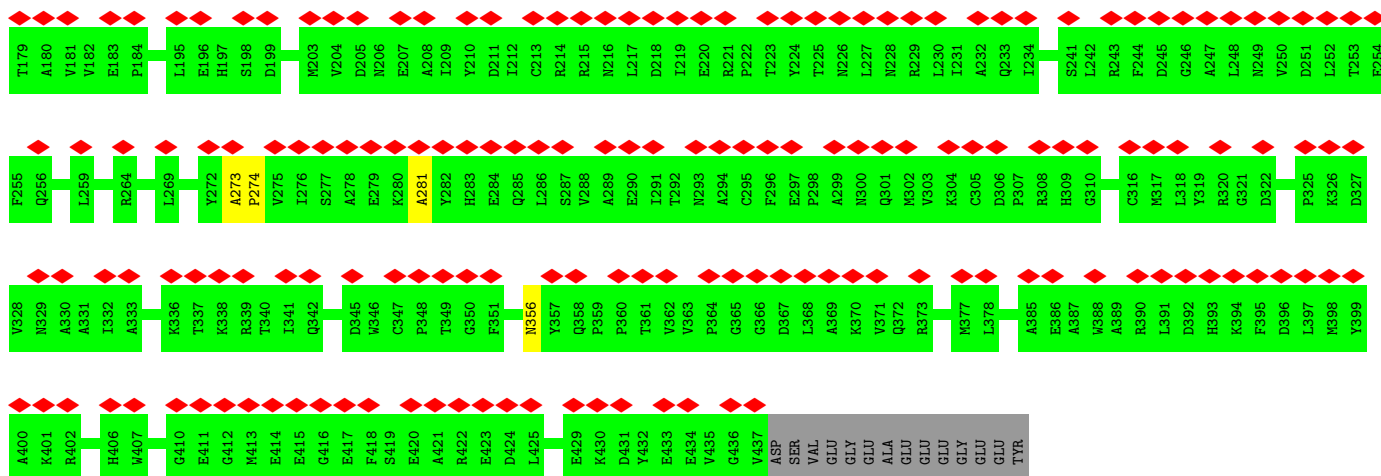


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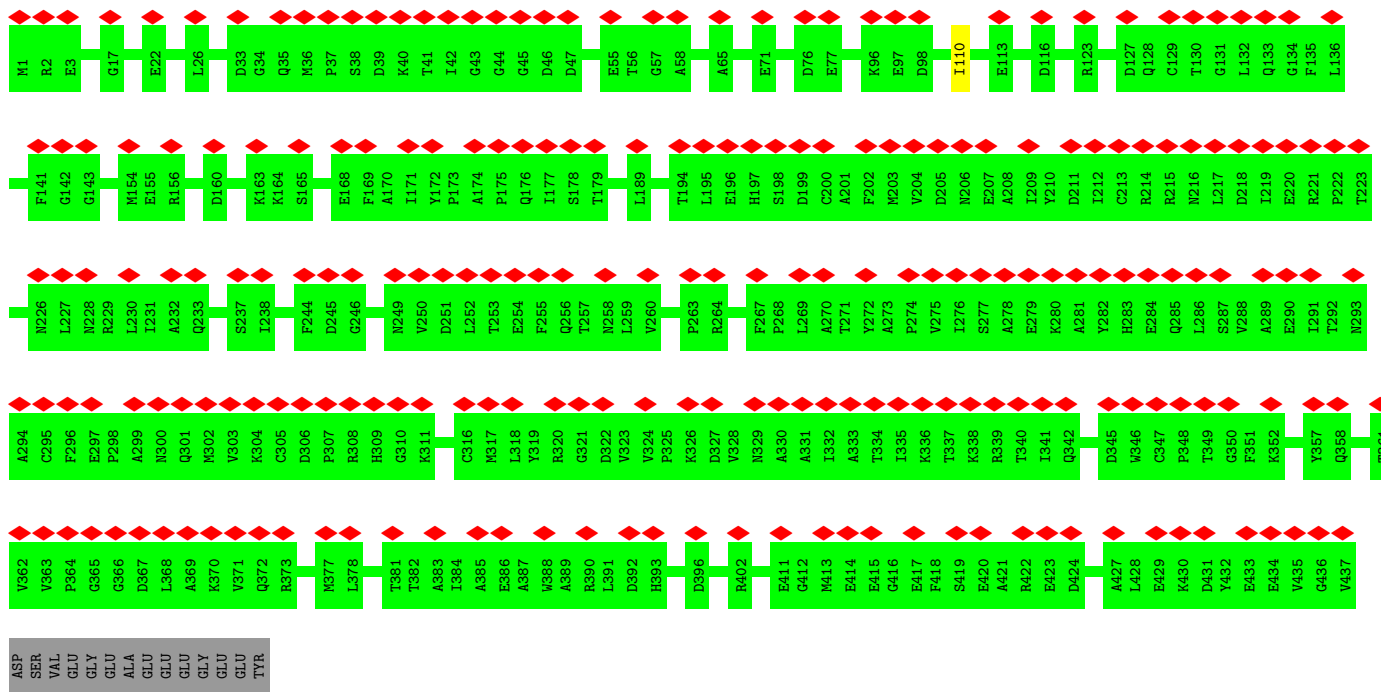


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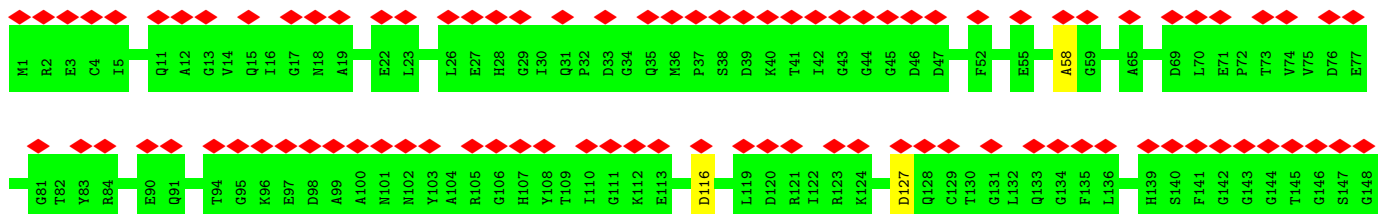
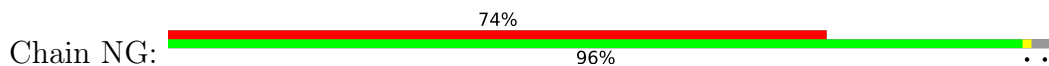




• Molecule 54: Tubulin alpha chain



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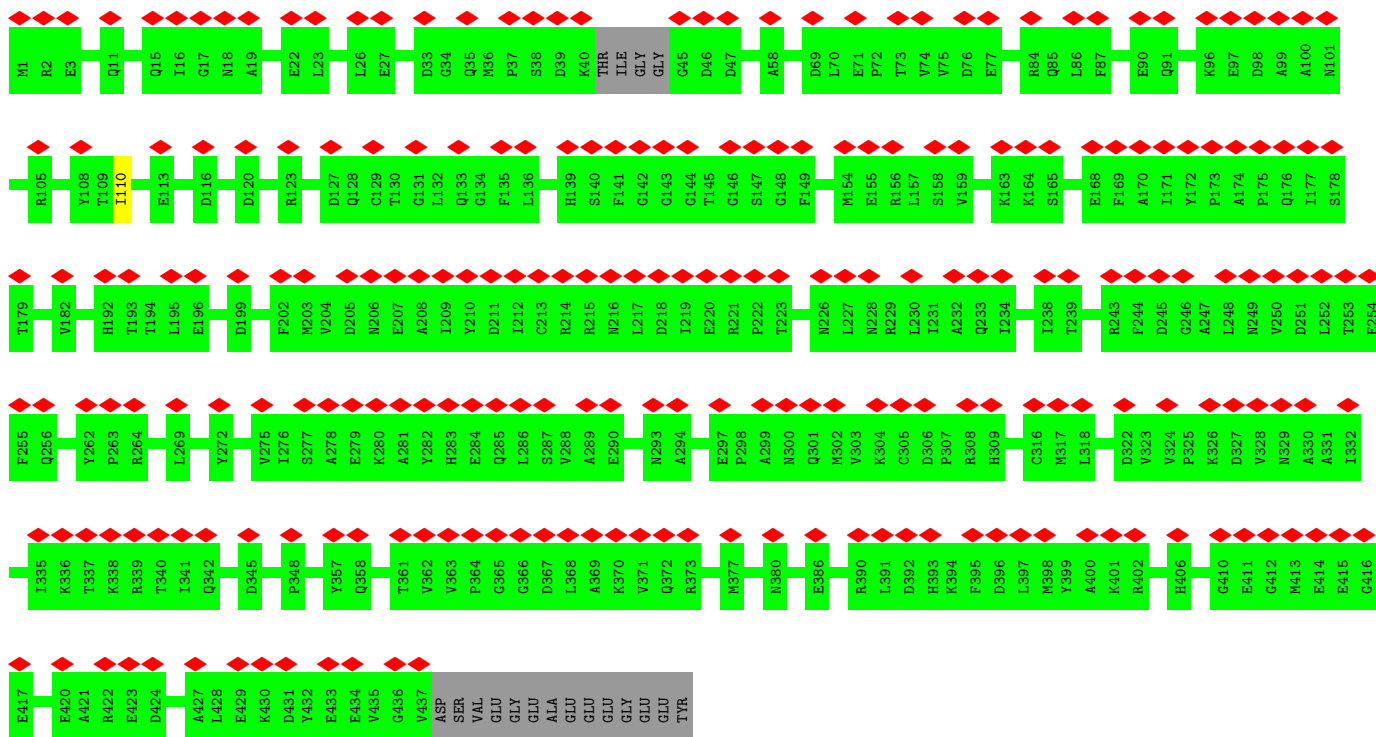


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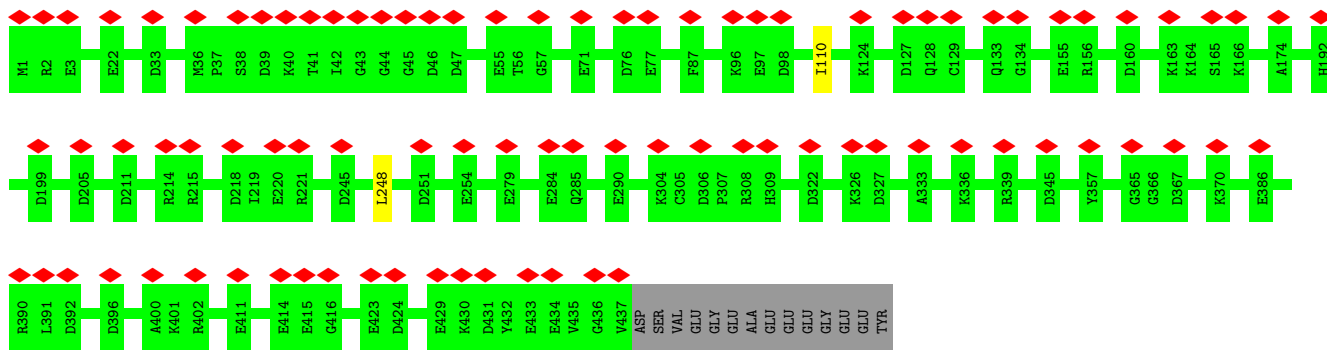


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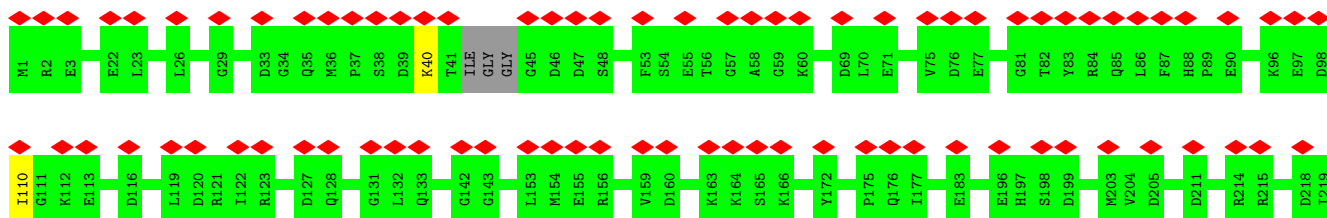


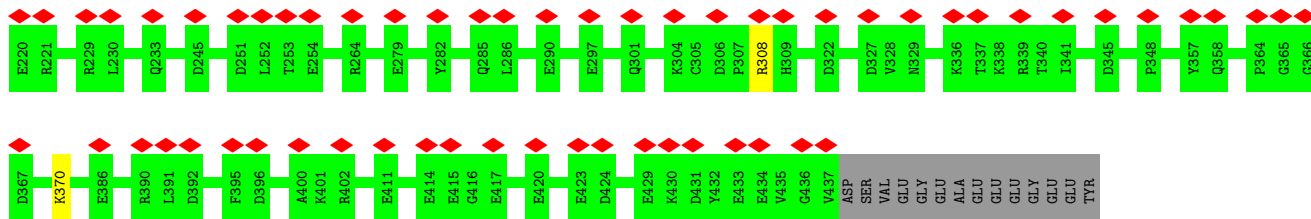


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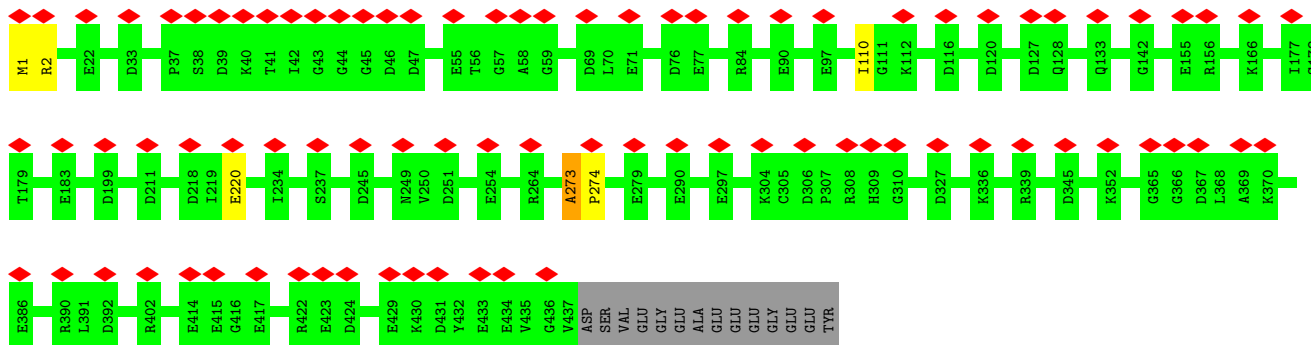


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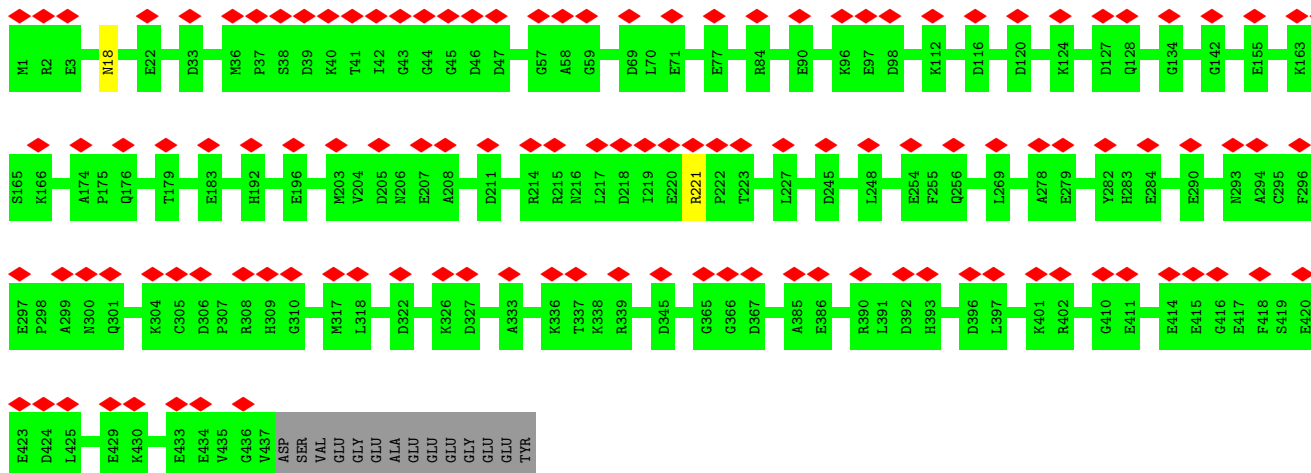




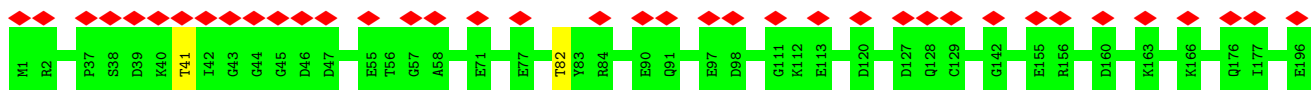
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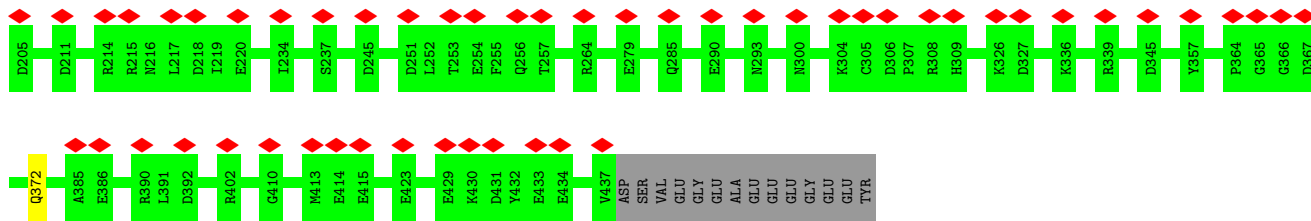


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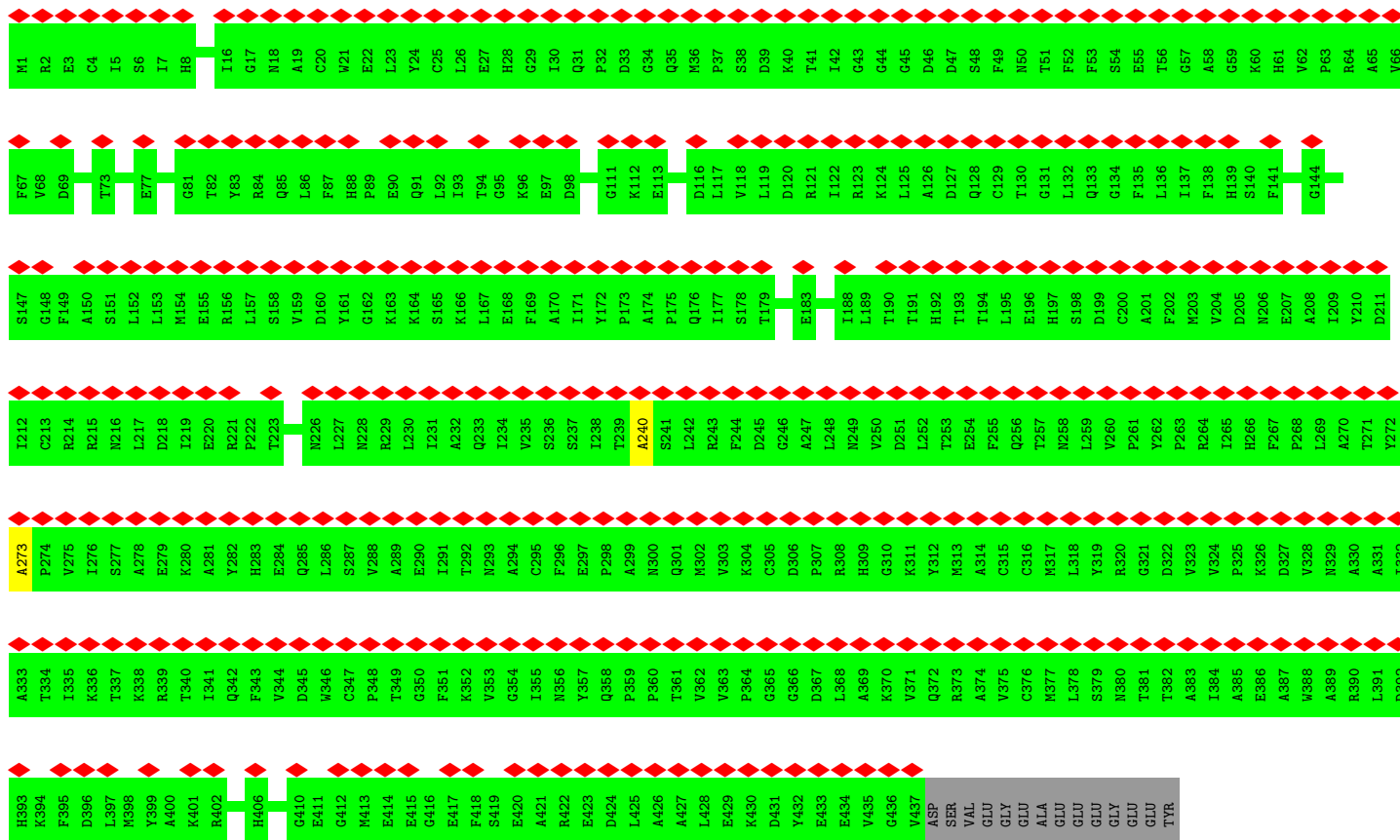
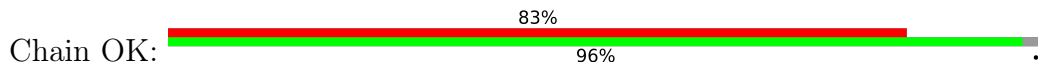


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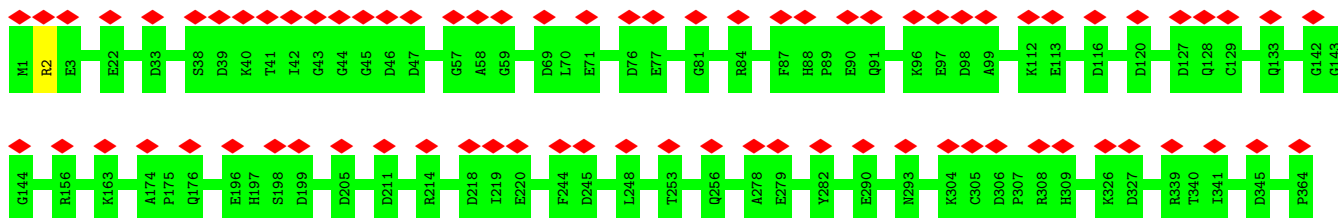


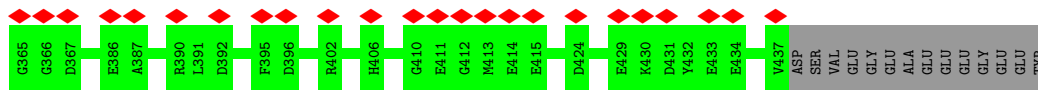


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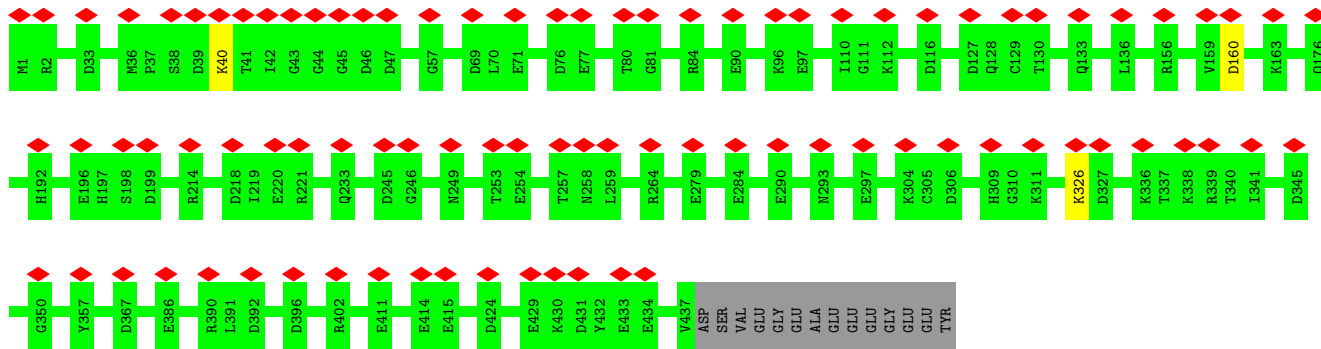


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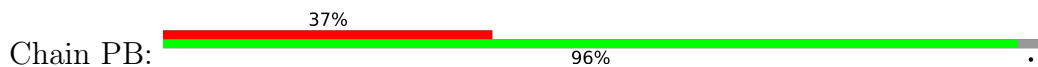




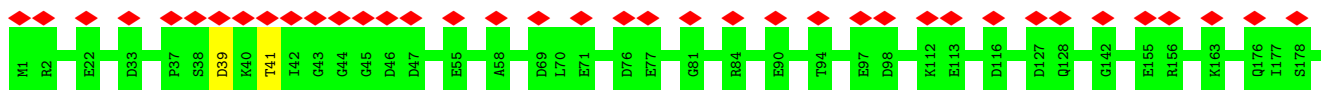
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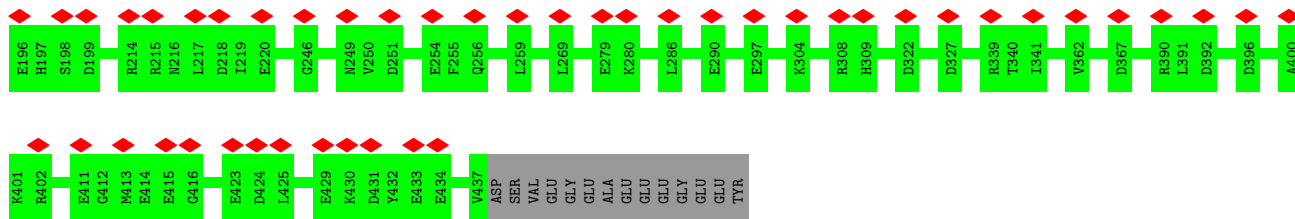
• Molecule 54: Tubulin alpha chain



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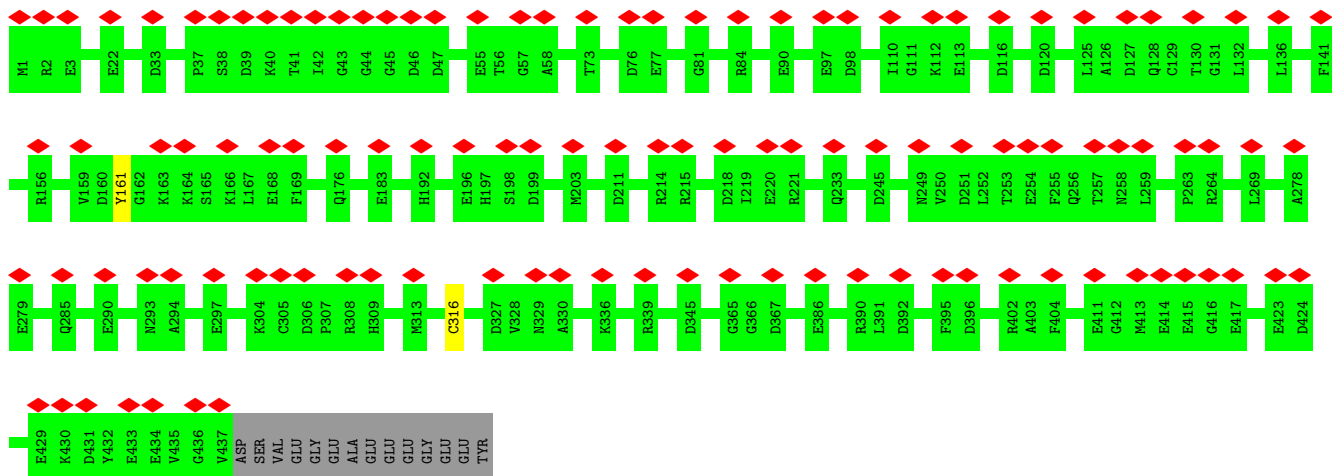




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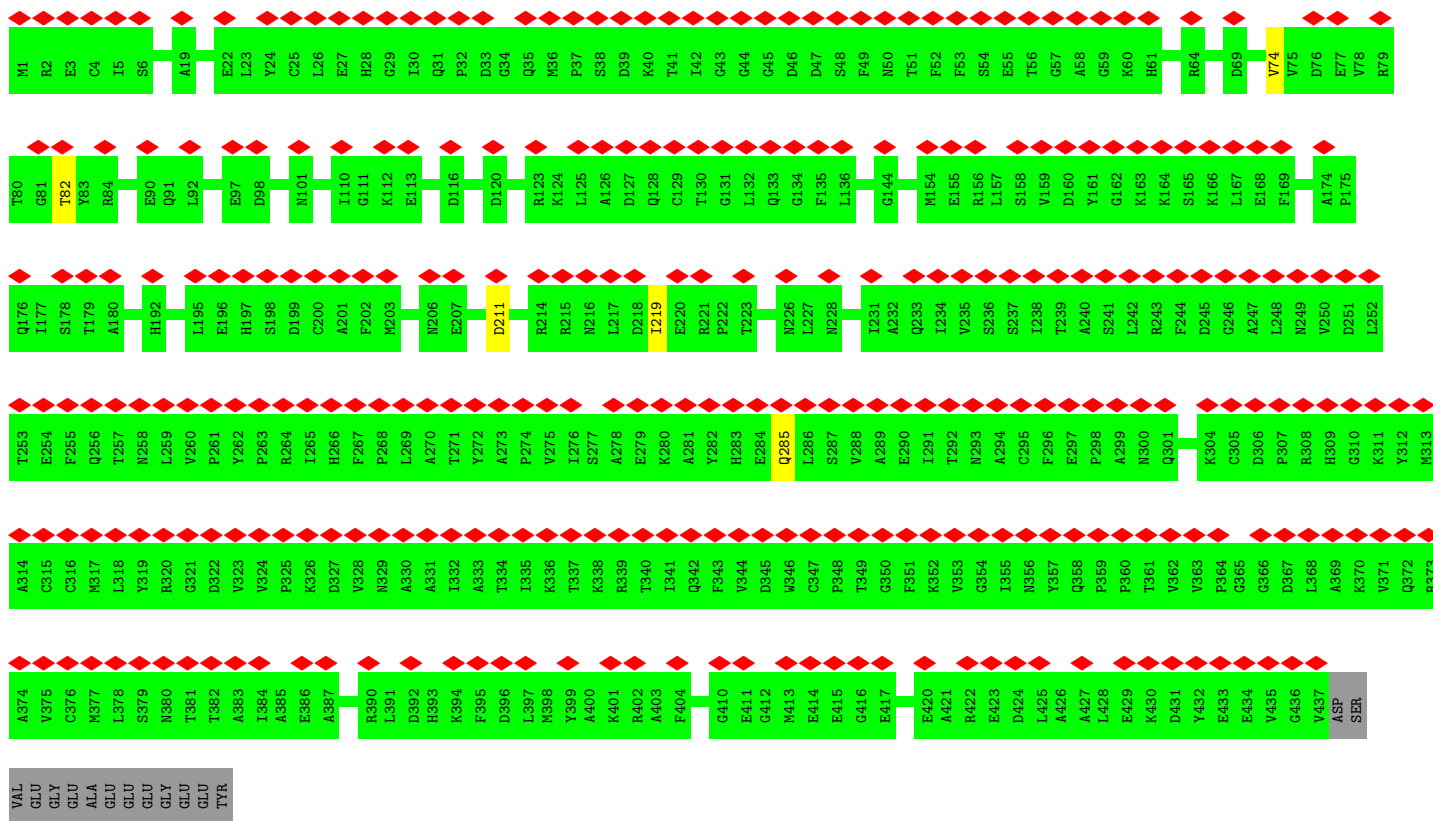


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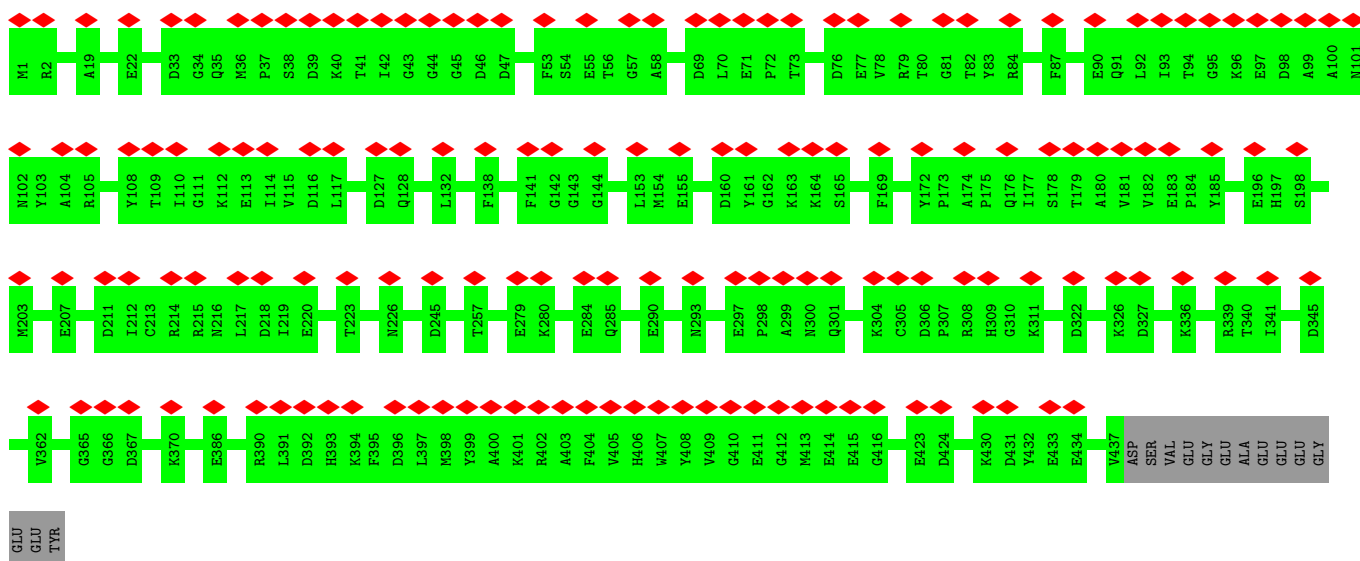


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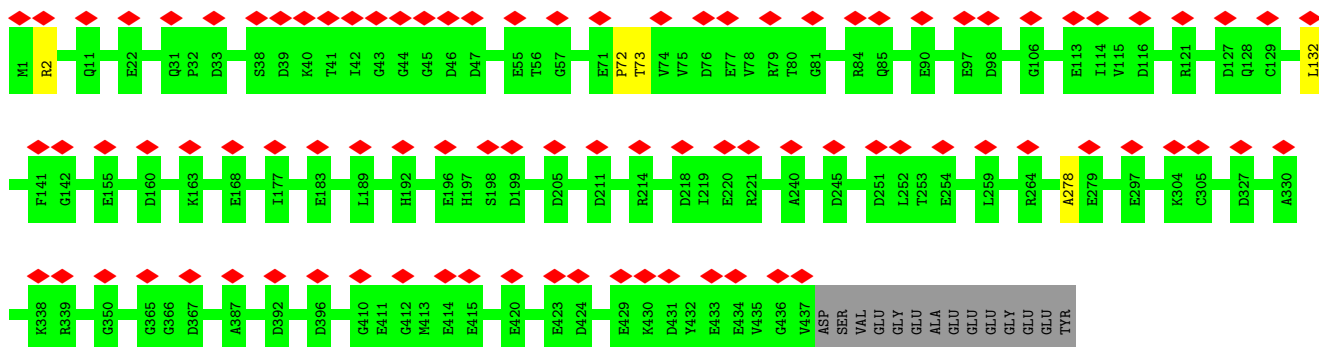


• Molecule 54: Tubulin alpha chain

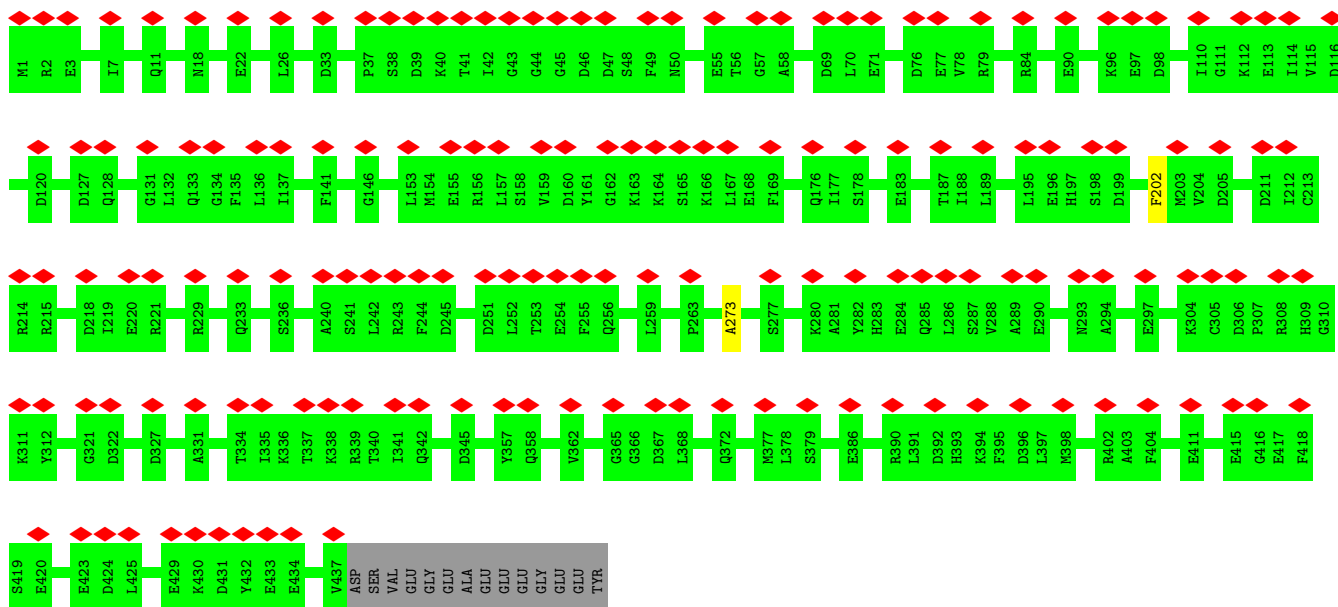
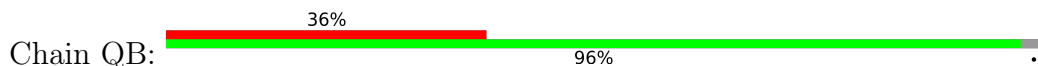


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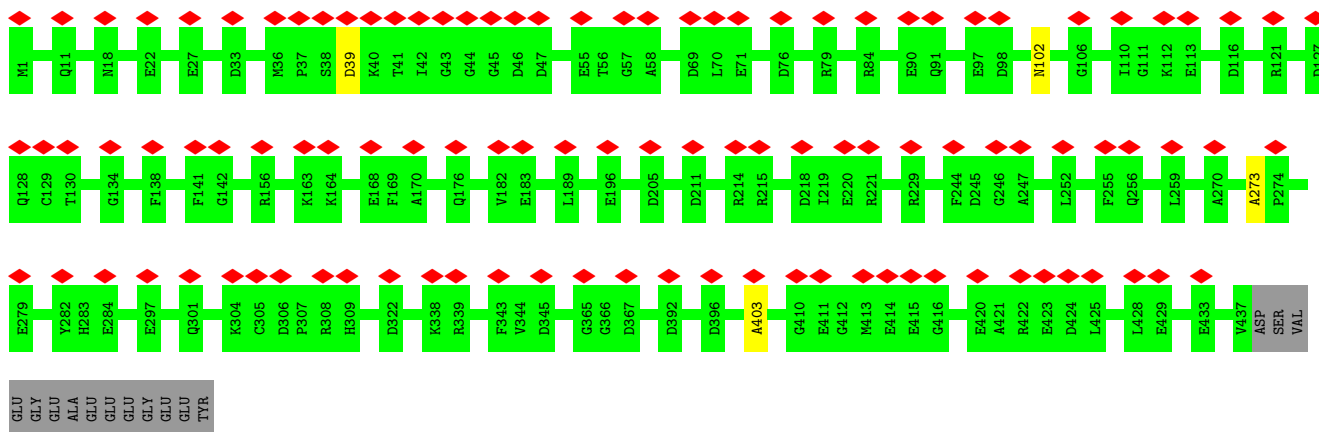




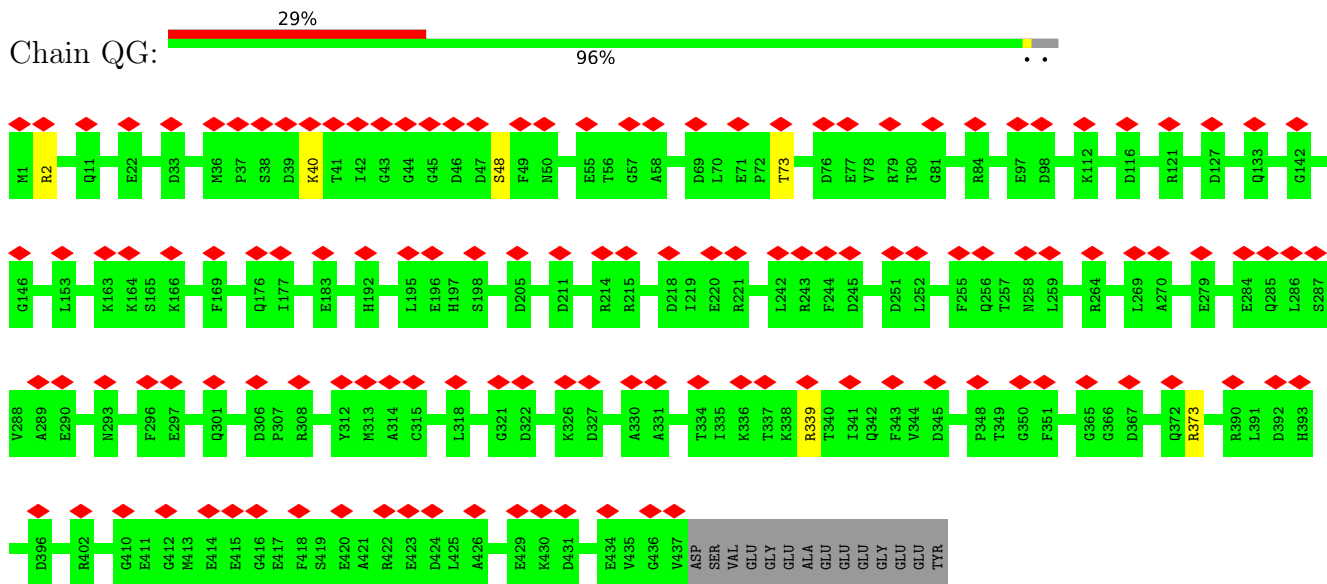
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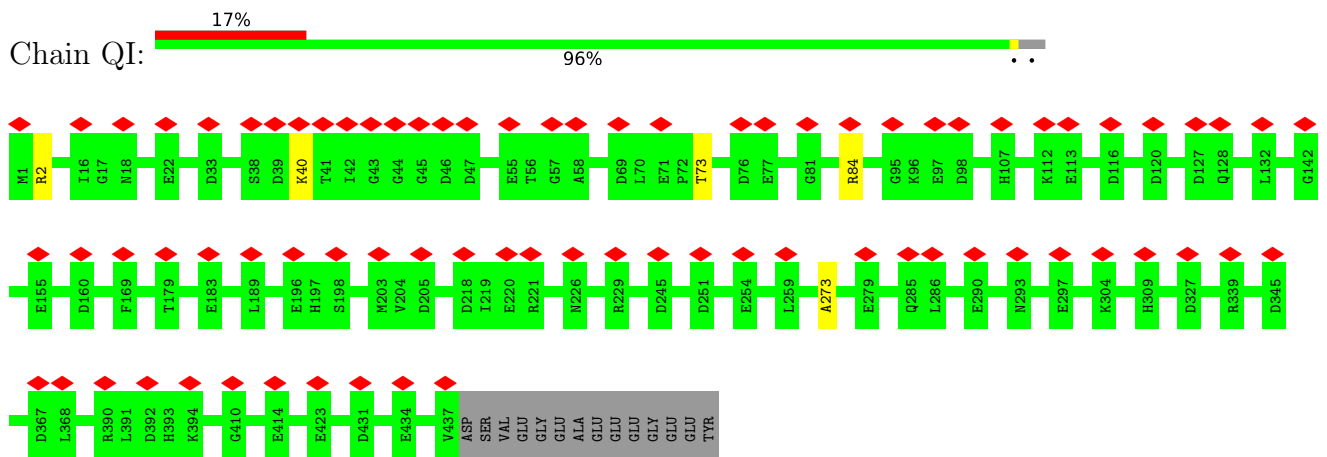
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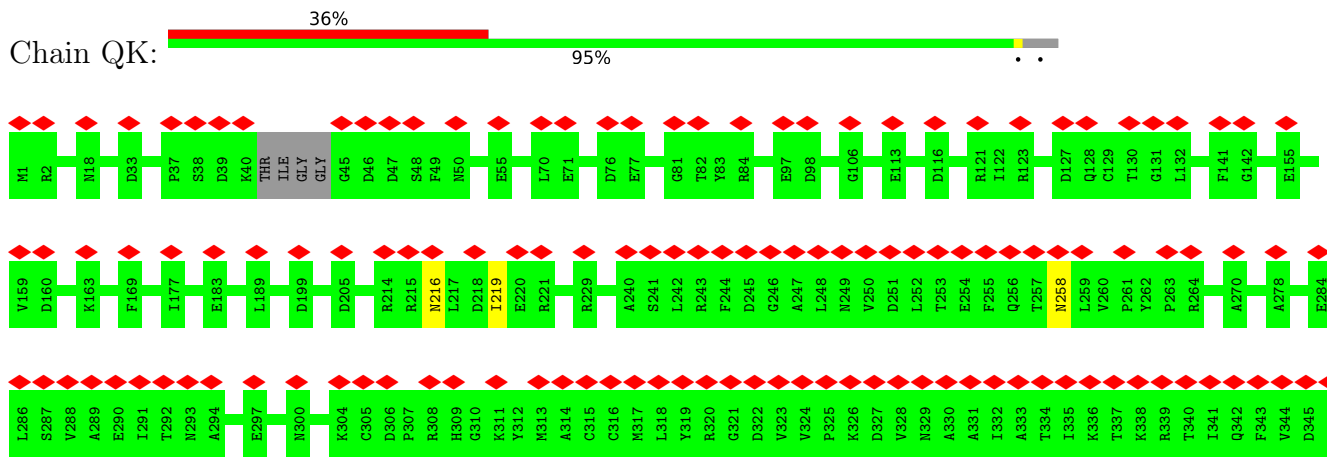
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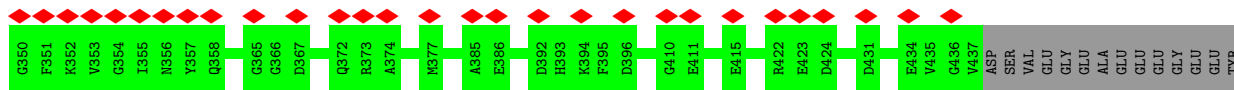


• Molecule 54: Tubulin alpha chain

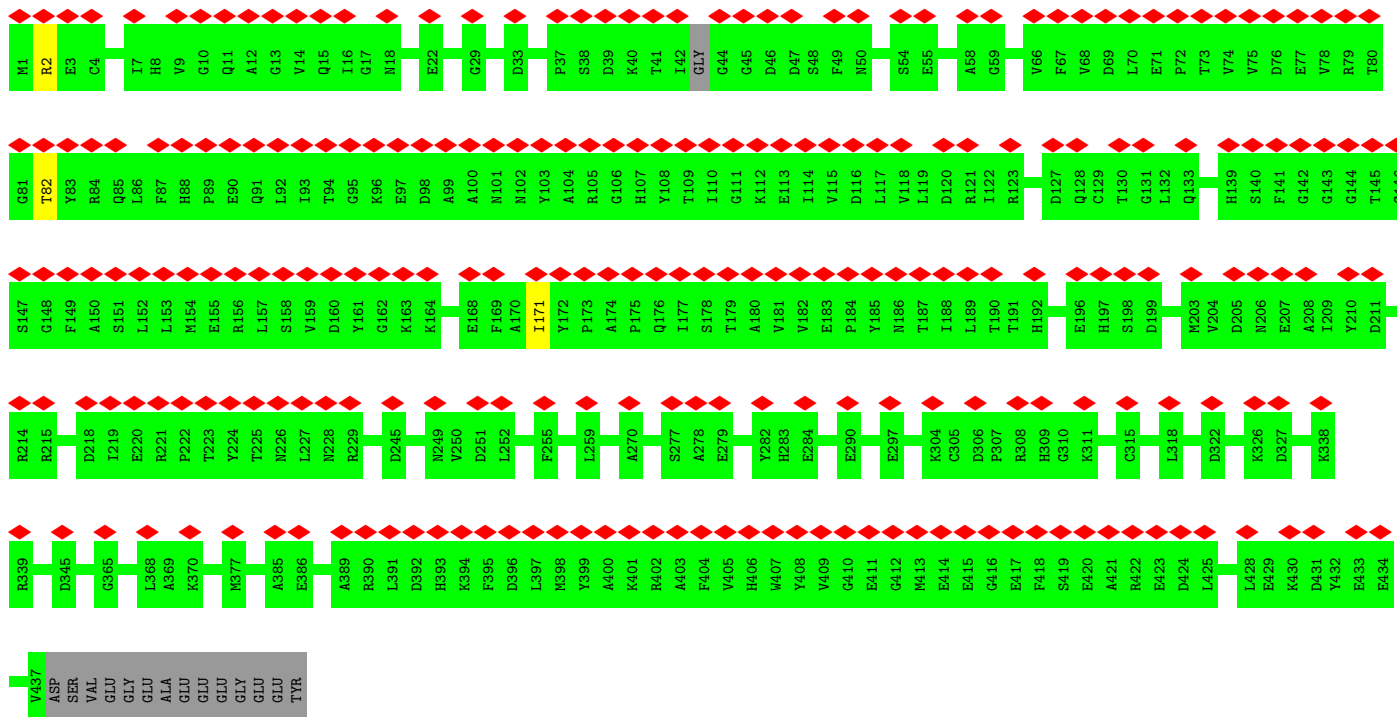


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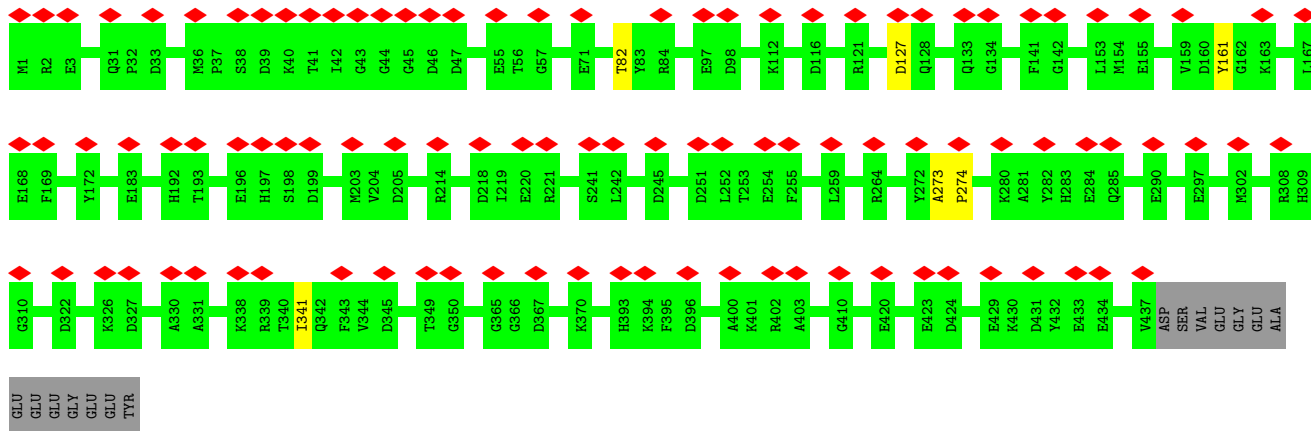




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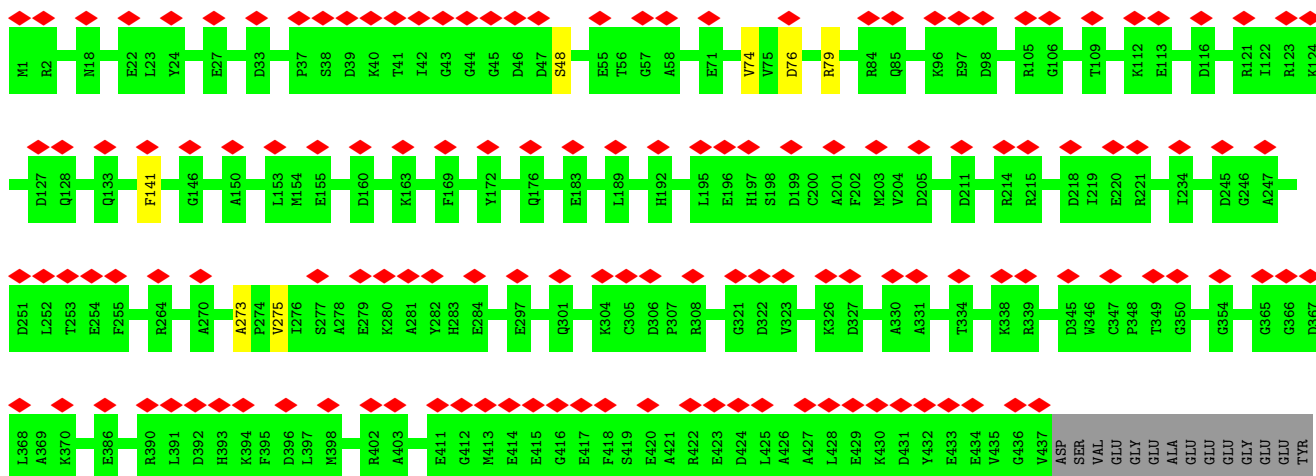


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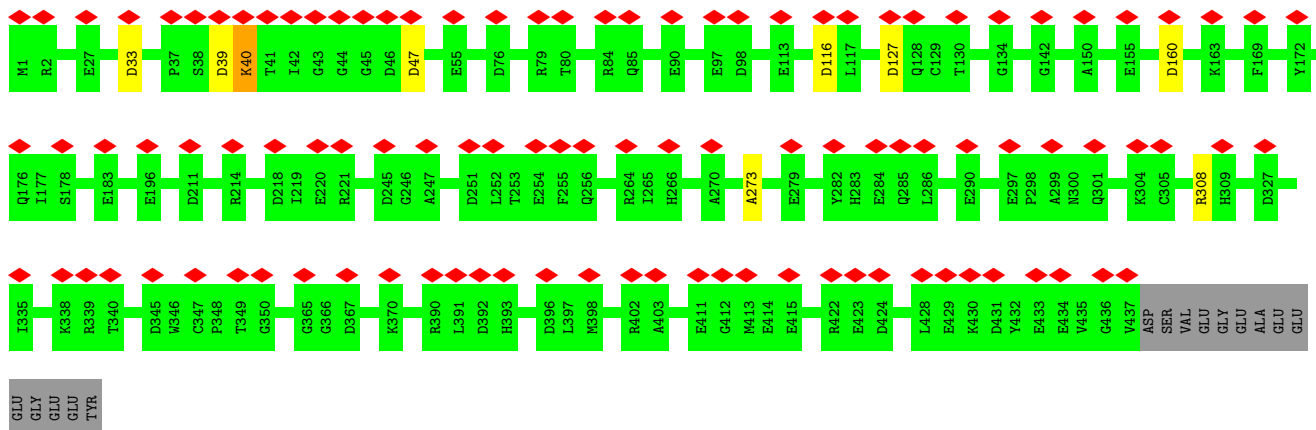


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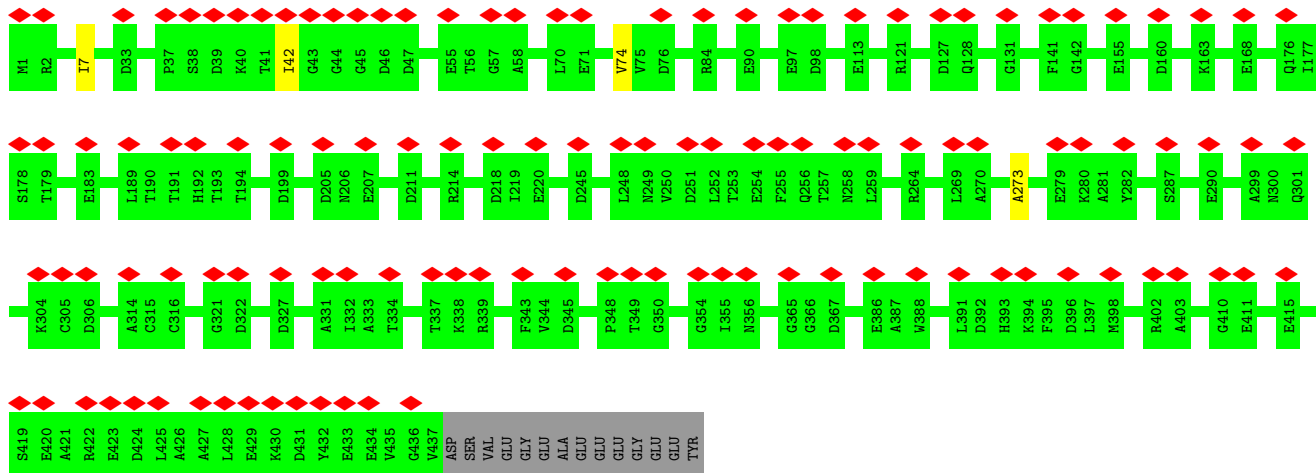




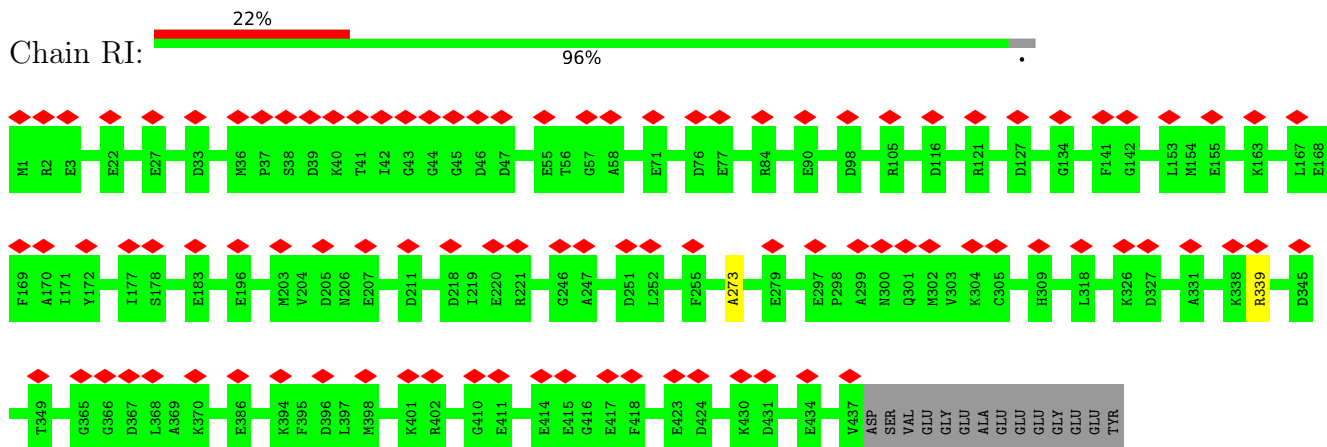
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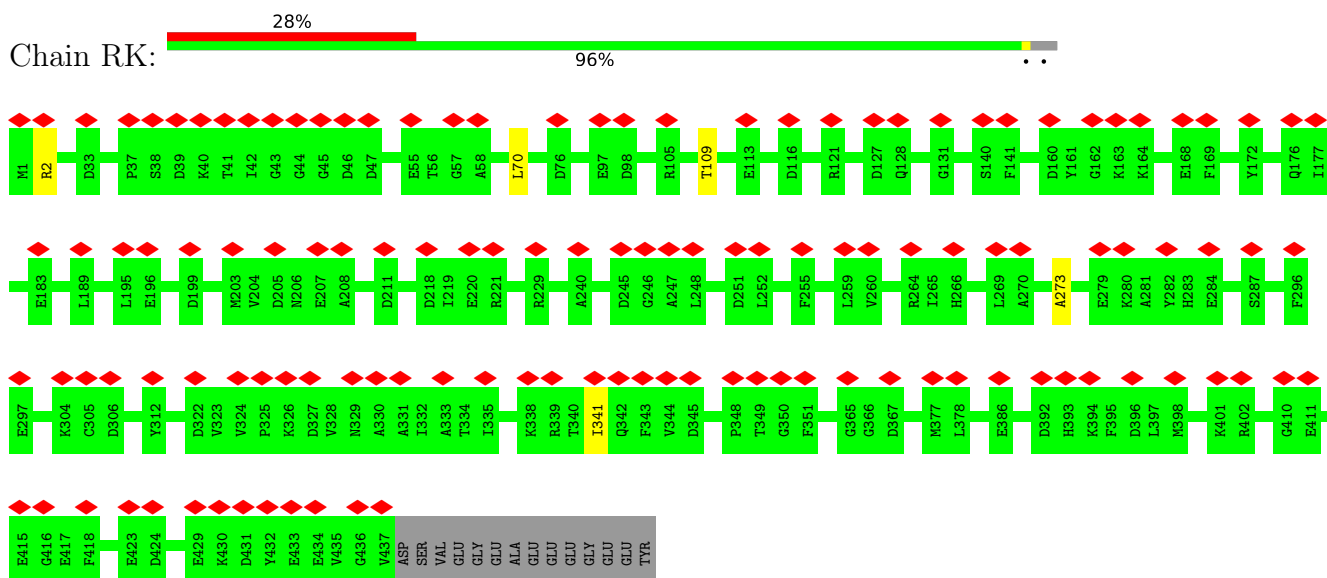
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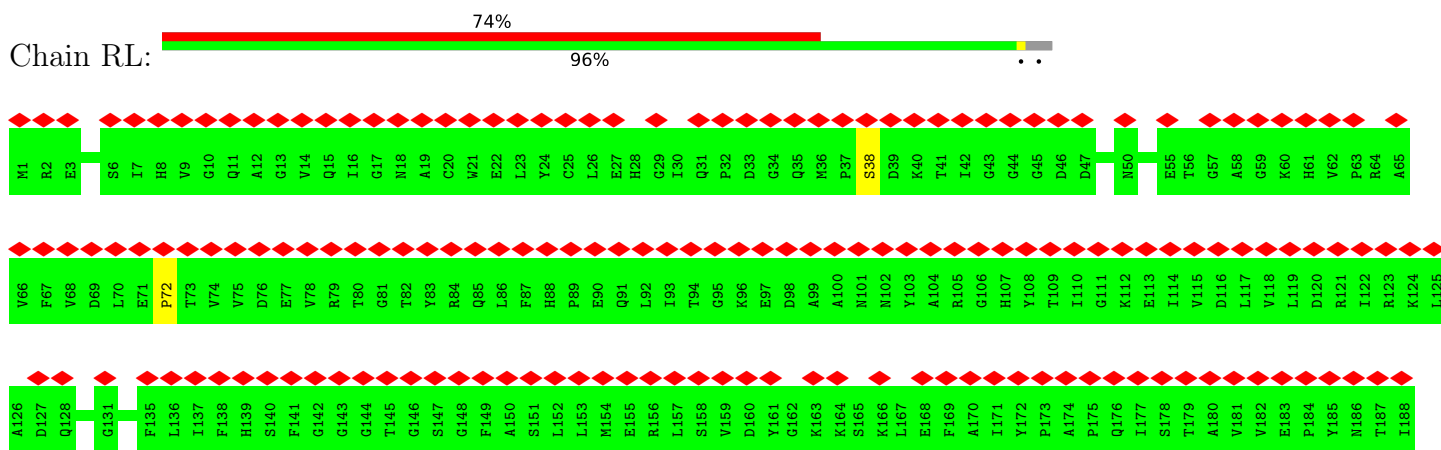
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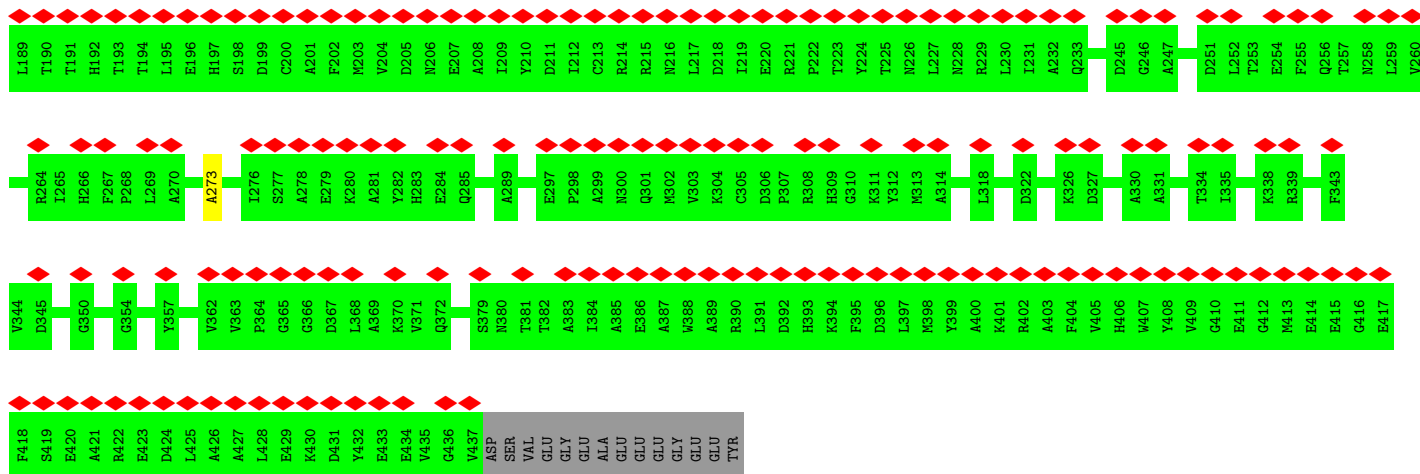


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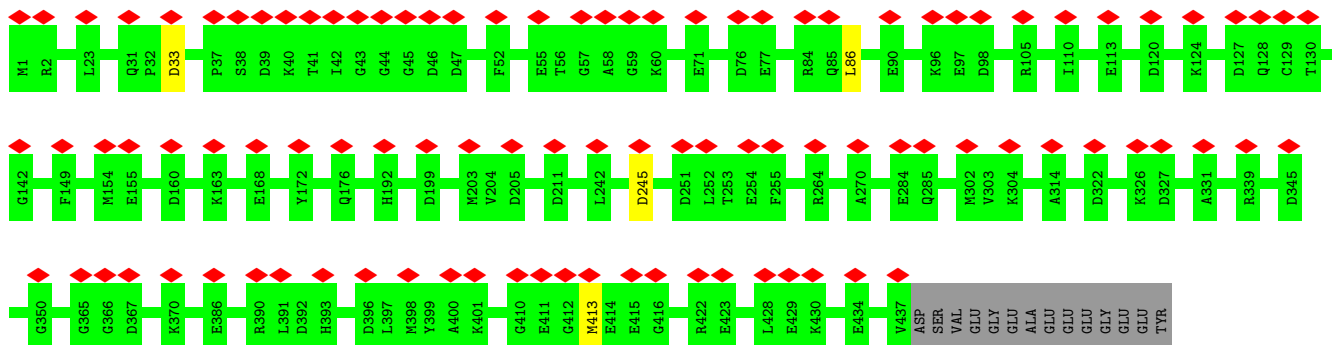


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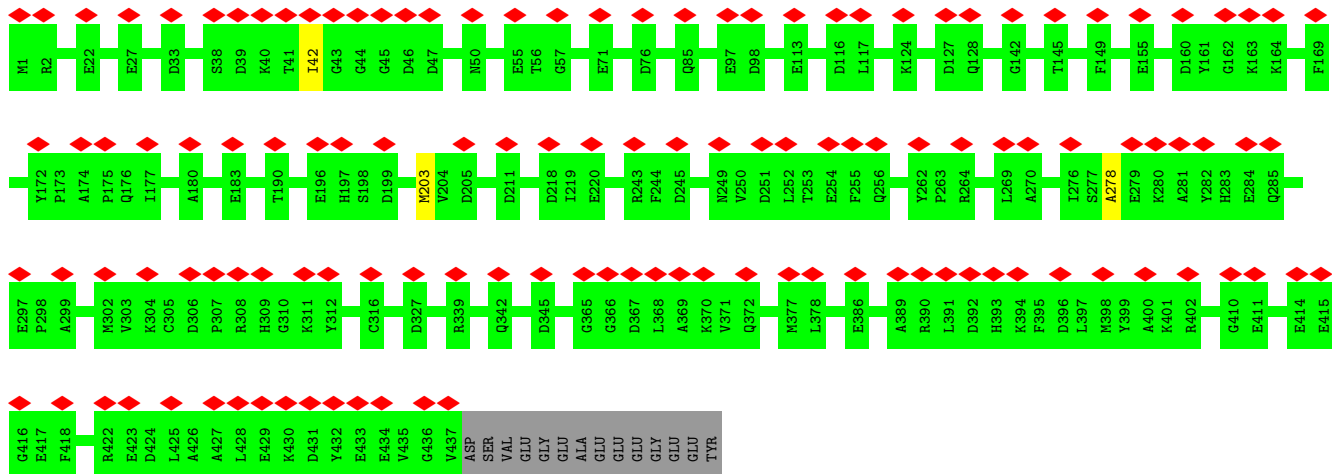




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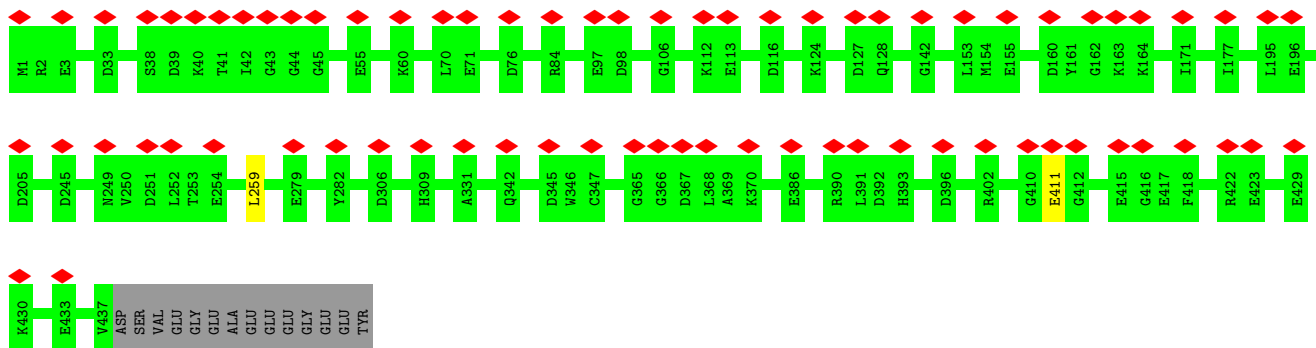


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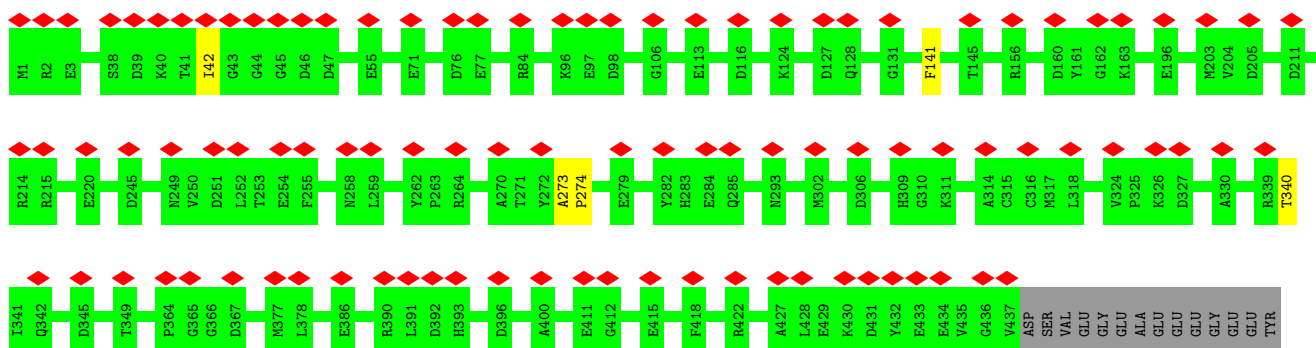


• Molecule 54: Tubulin alpha chain

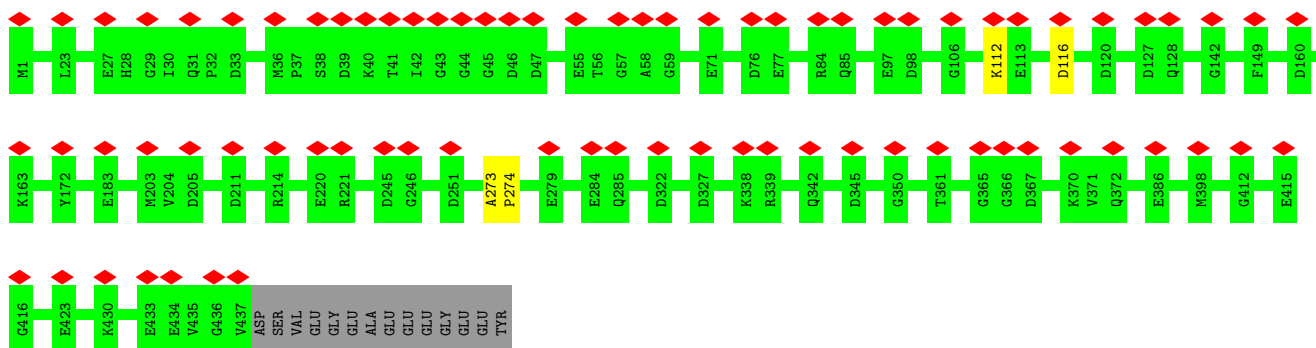




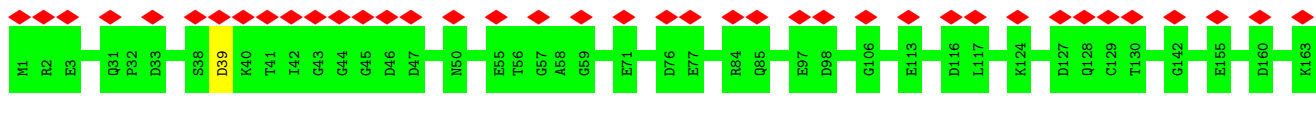
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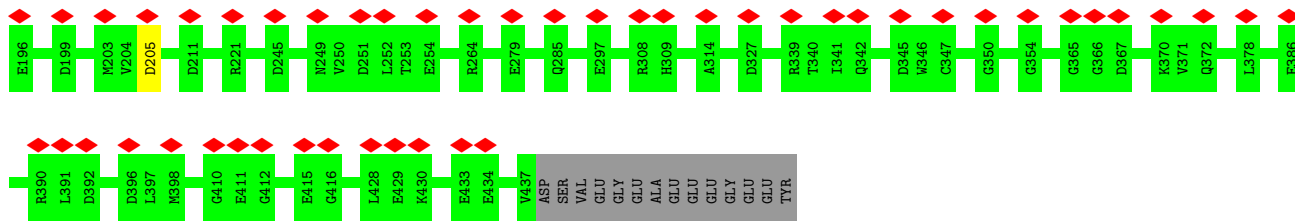


• Molecule 54: Tubulin alpha chain

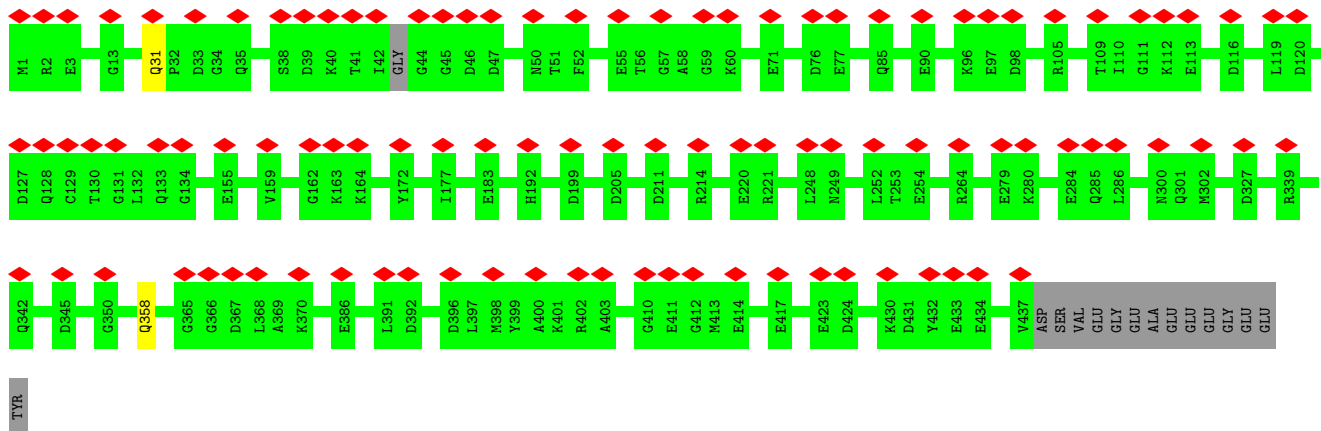


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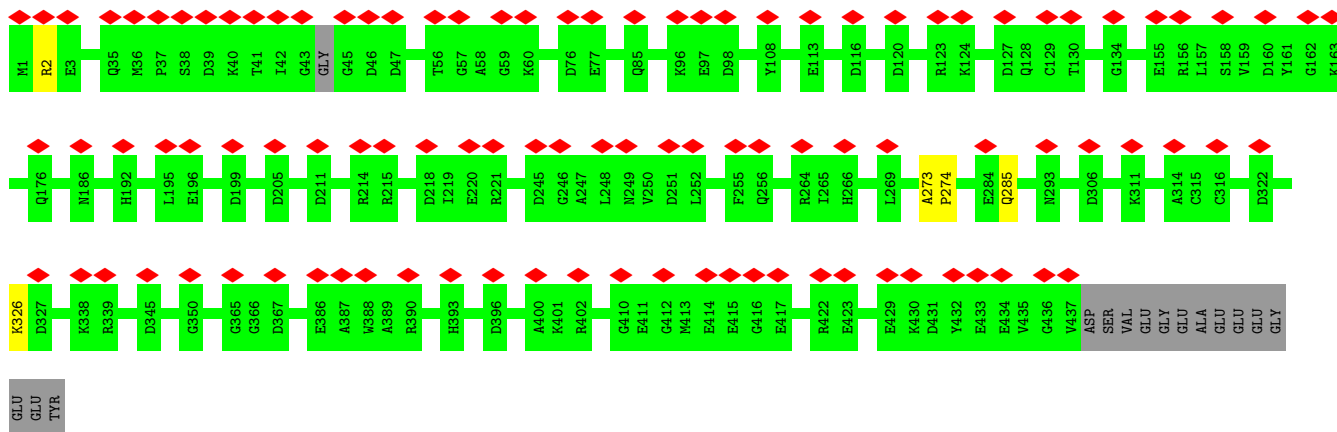




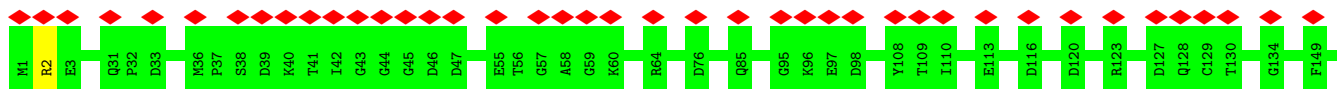
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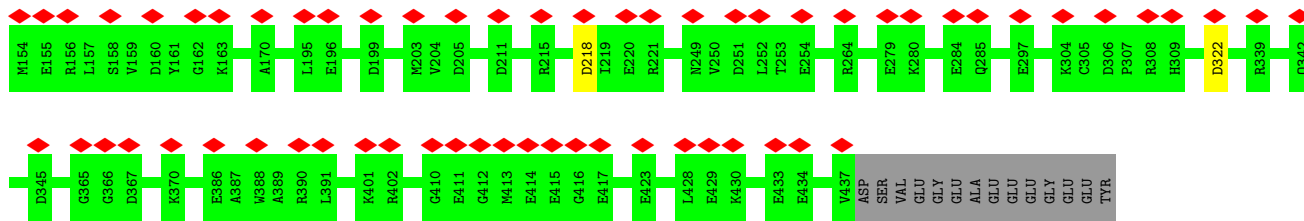


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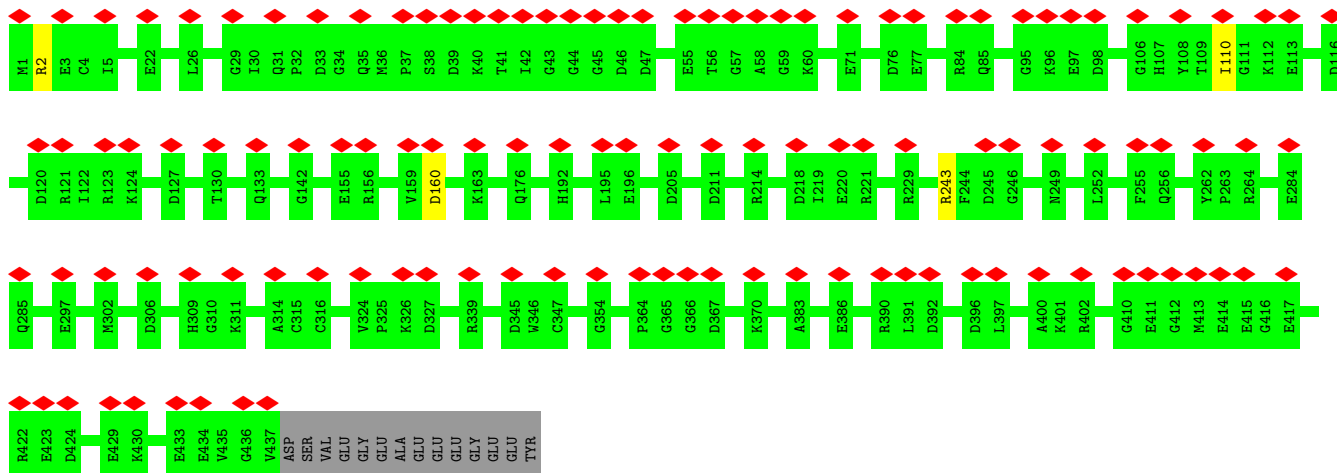


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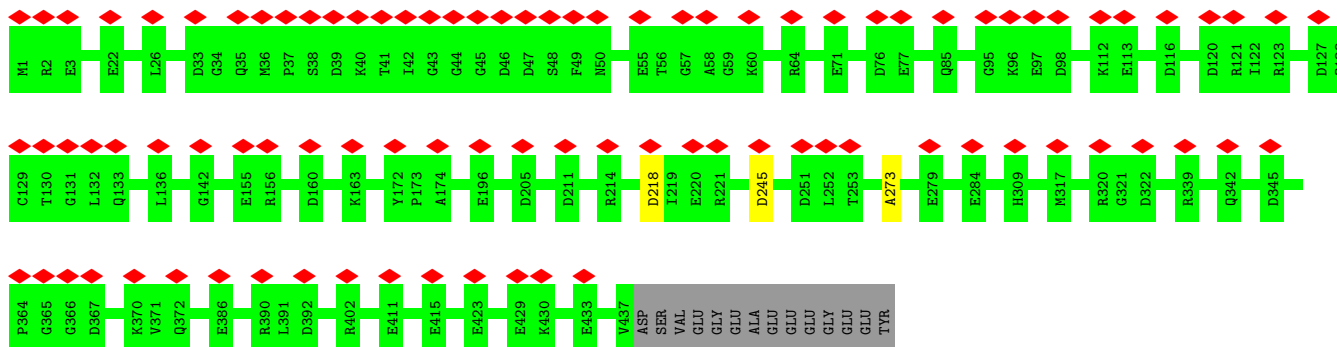




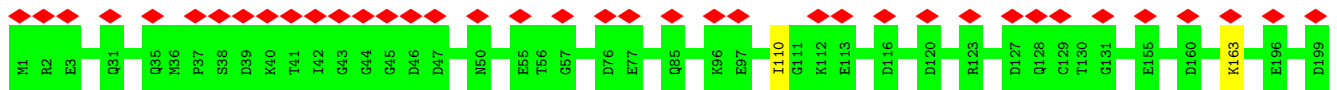
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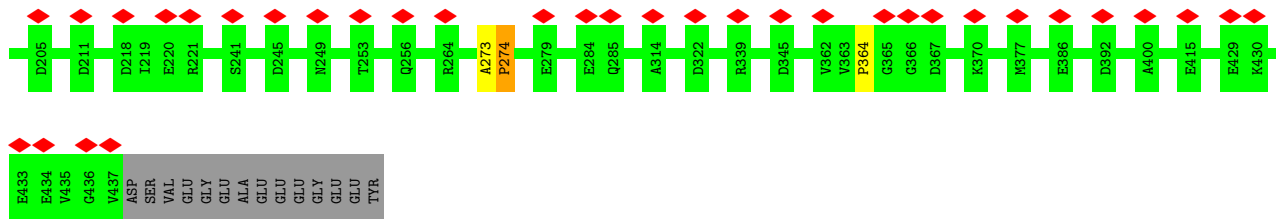


• Molecule 54: Tubulin alpha chain

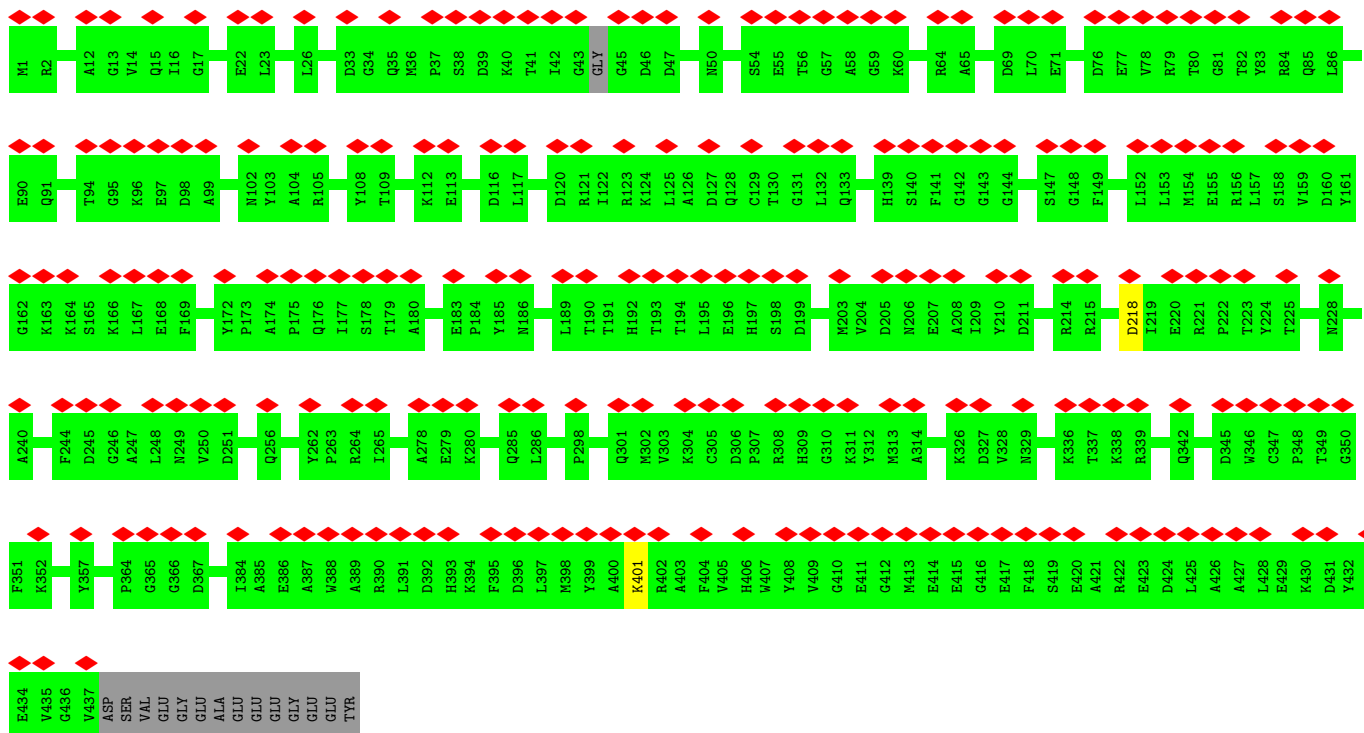


• Molecule 54: Tubulin alpha chain

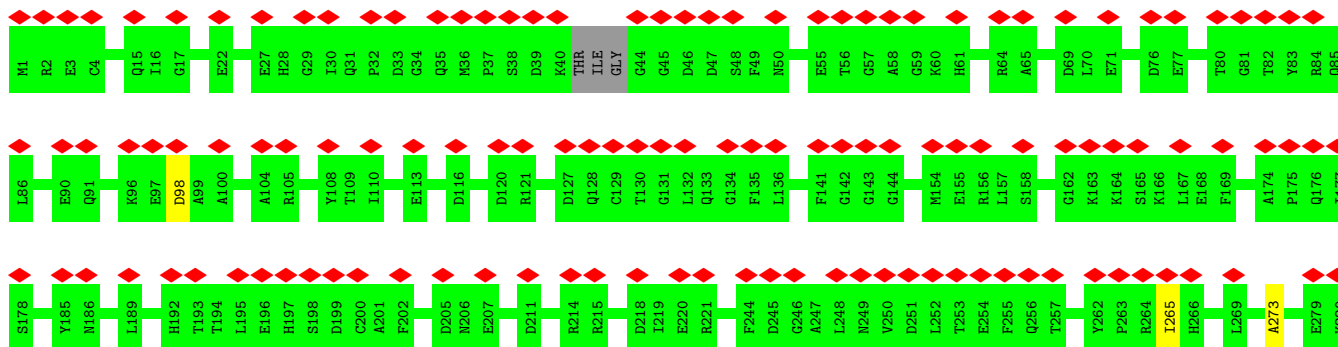


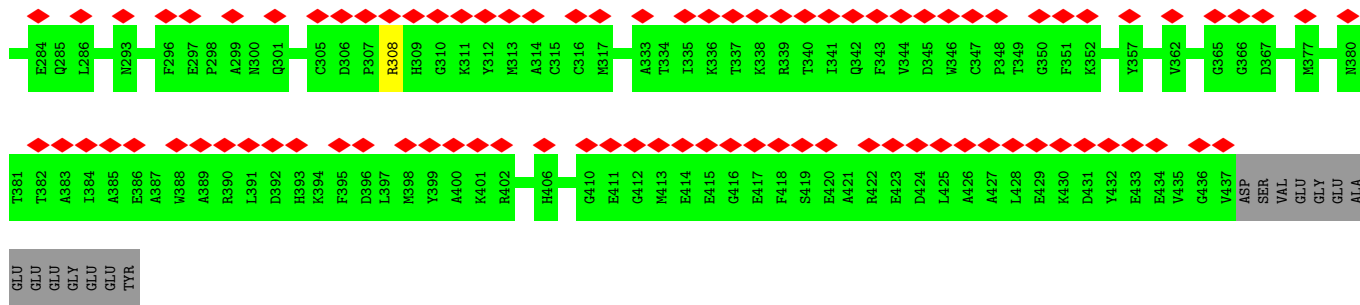


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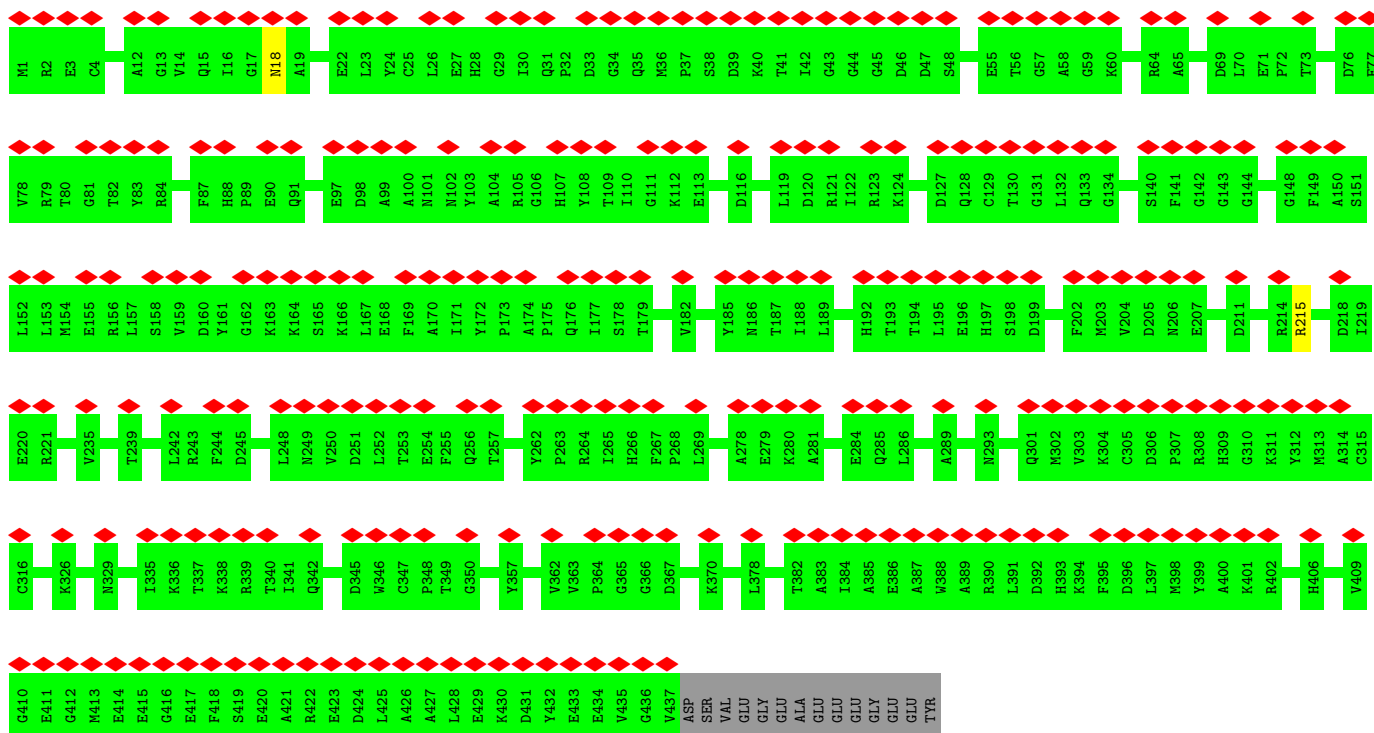


• Molecule 54: Tubulin alpha chain

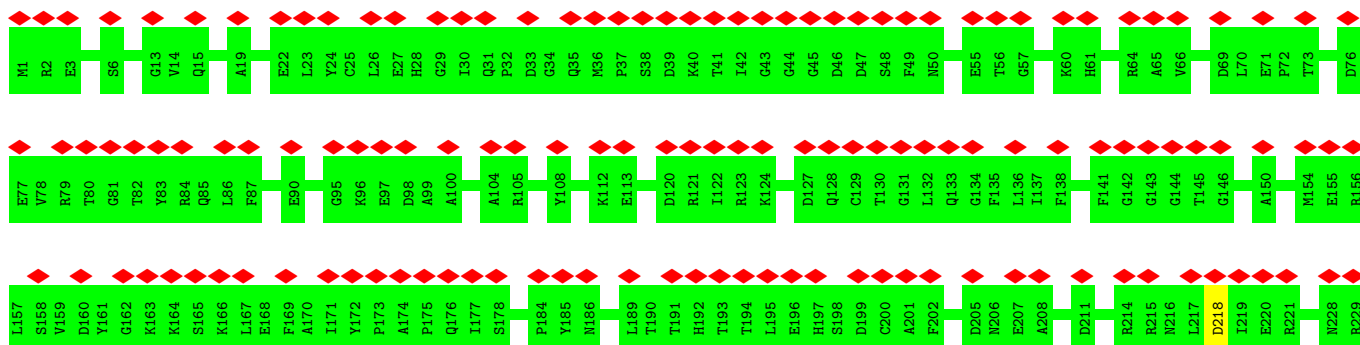


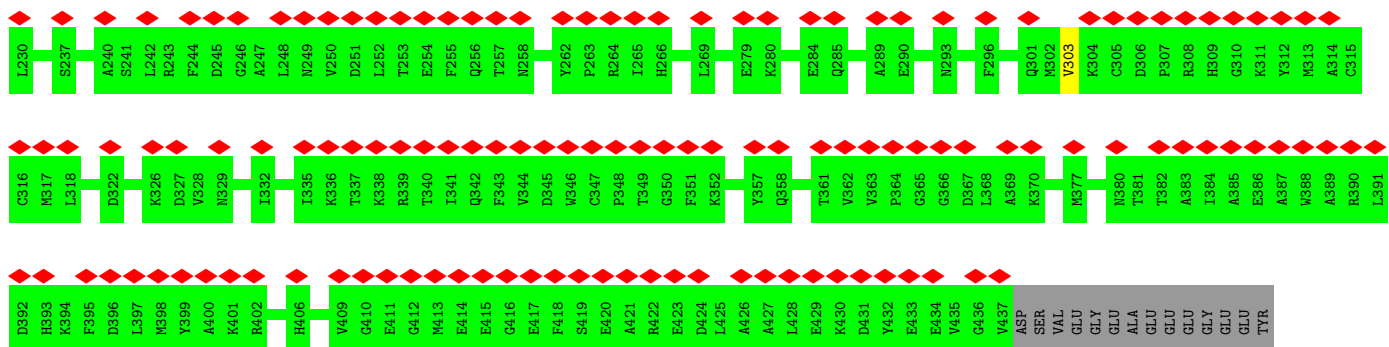


• Molecule 54: Tubulin alpha chain

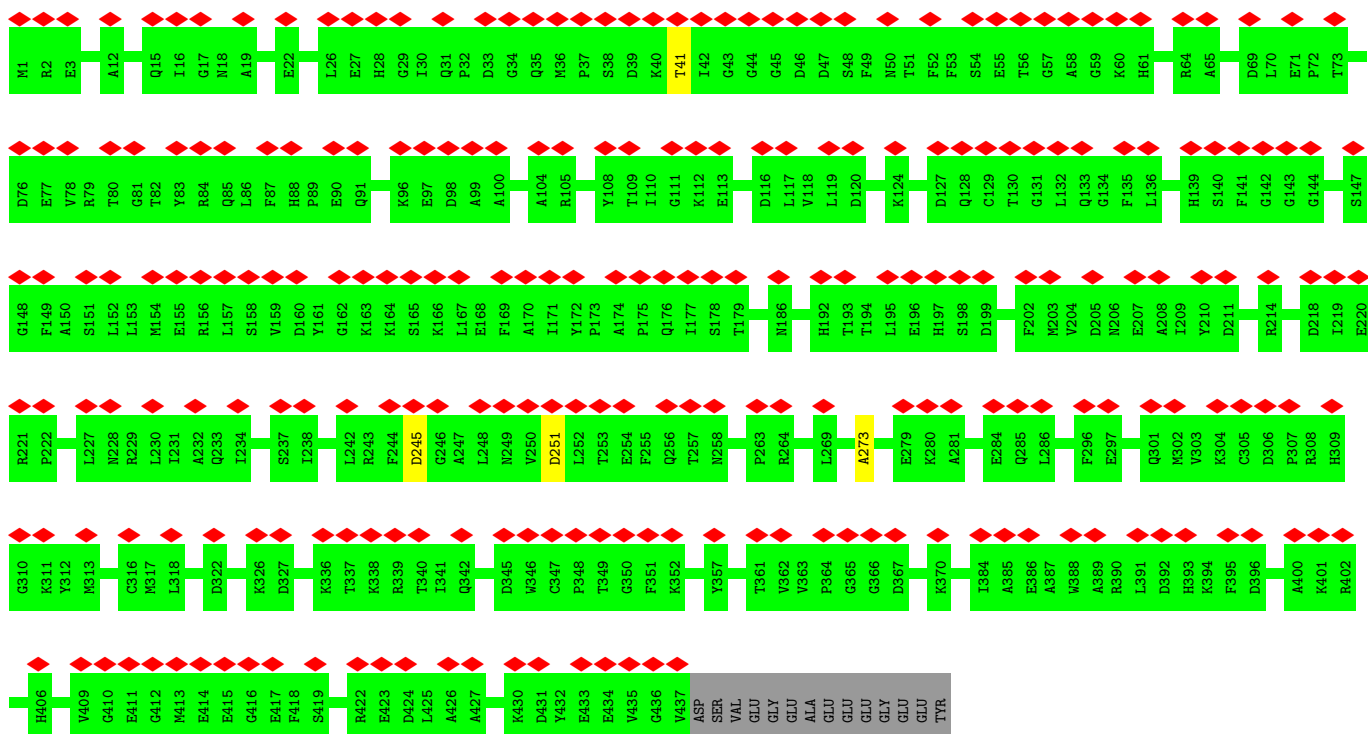


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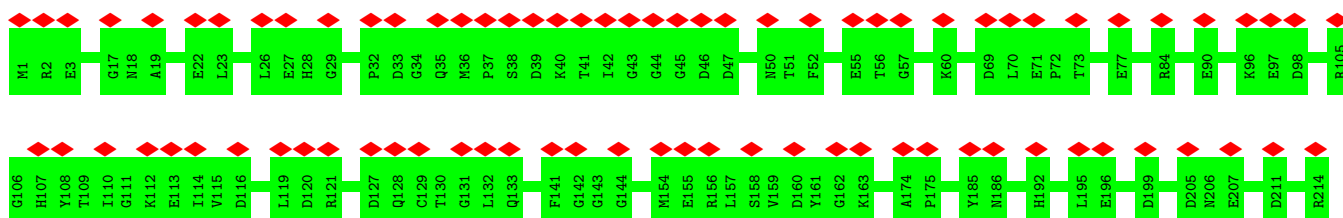


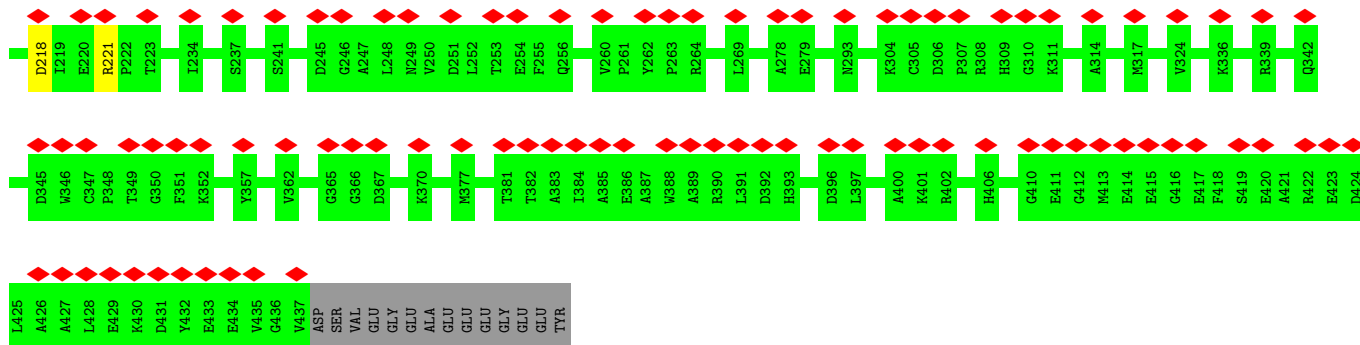


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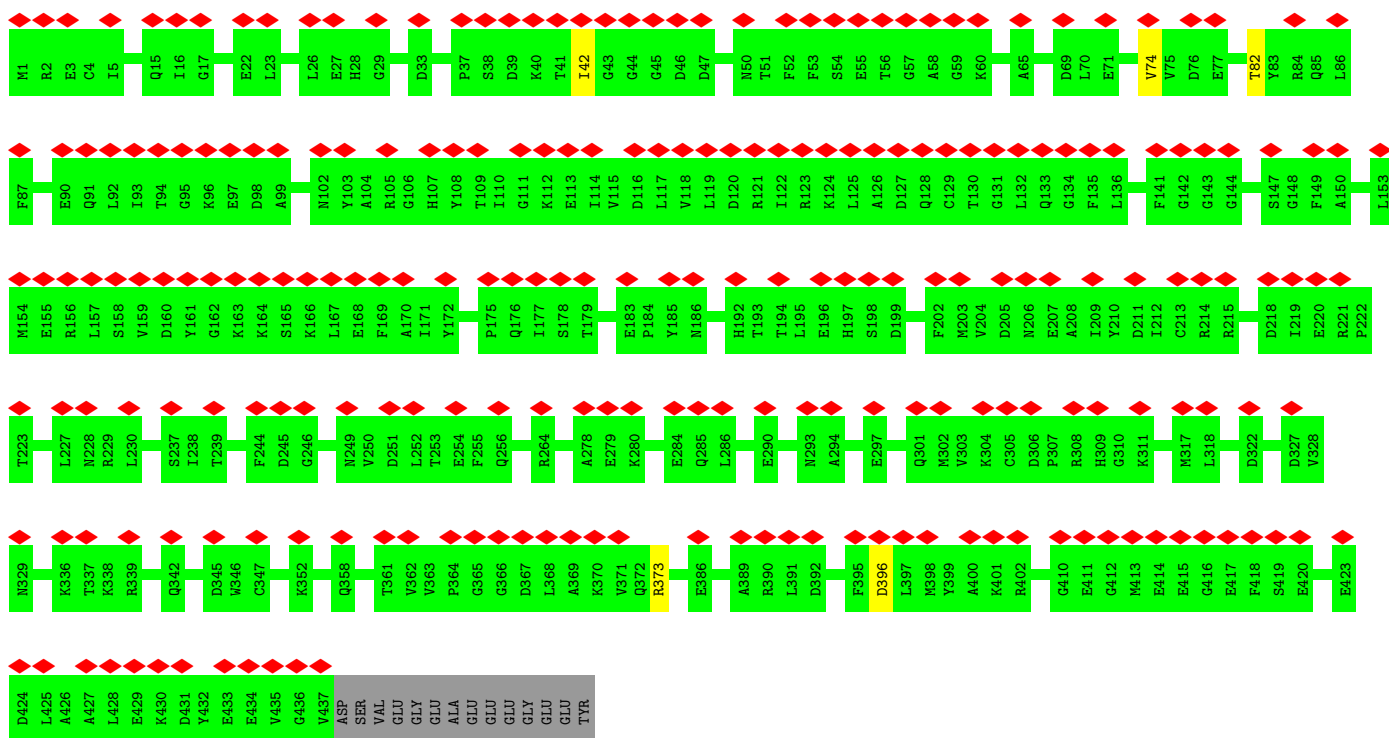


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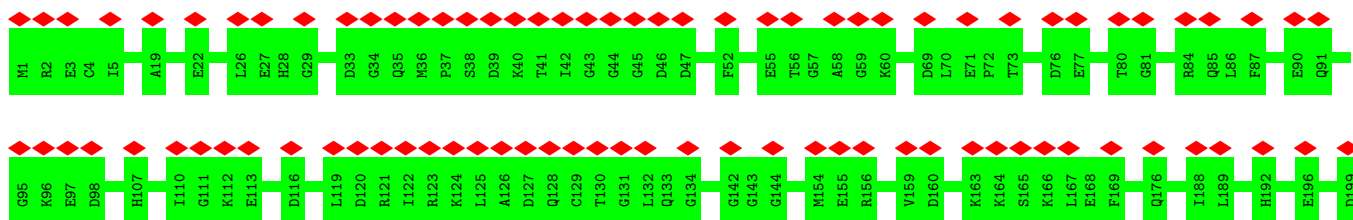
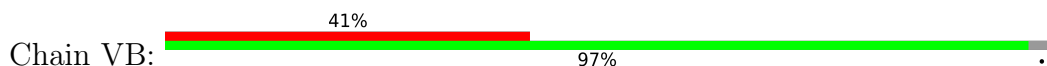


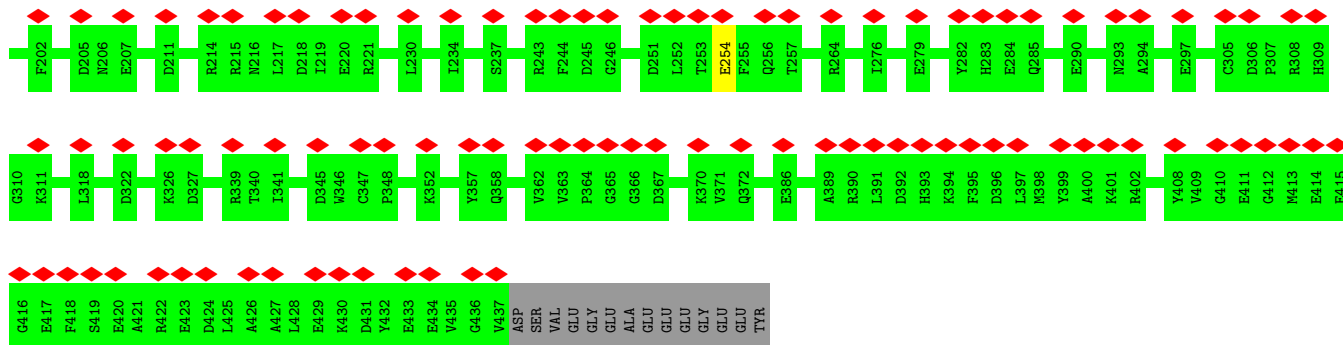


• Molecule 54: Tubulin alpha chain

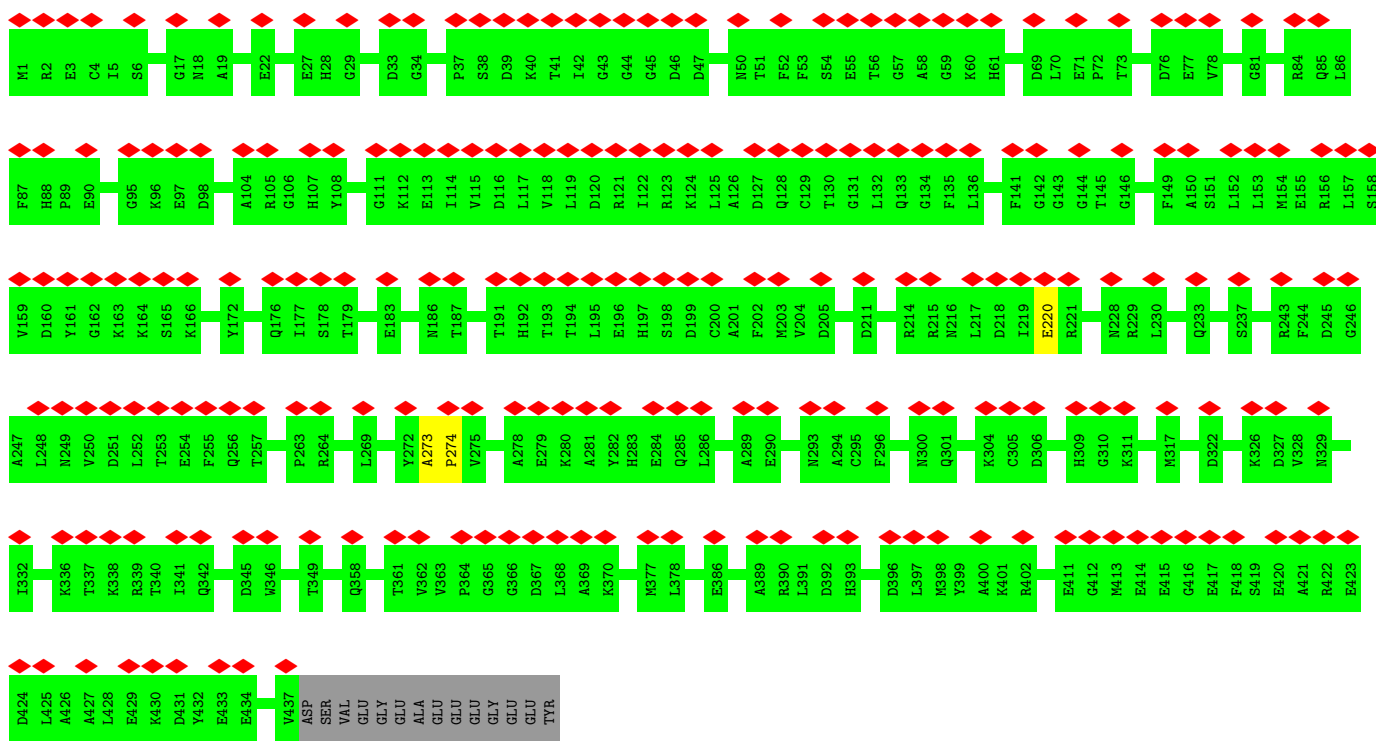


• Molecule 54: Tubulin alpha chain

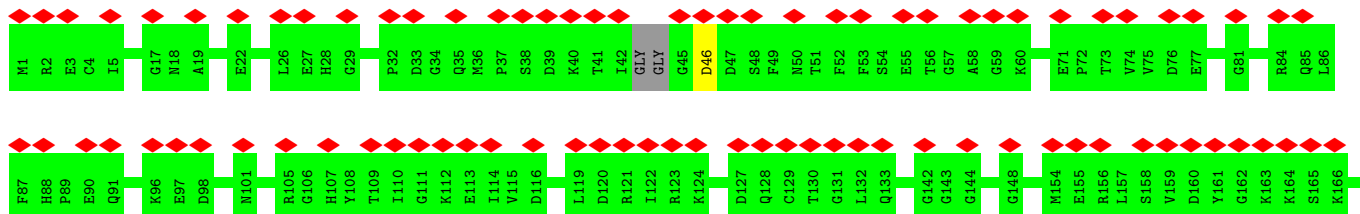




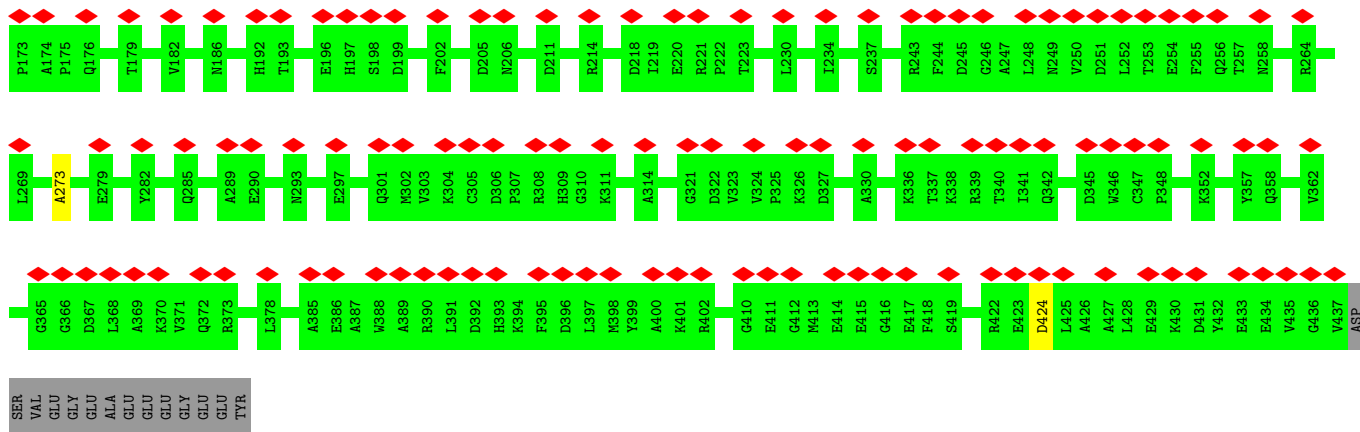
• Molecule 54: Tubulin alpha chain



• Molecule 54: Tubulin alpha chain

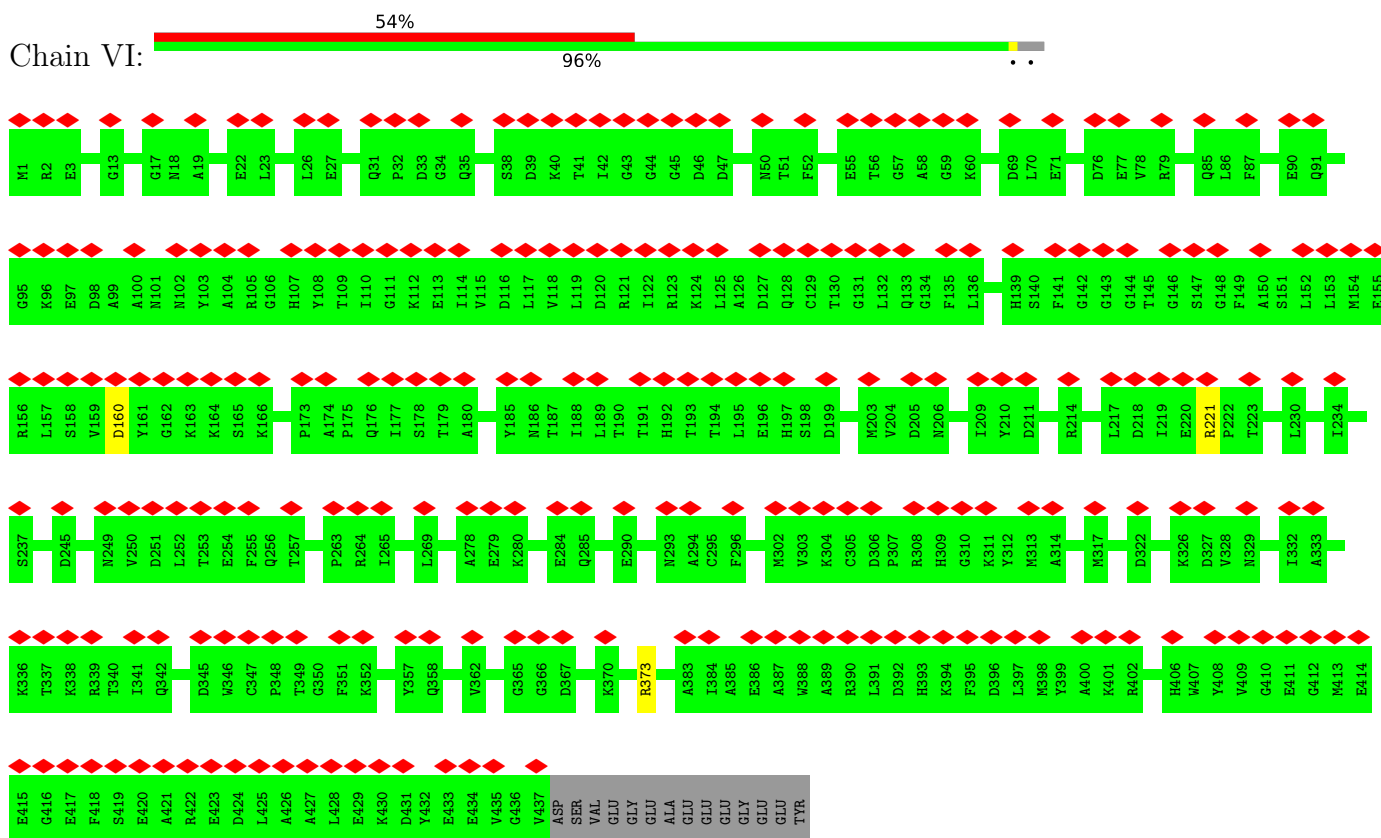






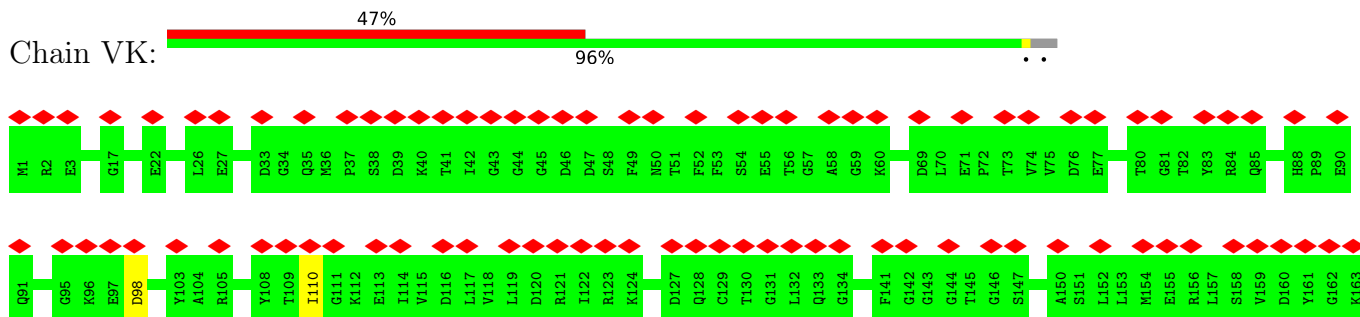
• Molecule 54: Tubulin alpha chain

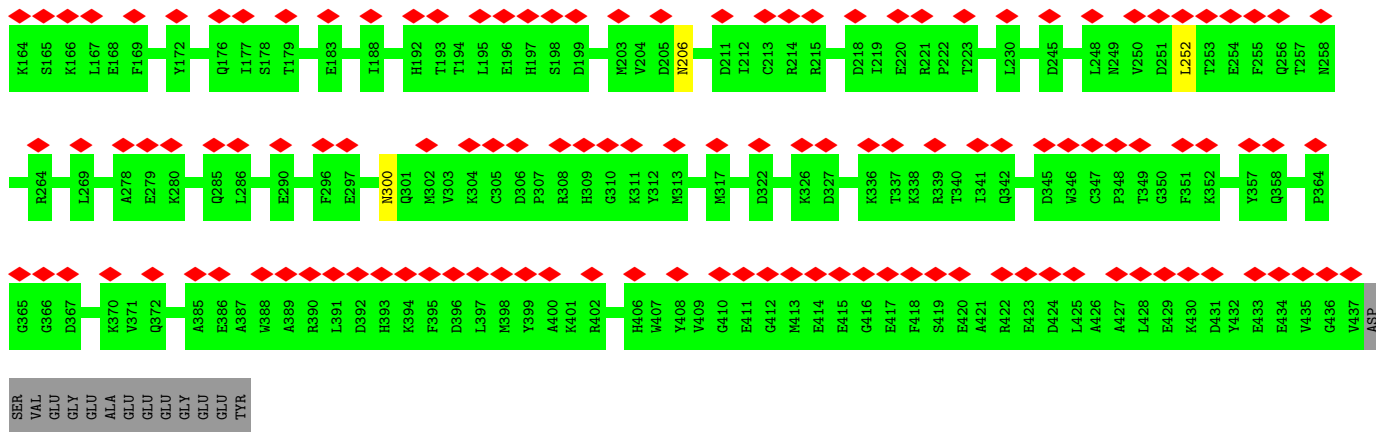
Chain VI:



• Molecule 54: Tubulin alpha chain

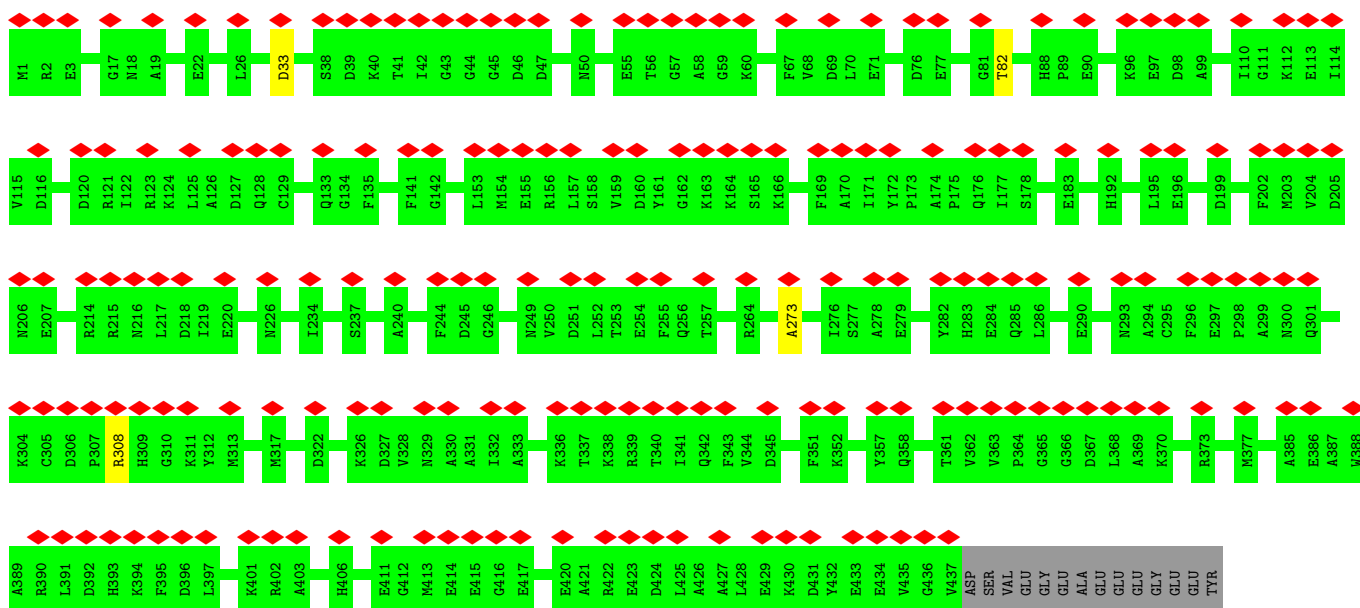
Chain VK:





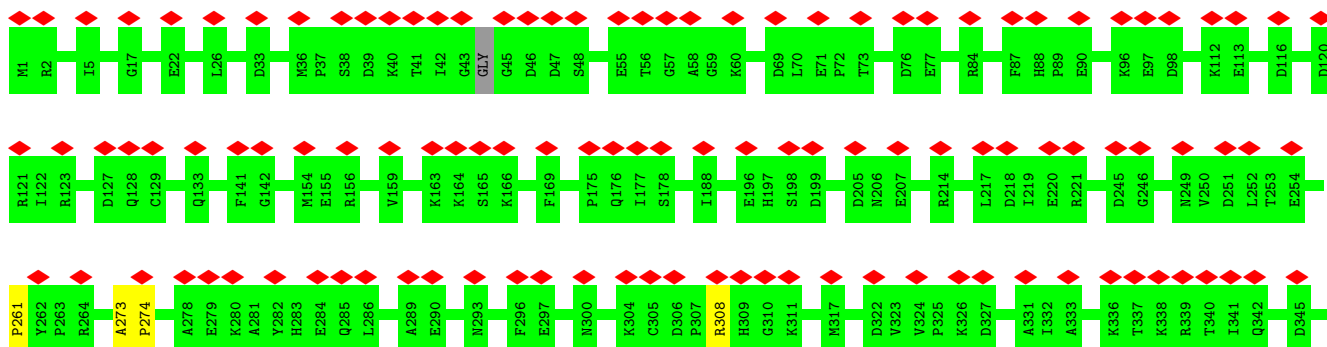
• Molecule 54: Tubulin alpha chain

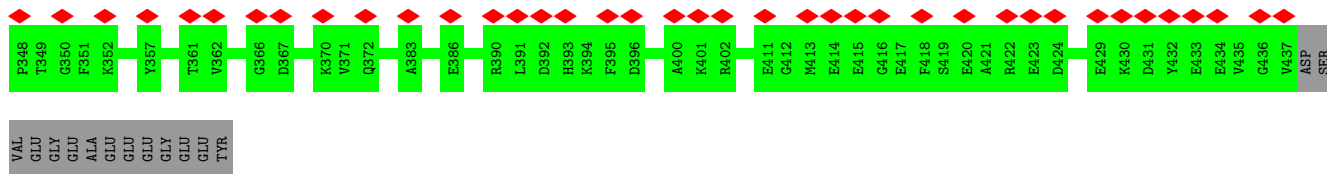
Chain WA:



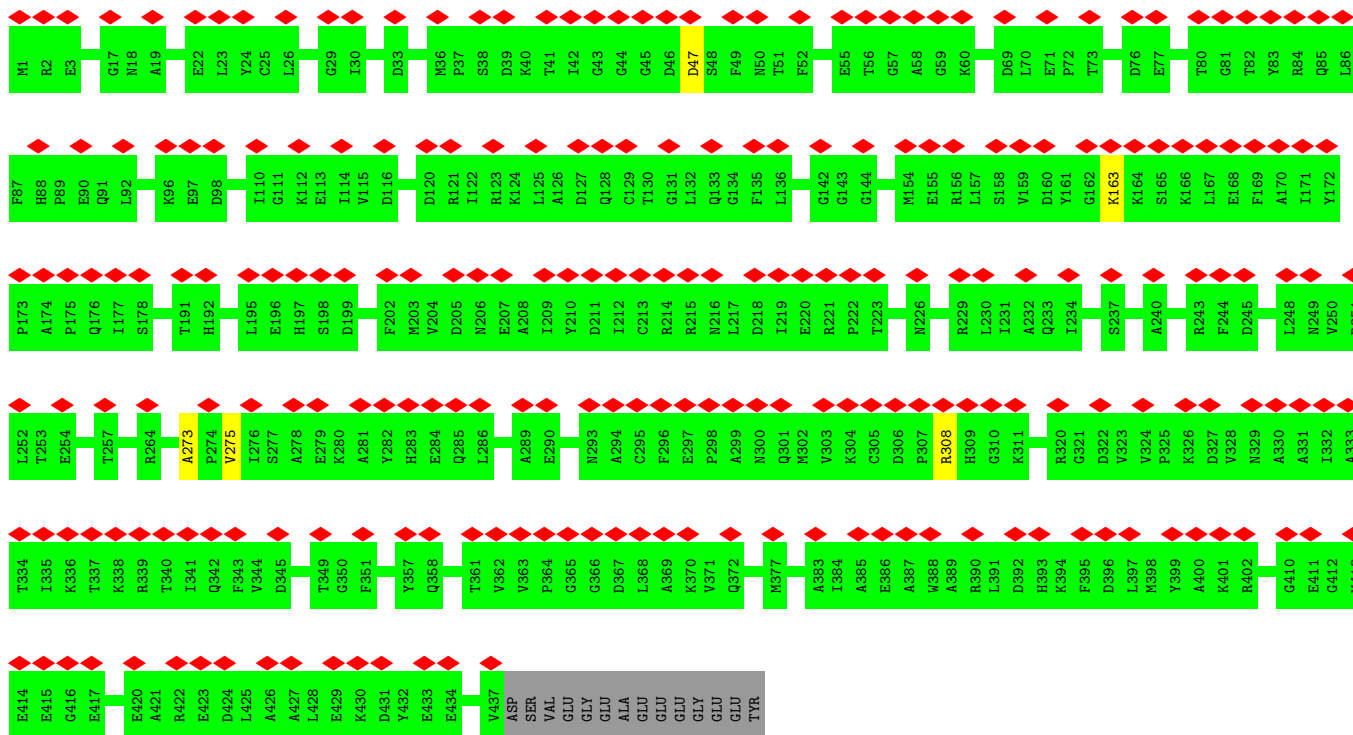
• Molecule 54: Tubulin alpha chain

Chain WB:

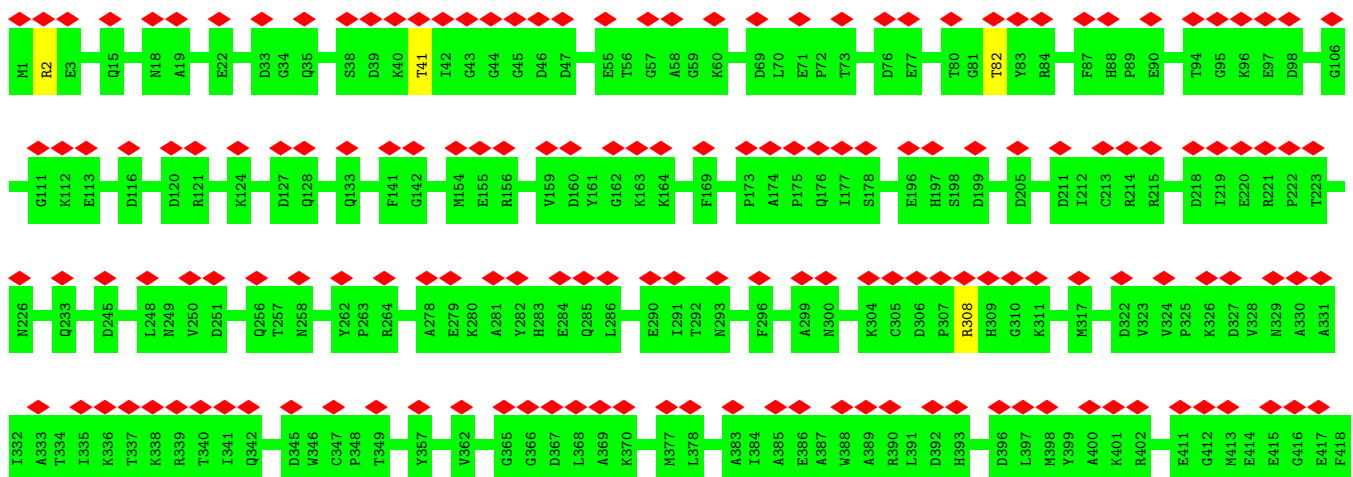


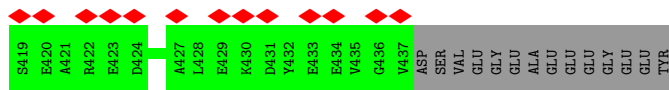


• Molecule 54: Tubulin alpha chain

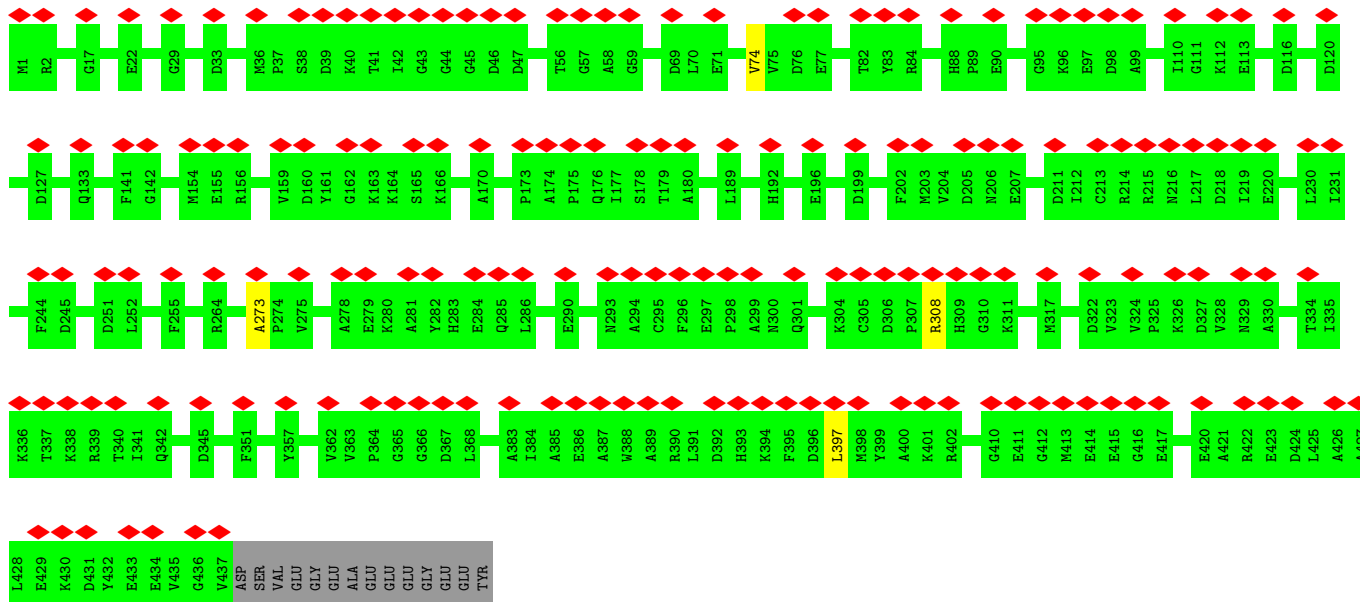
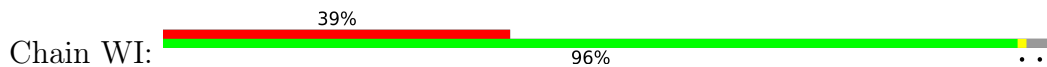


• Molecule 54: Tubulin alpha chain

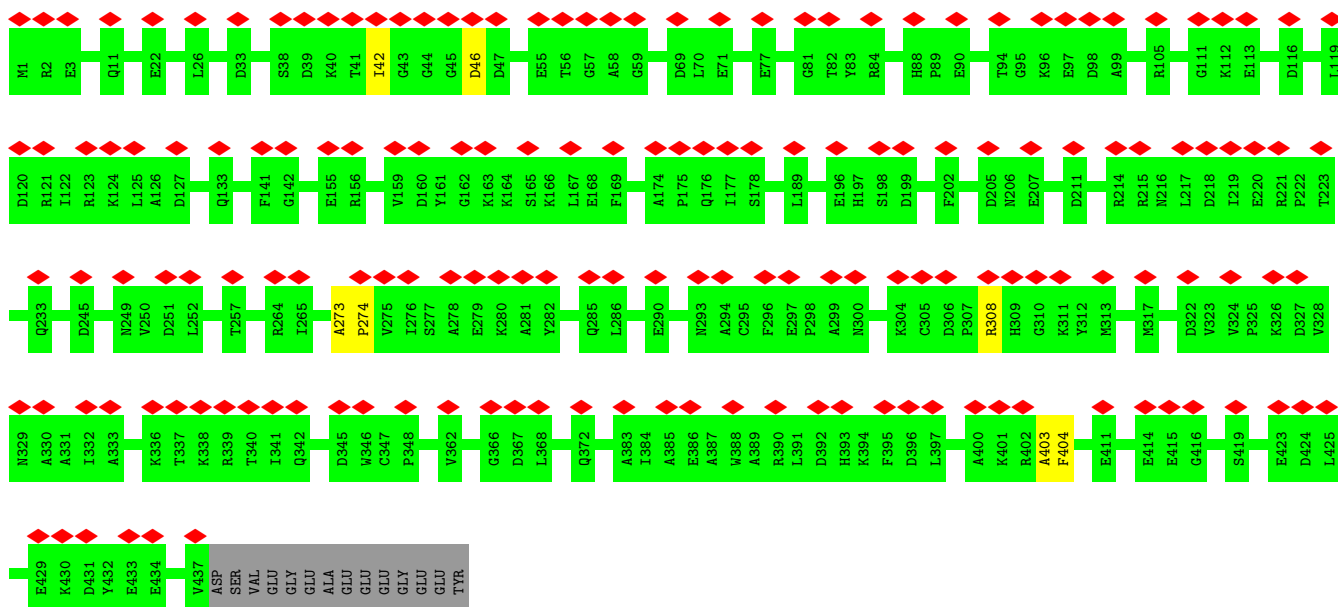




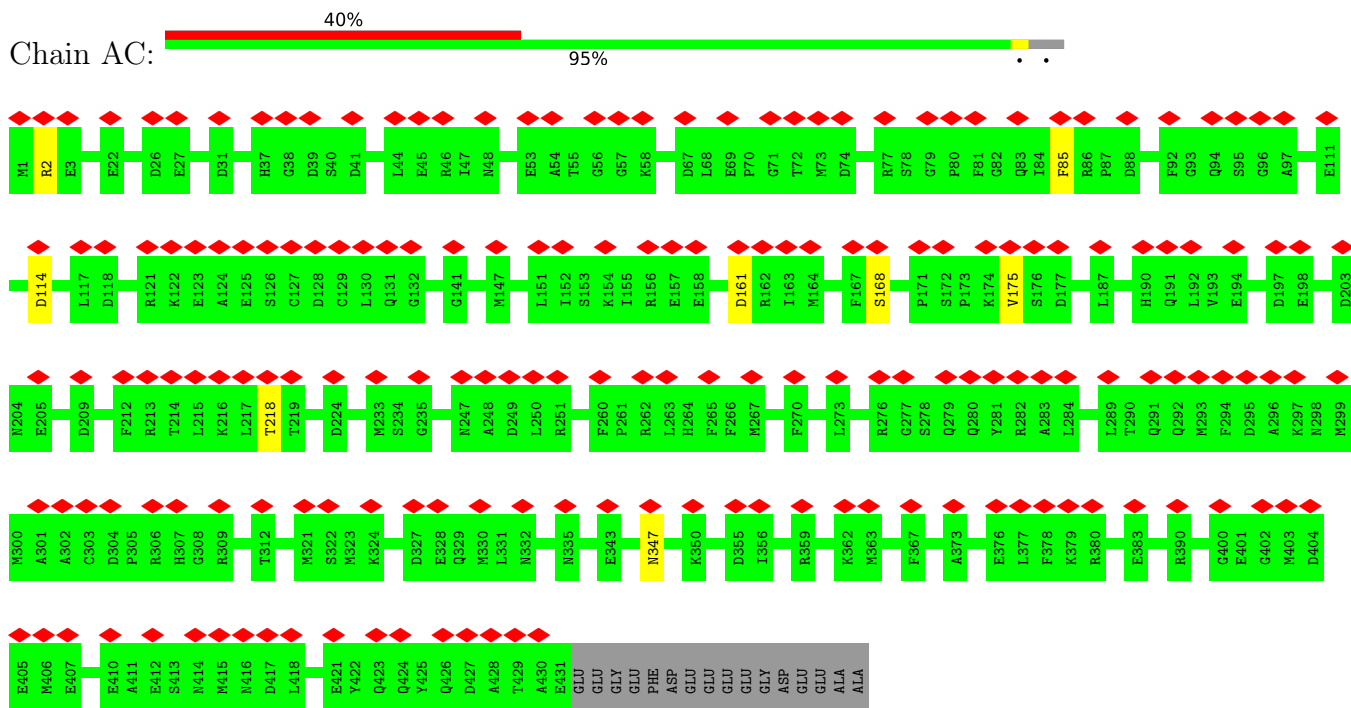
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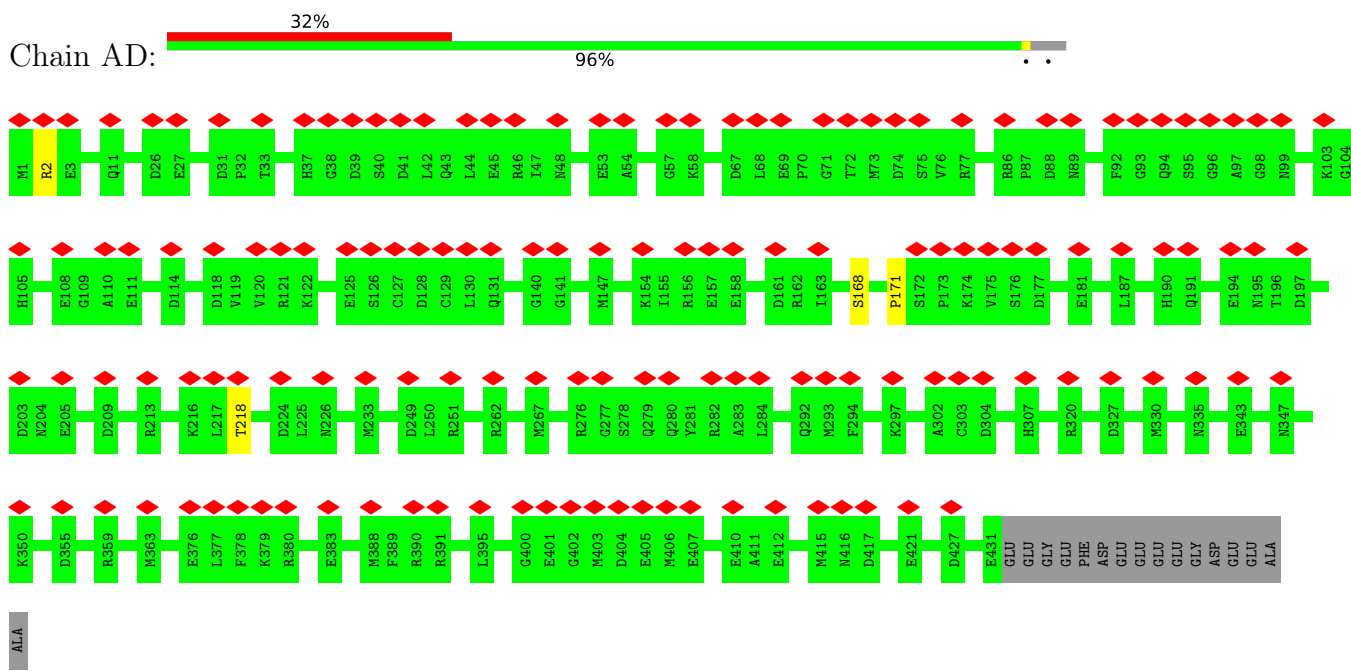
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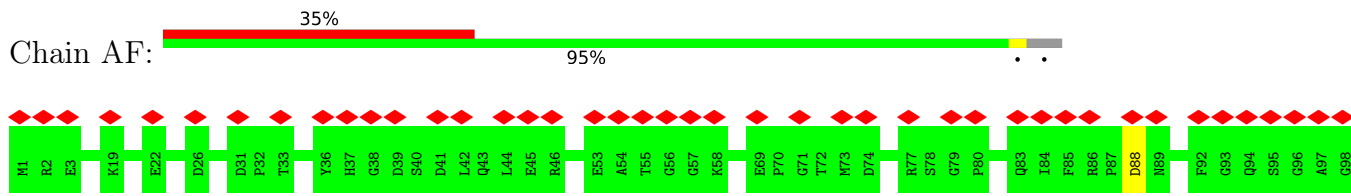
• Molecule 55: Tubulin beta chain

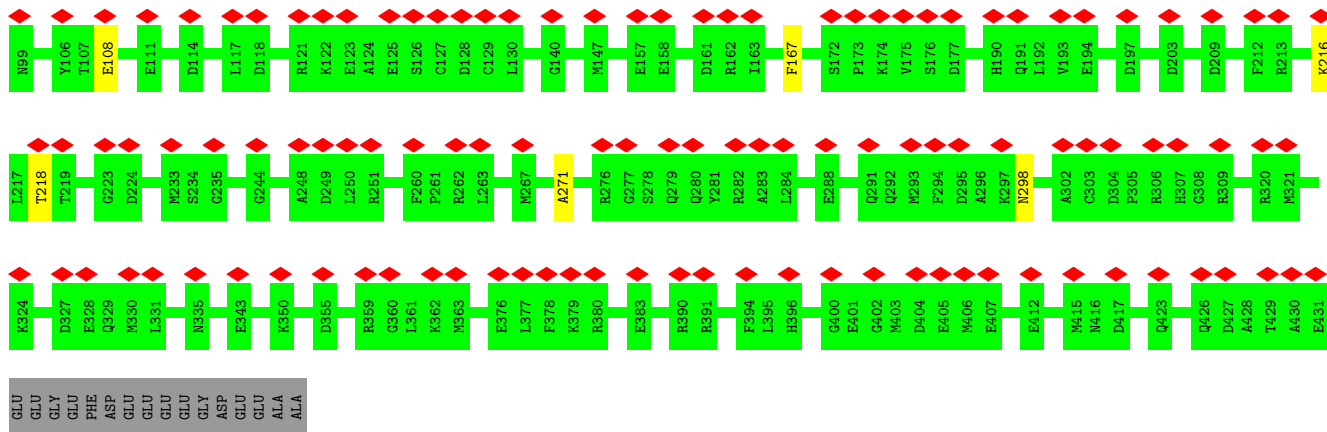


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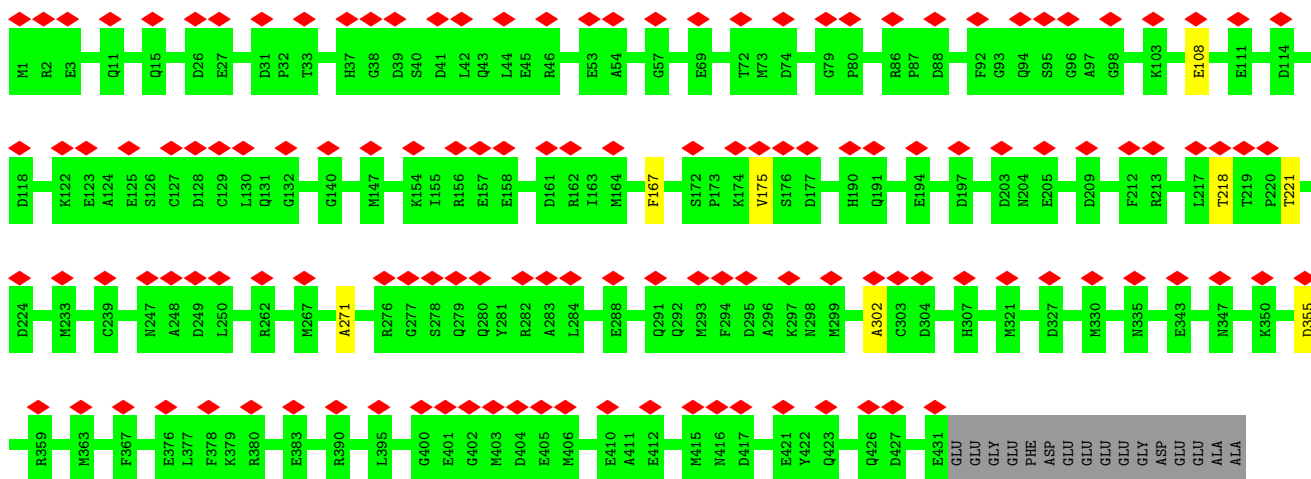


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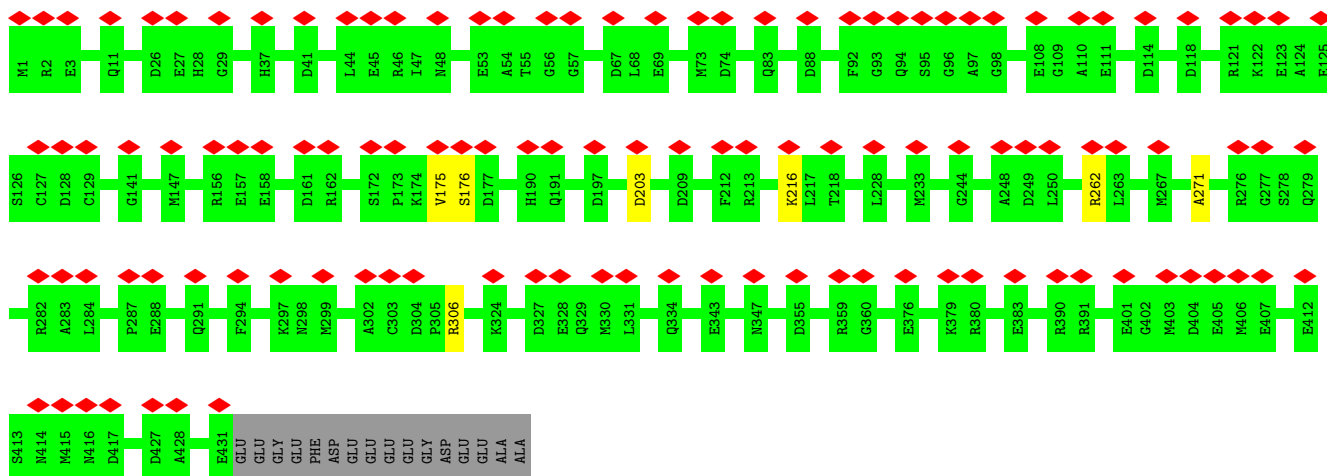




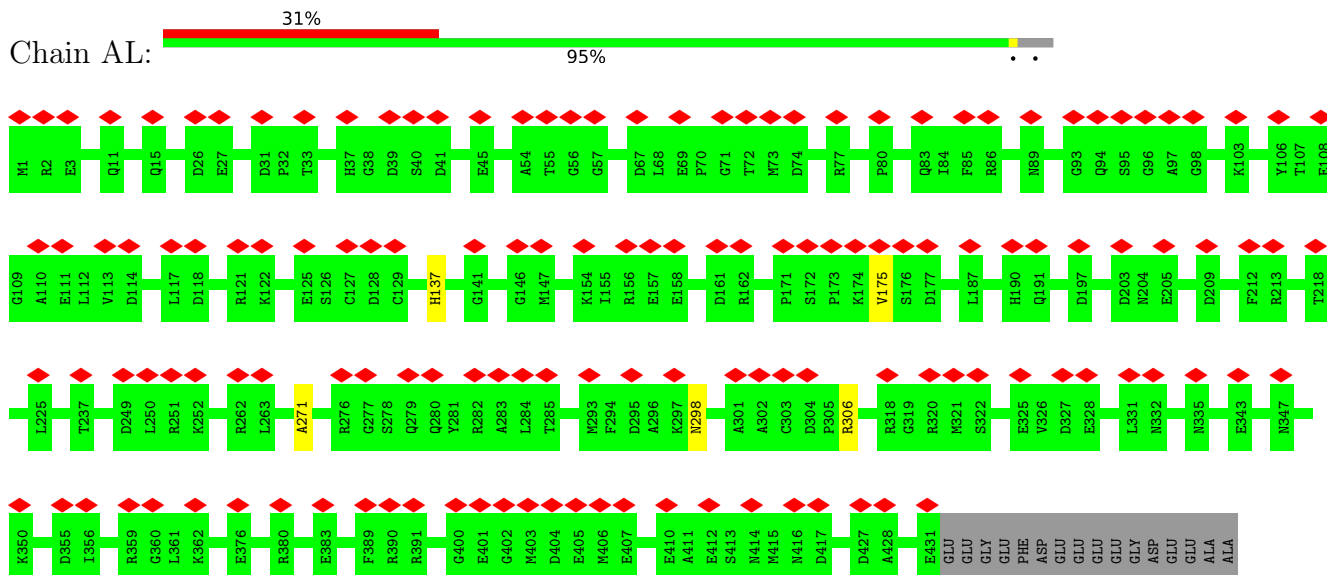
• Molecule 55: Tubulin beta chain



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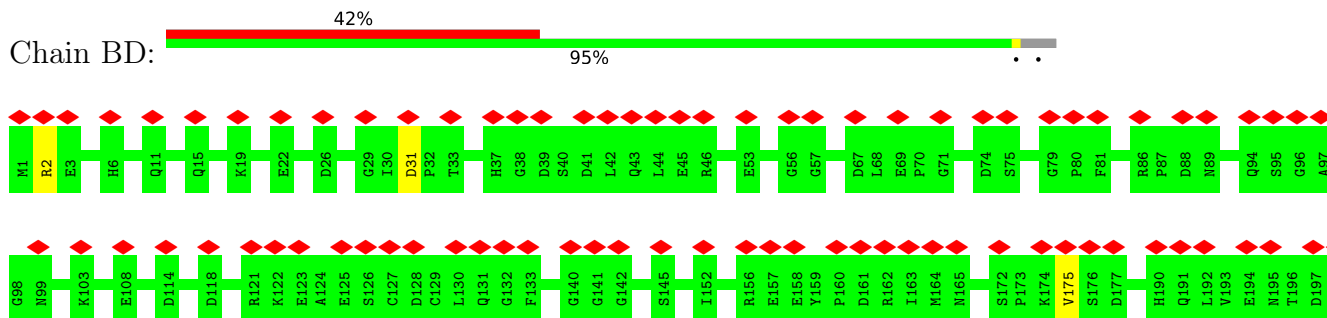
• Molecule 55: Tubulin beta chain

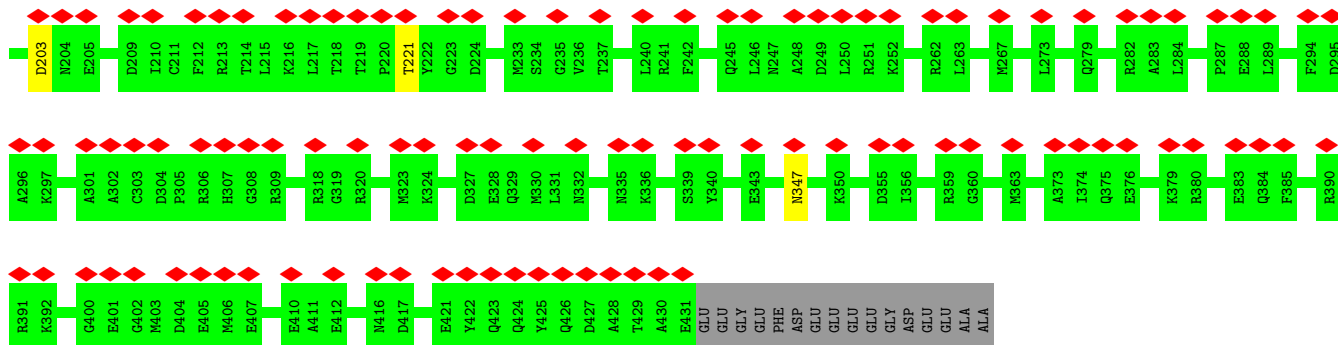


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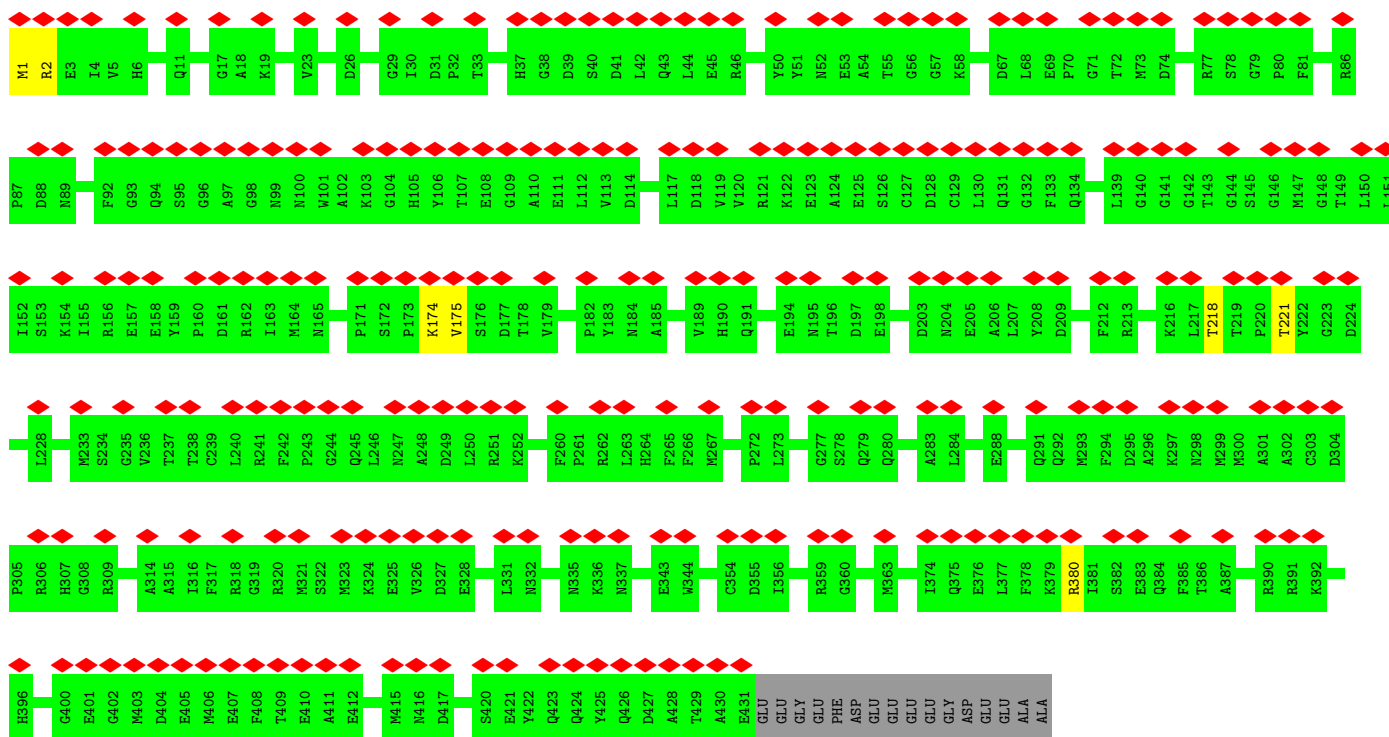


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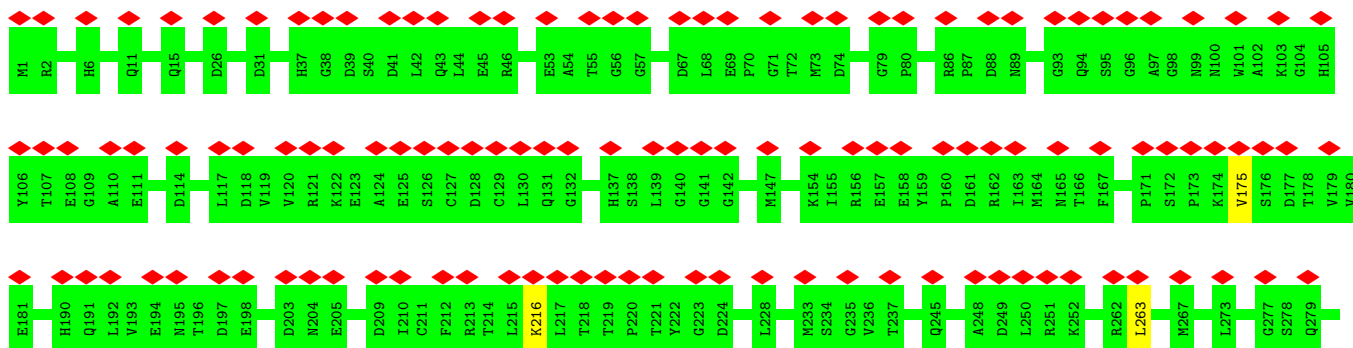




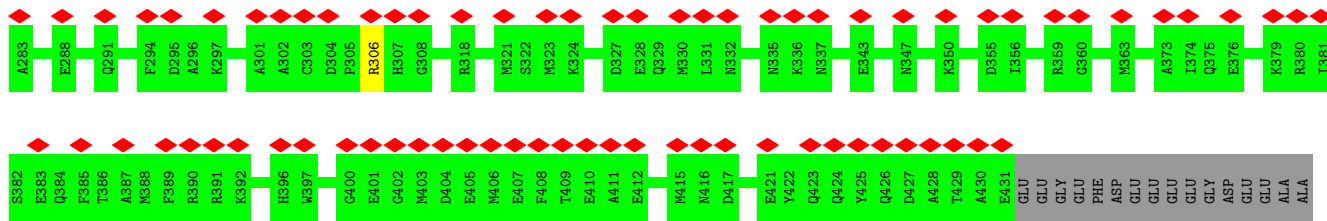
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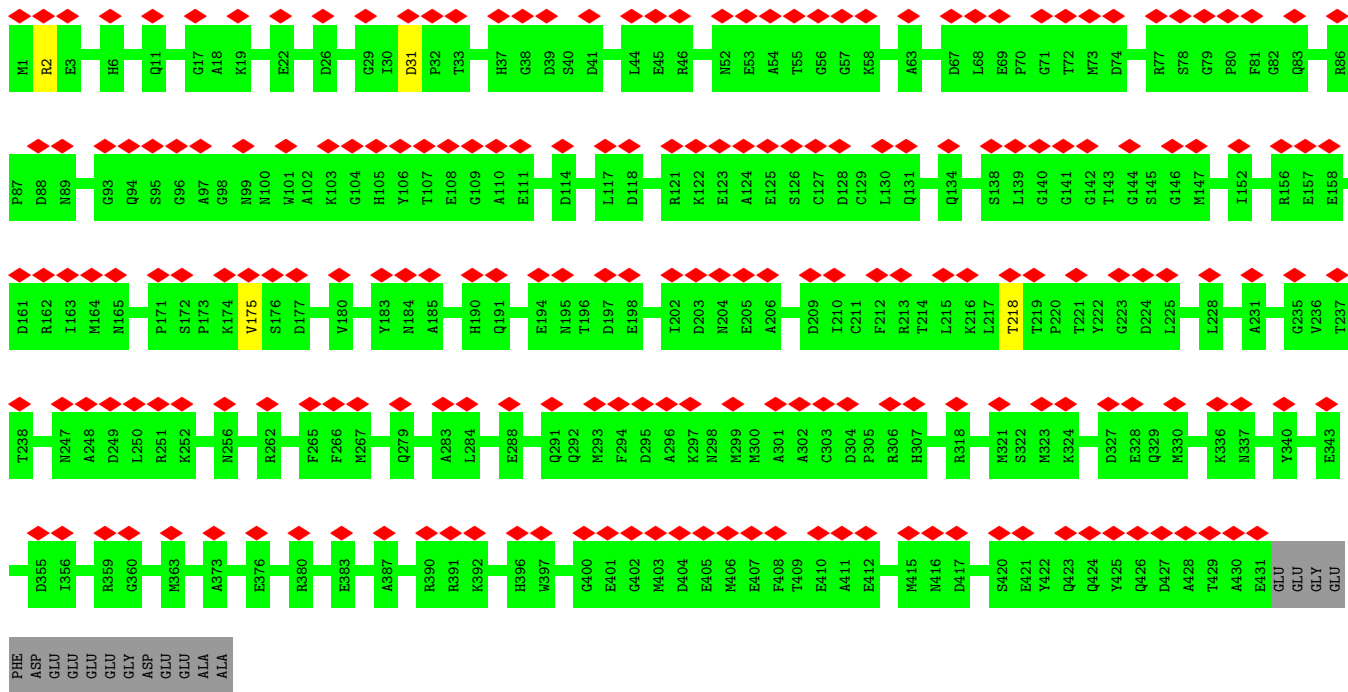
• Molecule 55: Tubulin beta chain



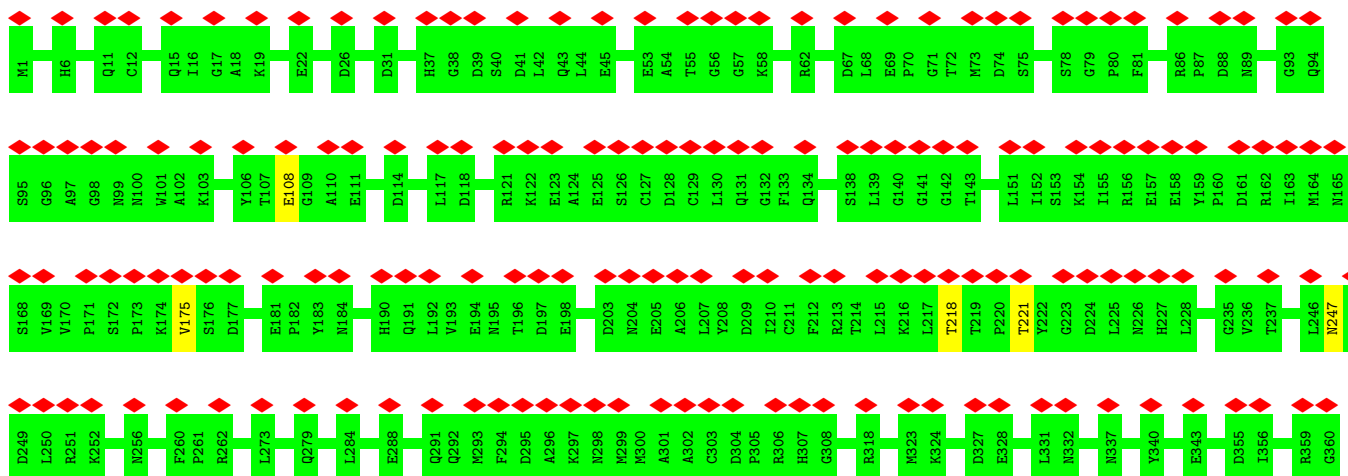


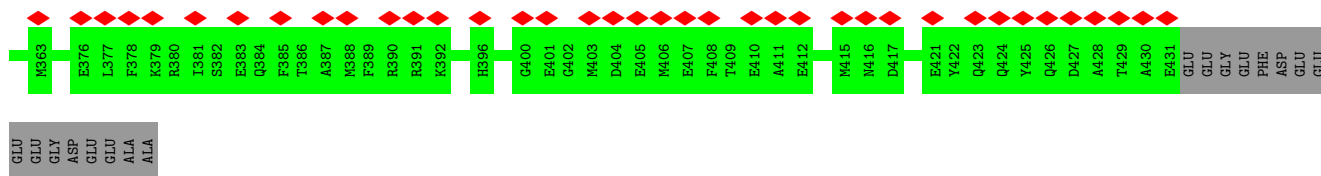


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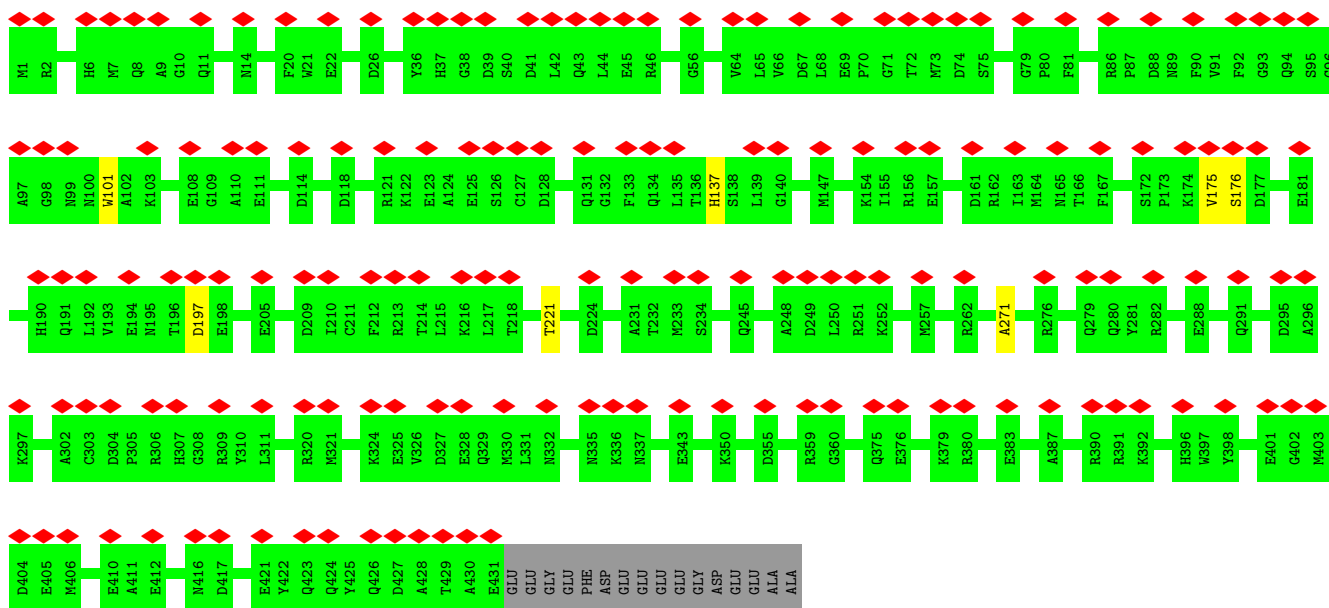
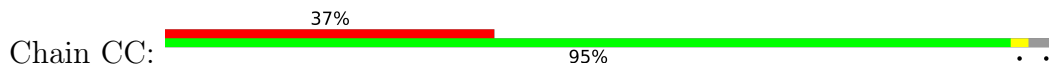


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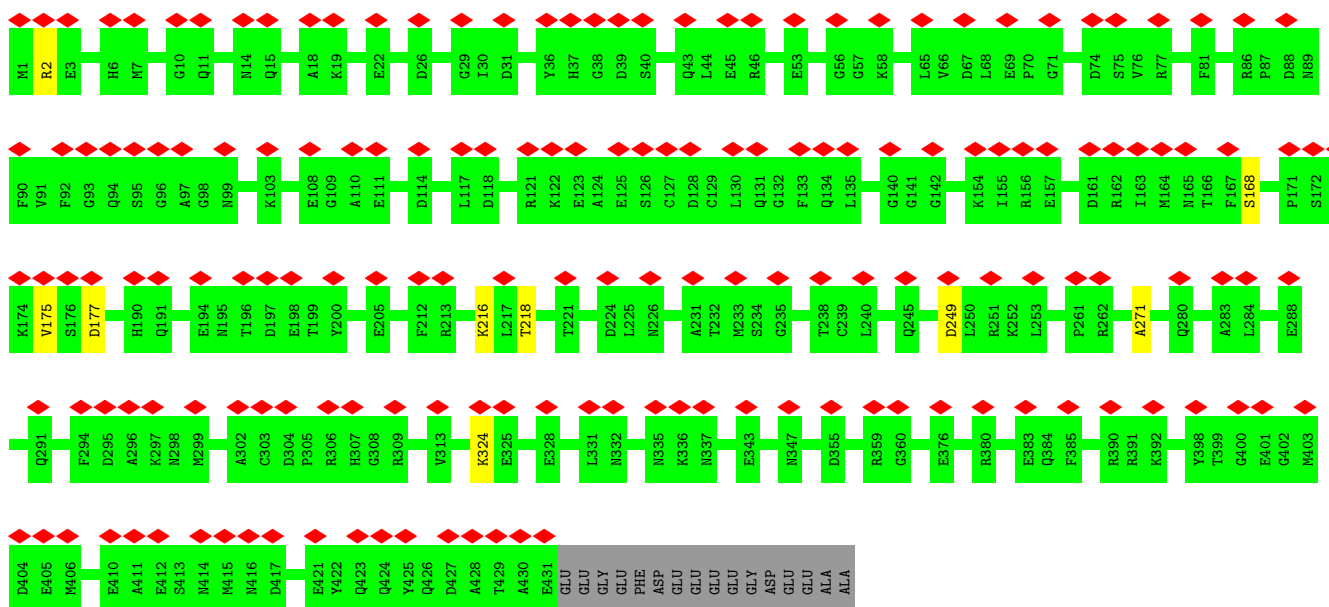
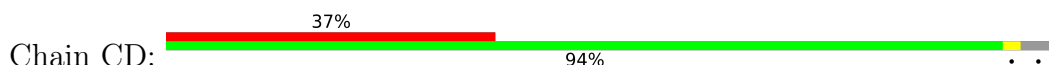




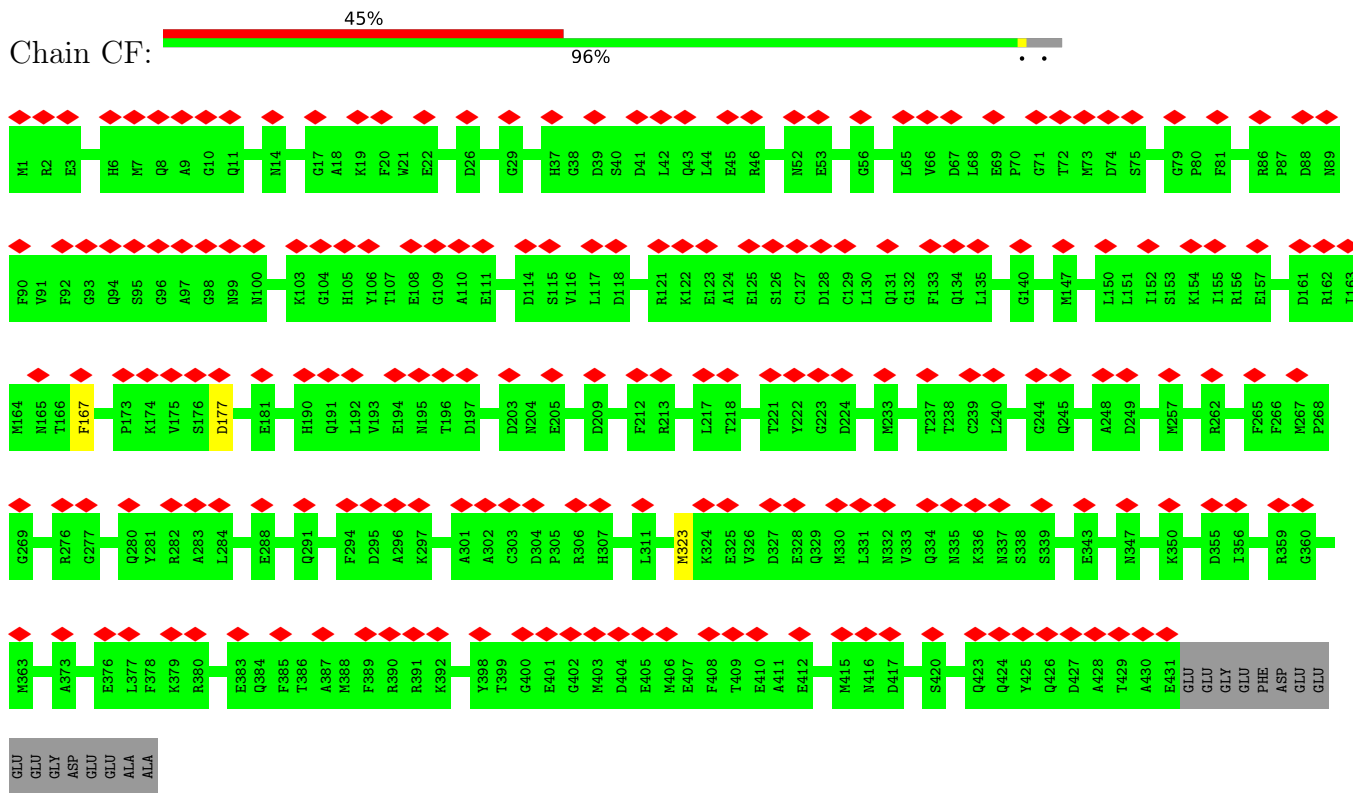
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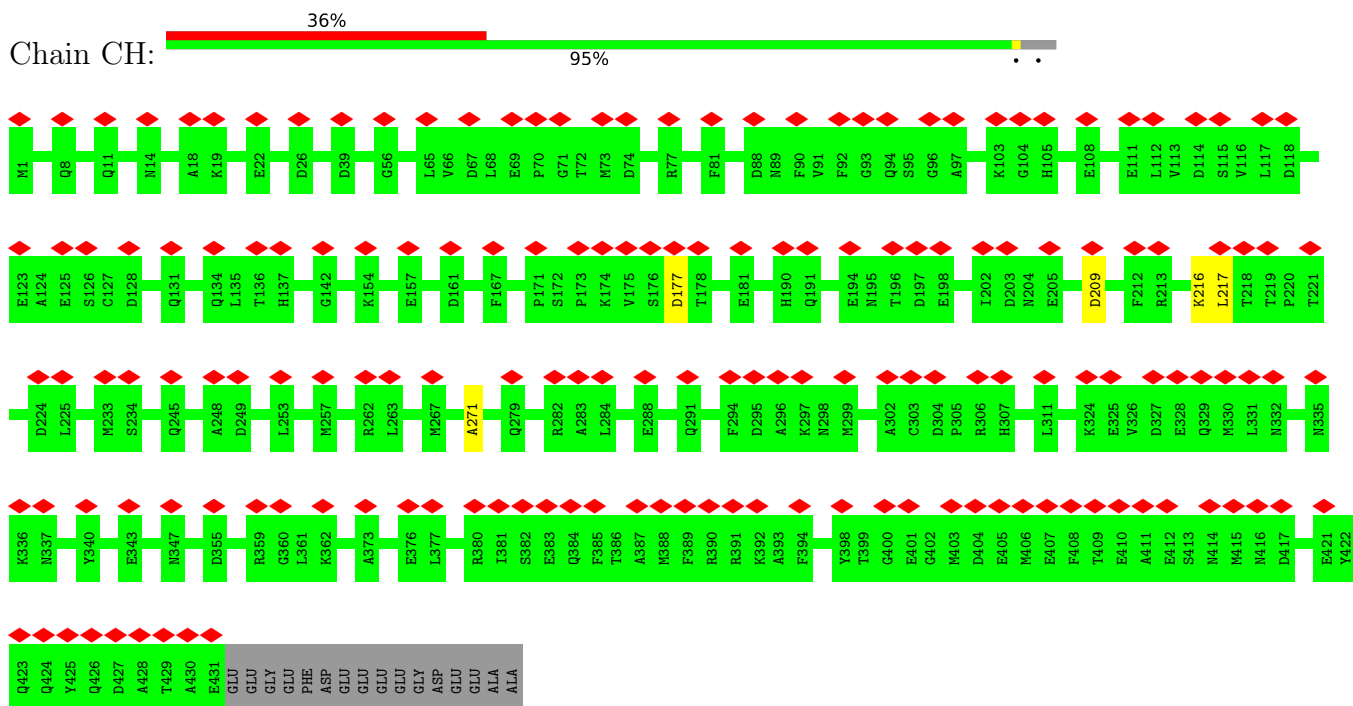
• Molecule 55: Tubulin beta chain



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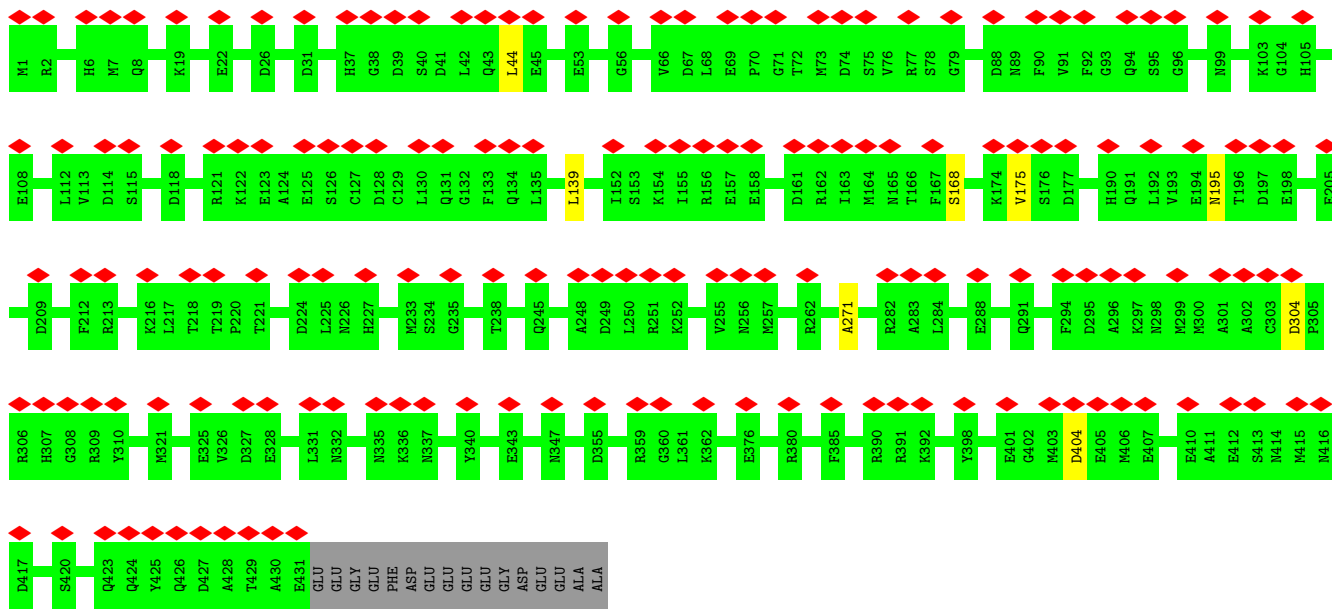


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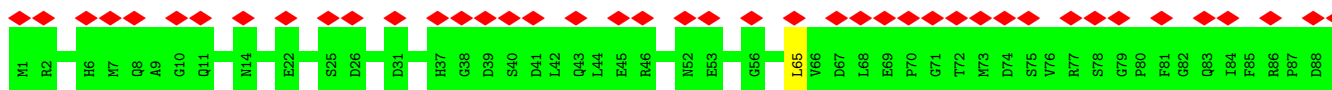


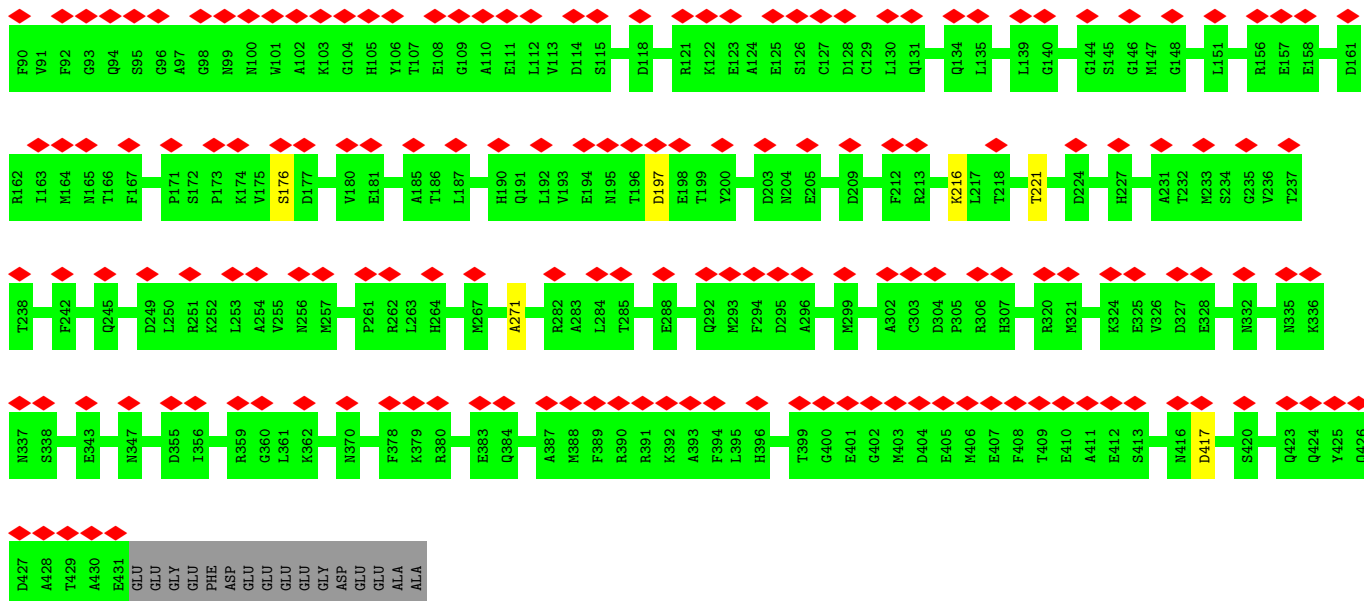


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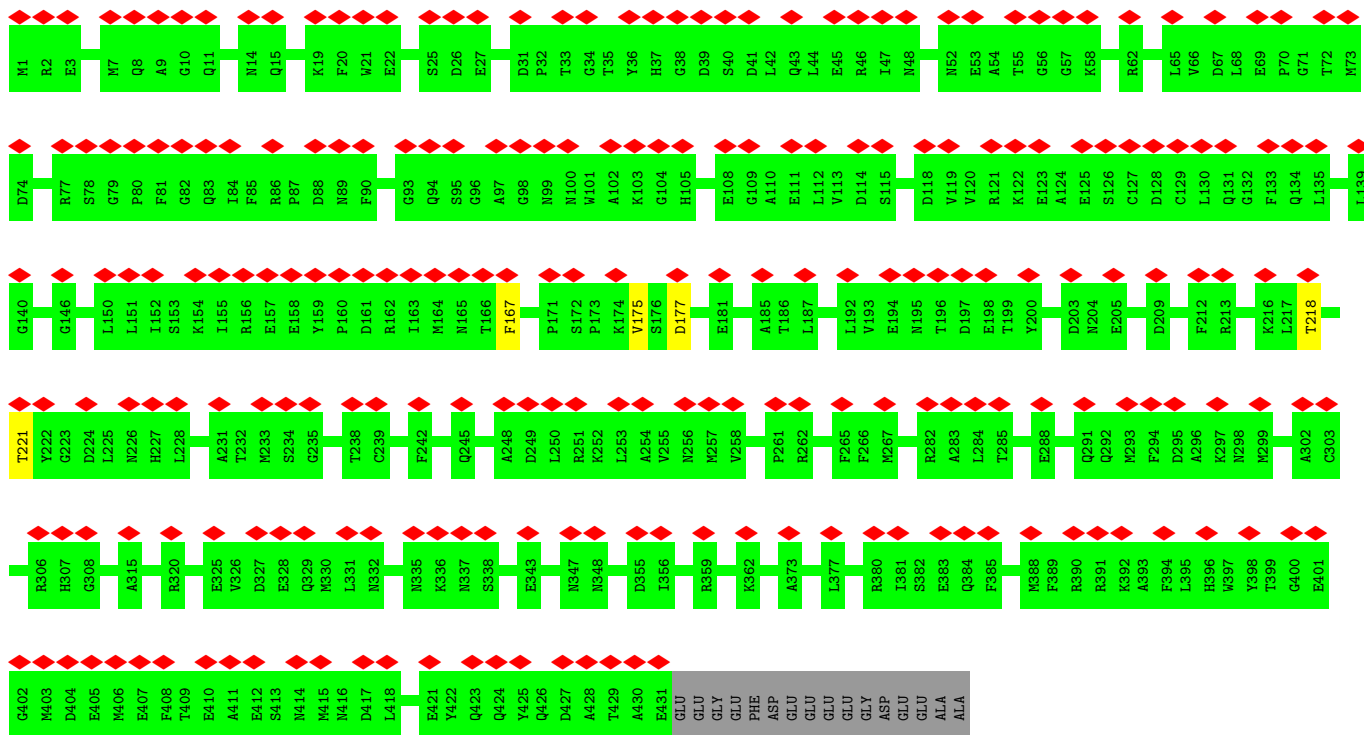


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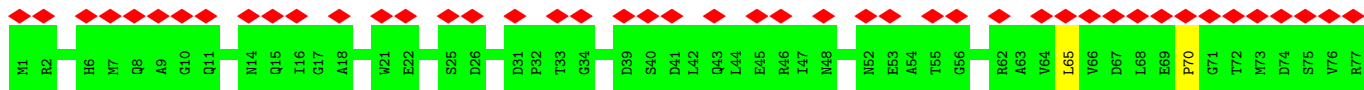




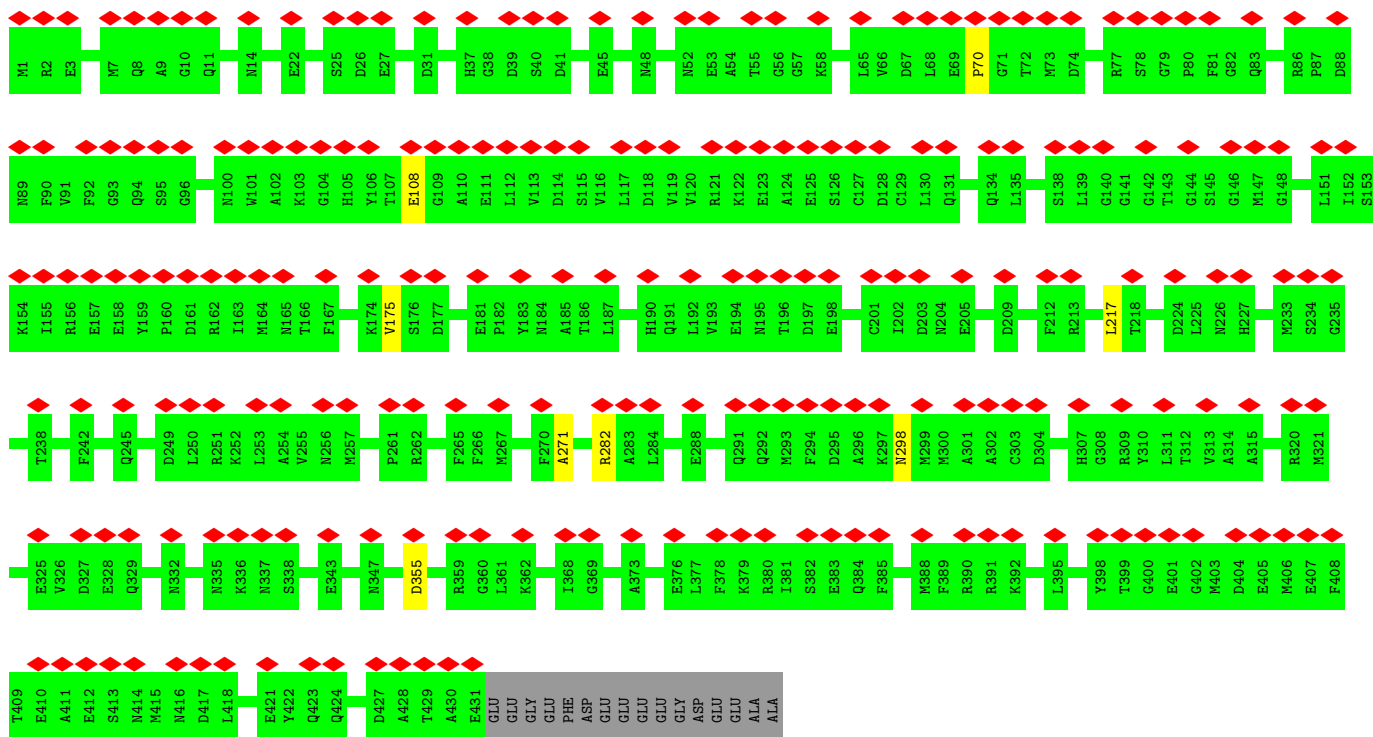
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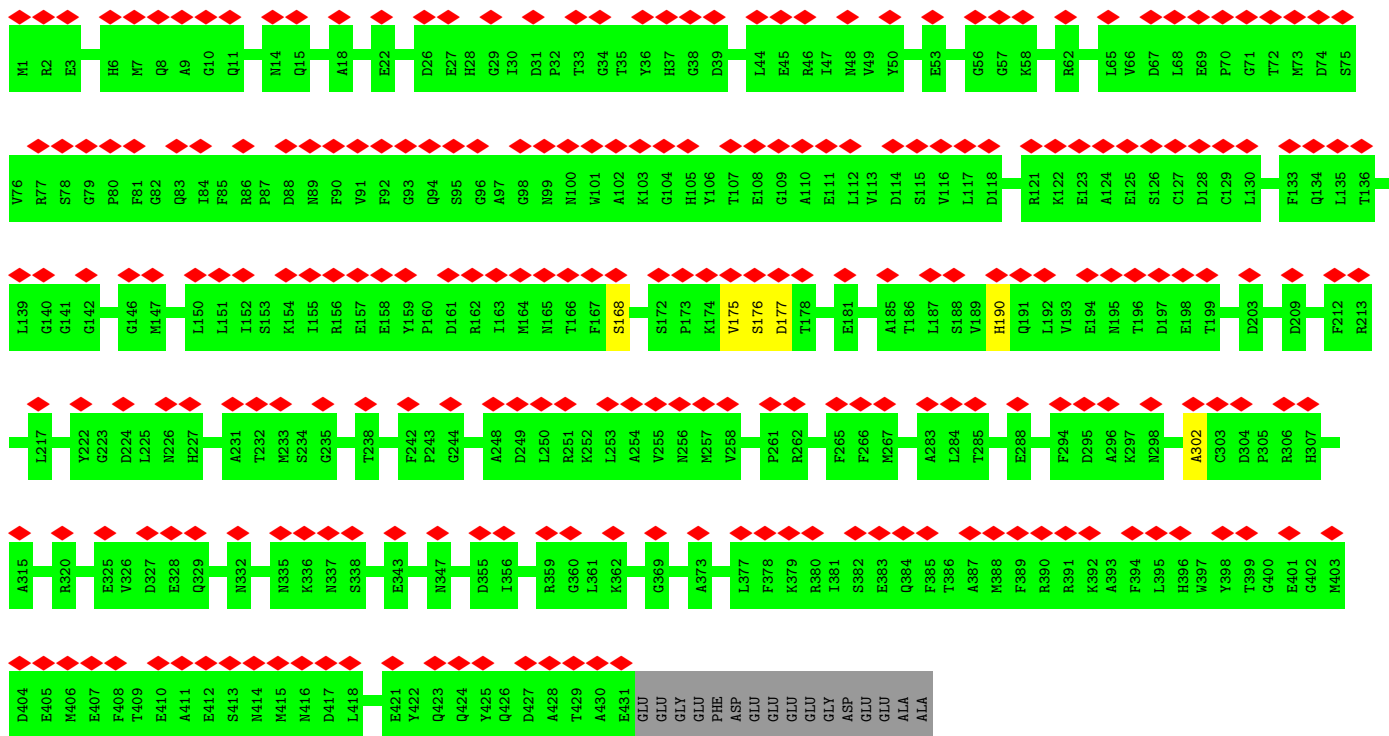
• Molecule 55: Tubulin beta chain







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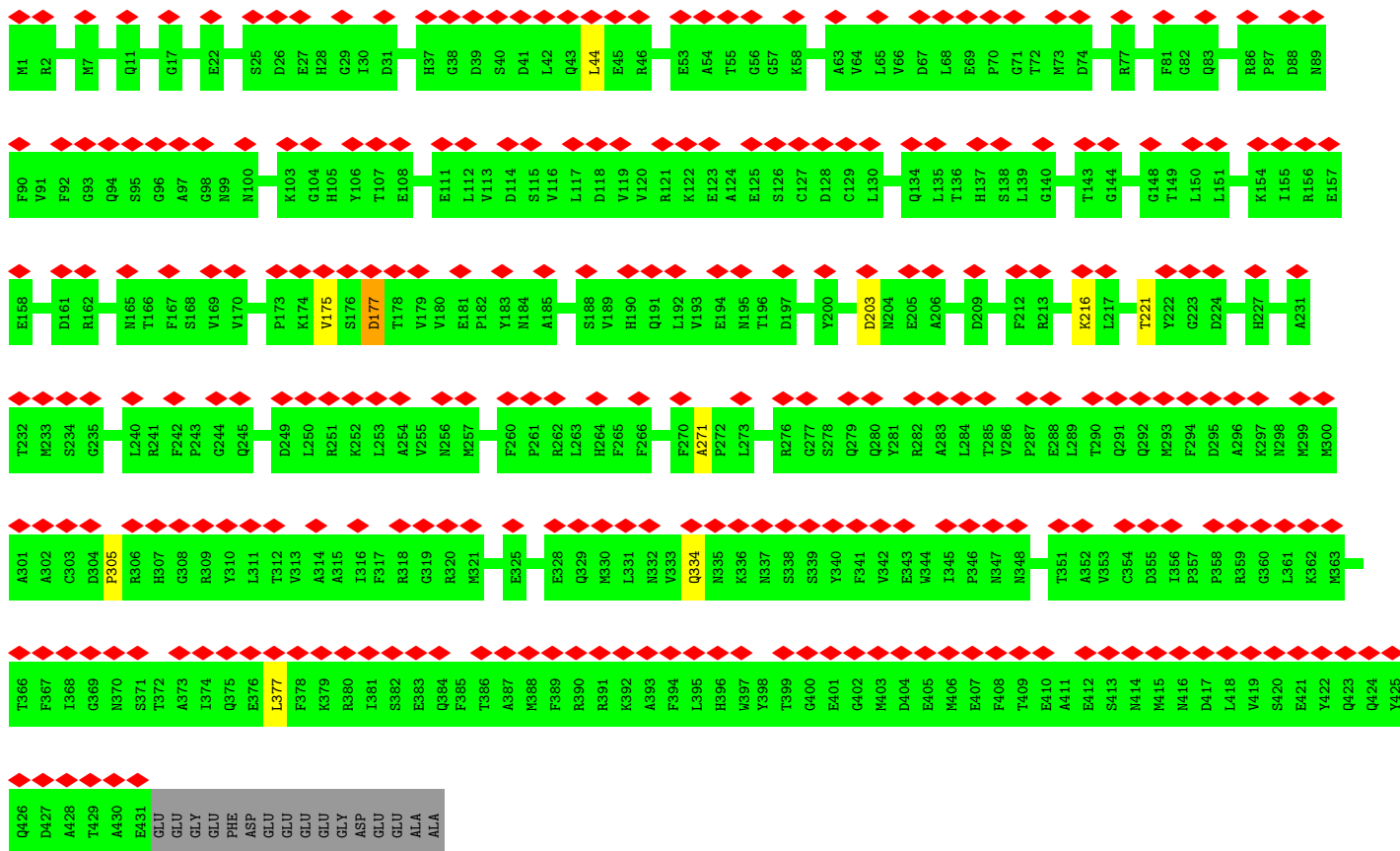


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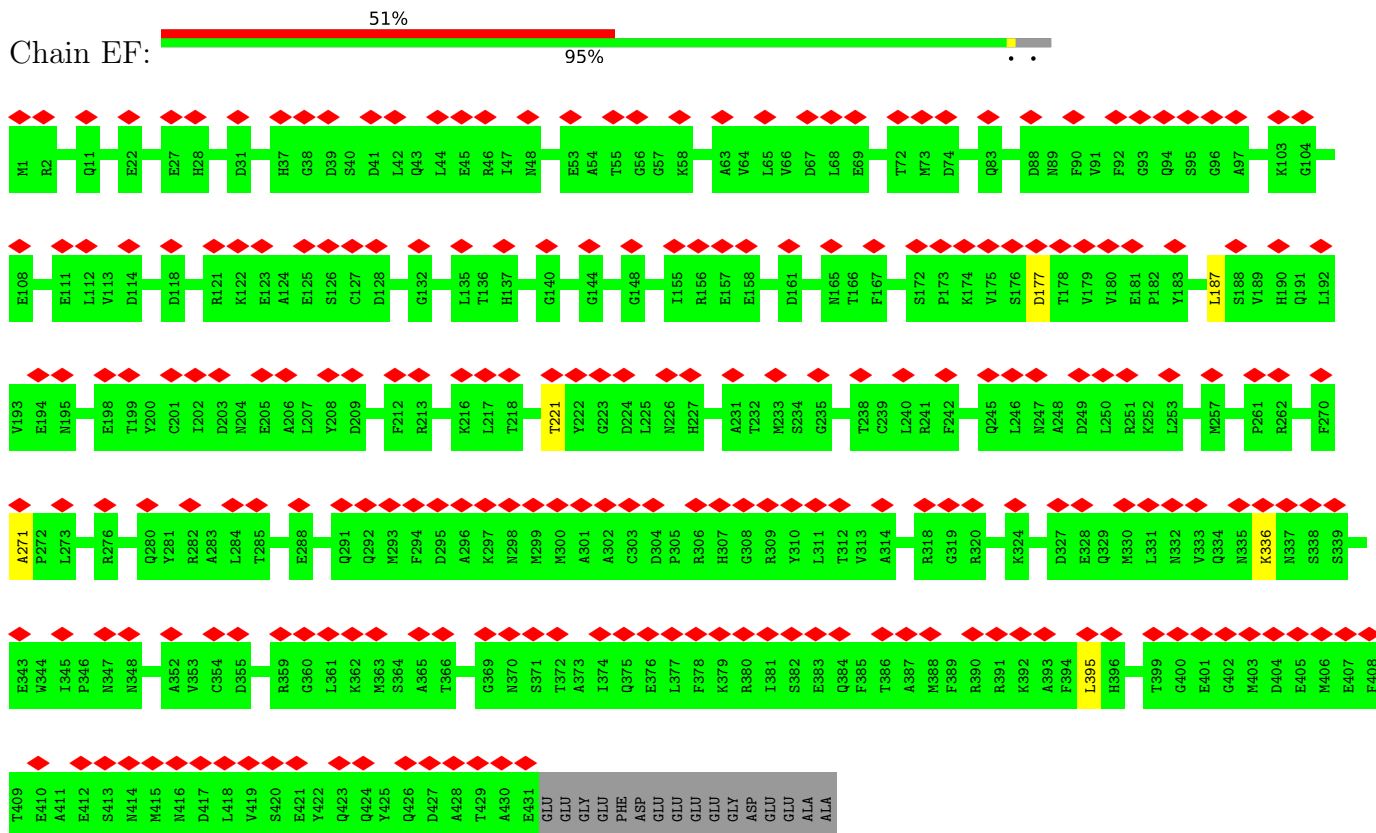


• Molecule 55: Tubulin beta chain

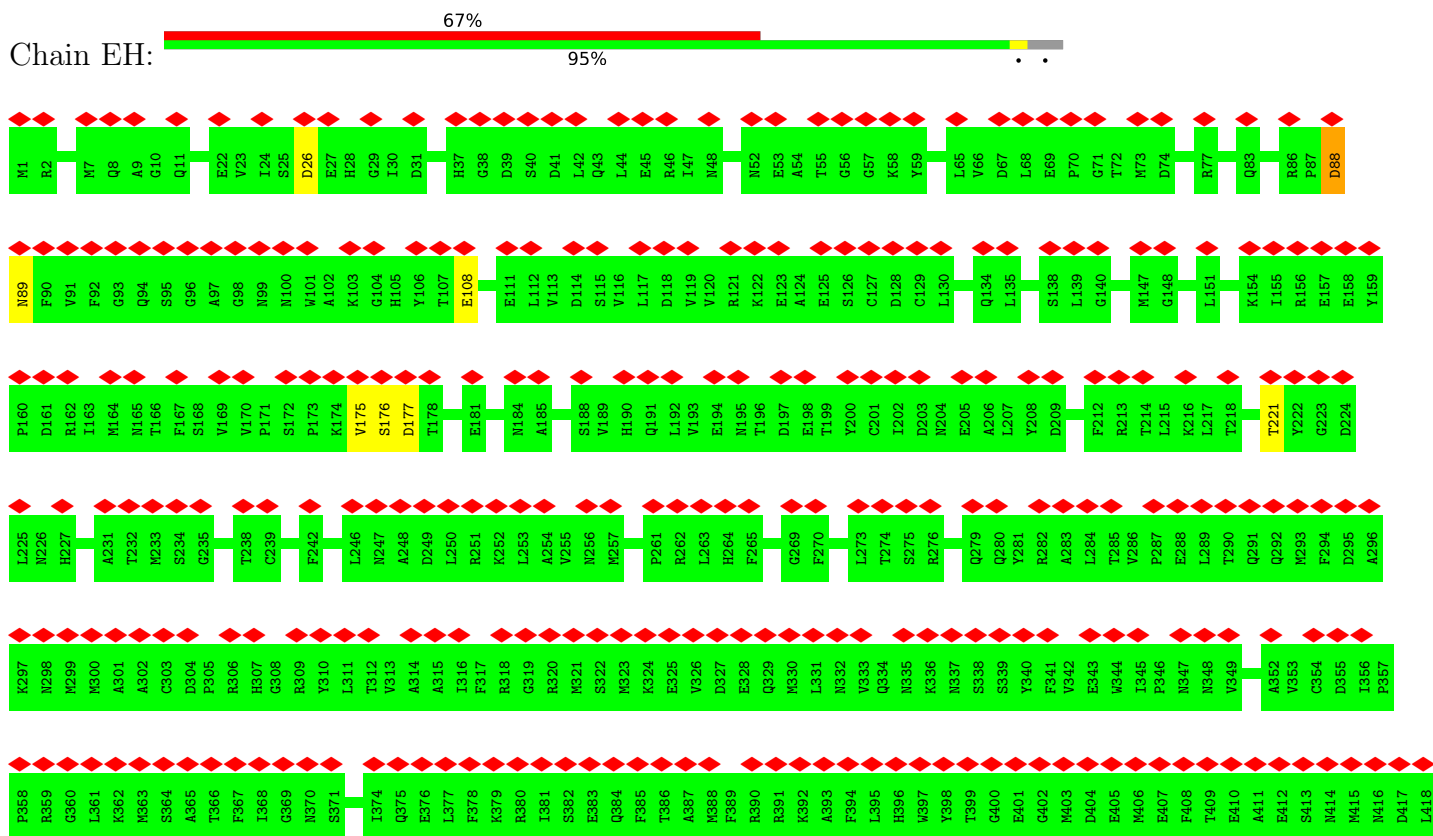


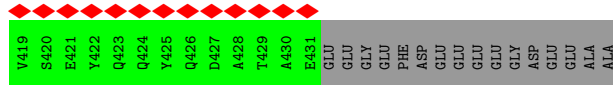


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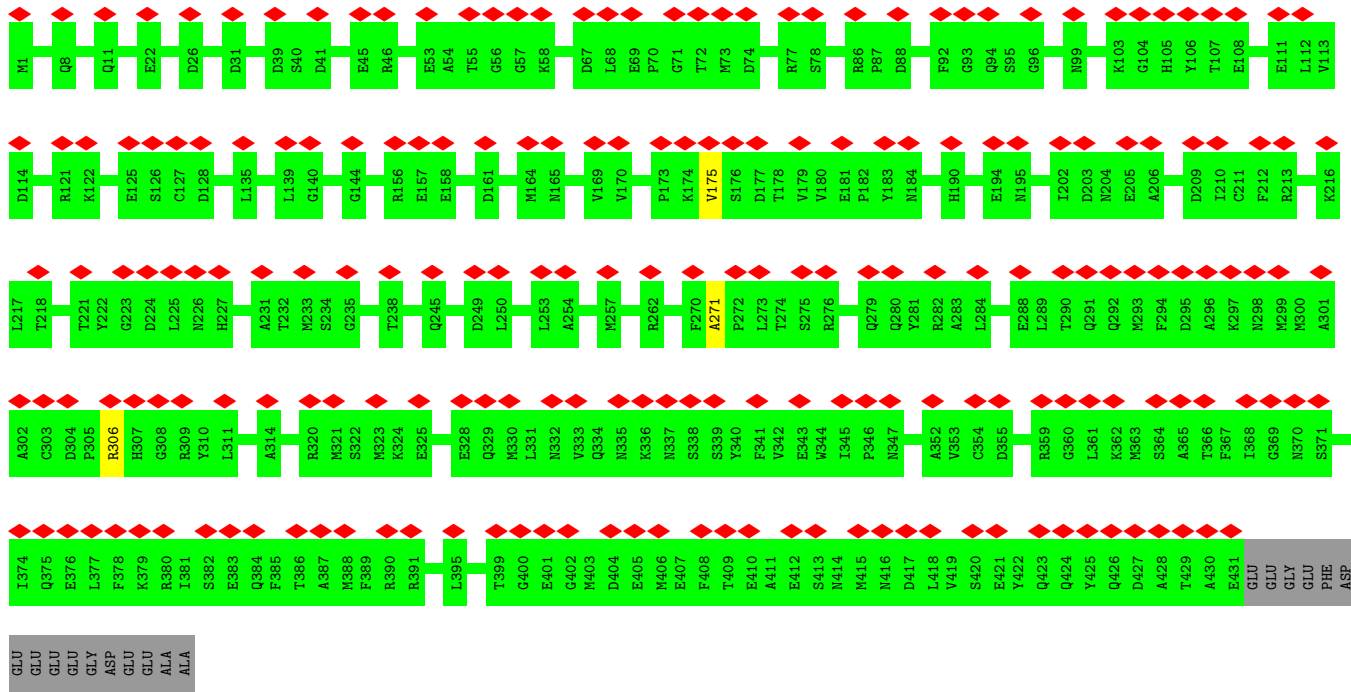


• Molecule 55: Tubulin beta chain

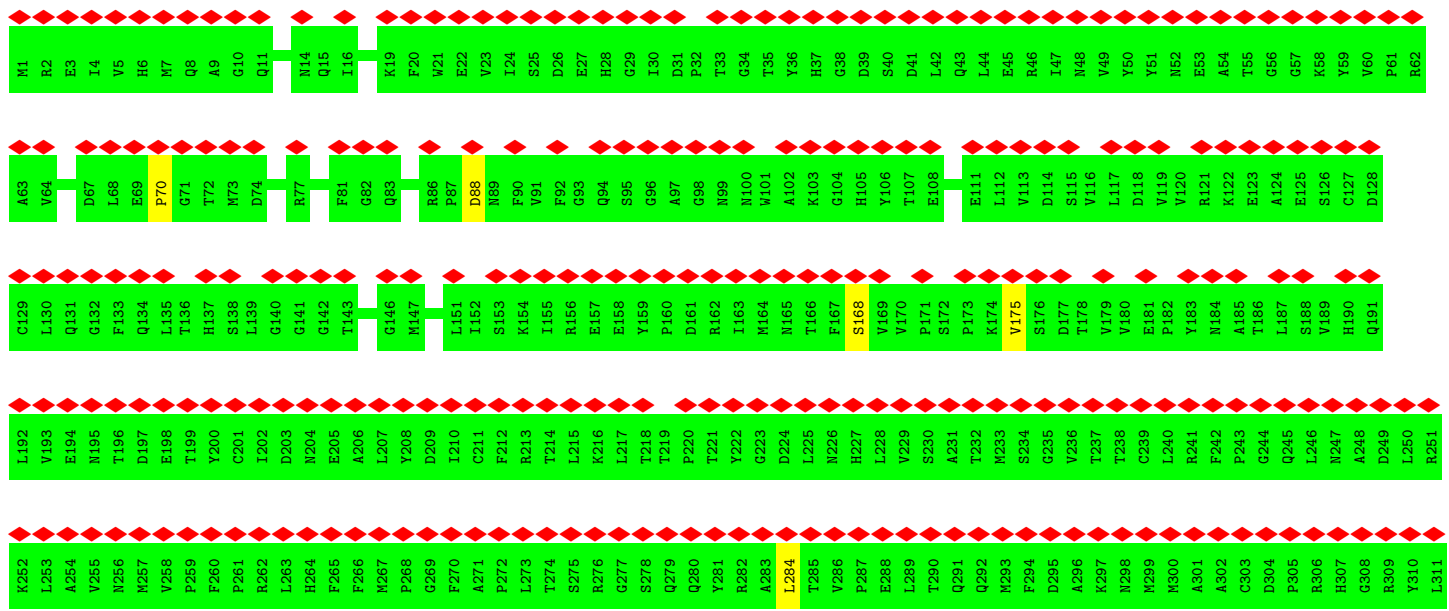
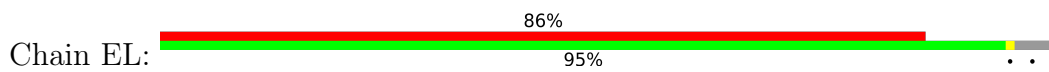


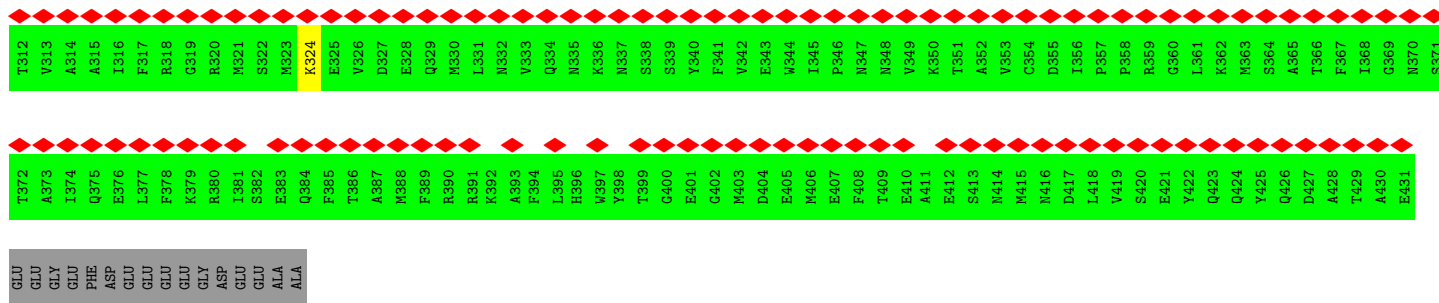


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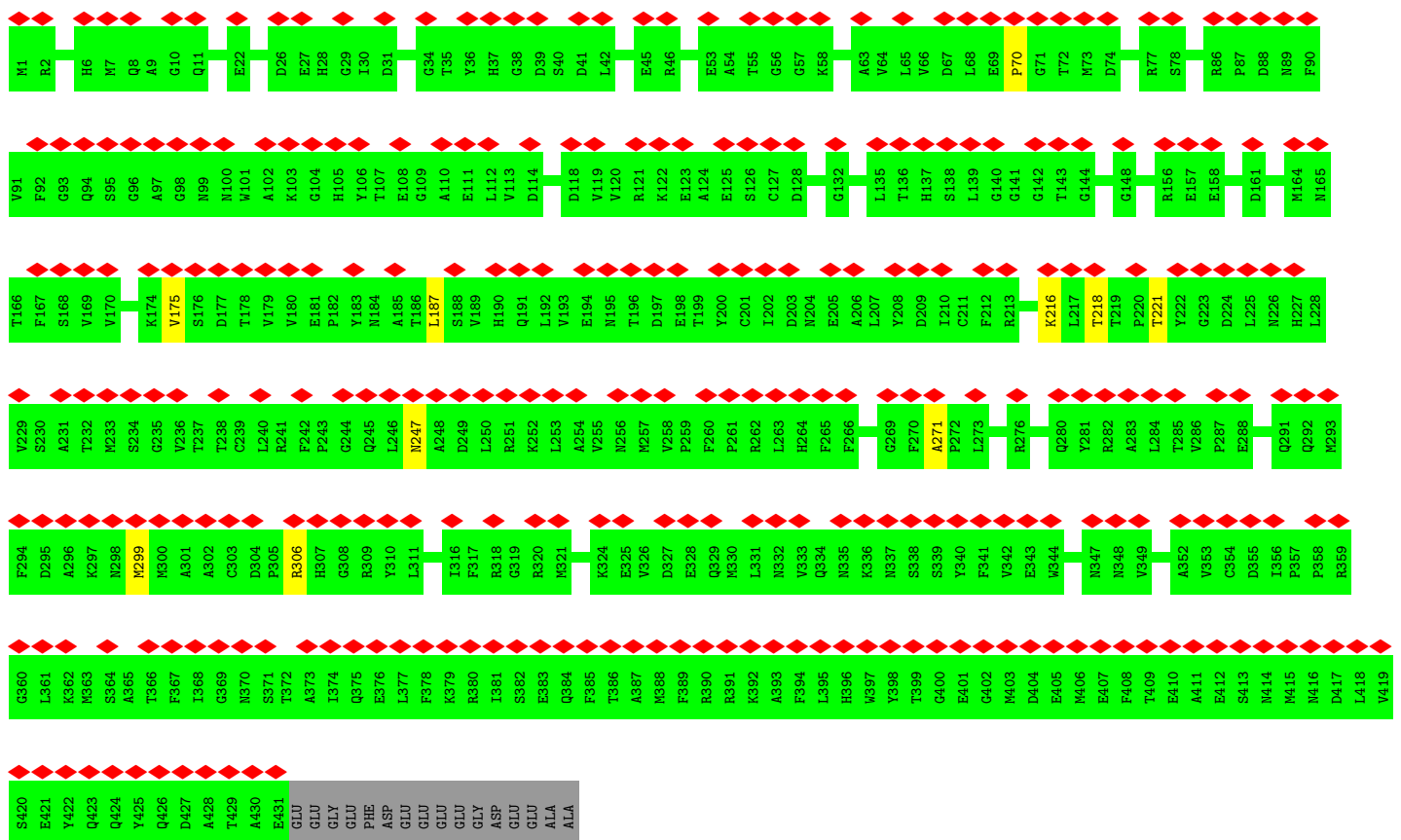


• Molecule 55: Tubulin beta chain

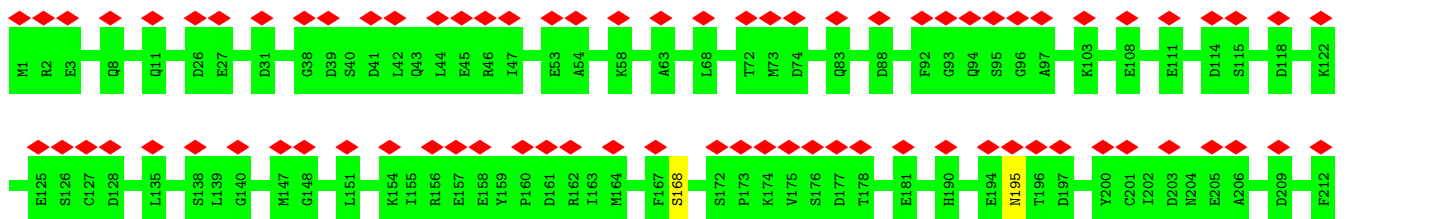


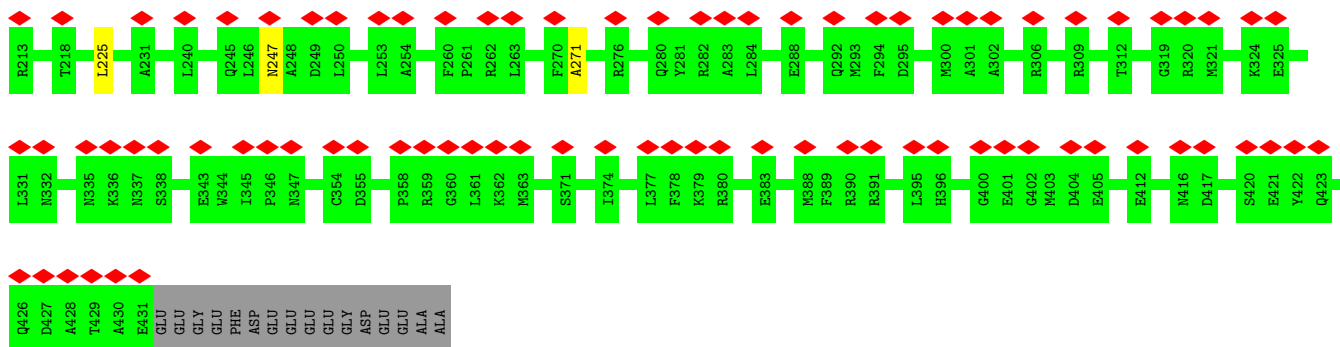


- Molecule 55: Tubulin beta chain

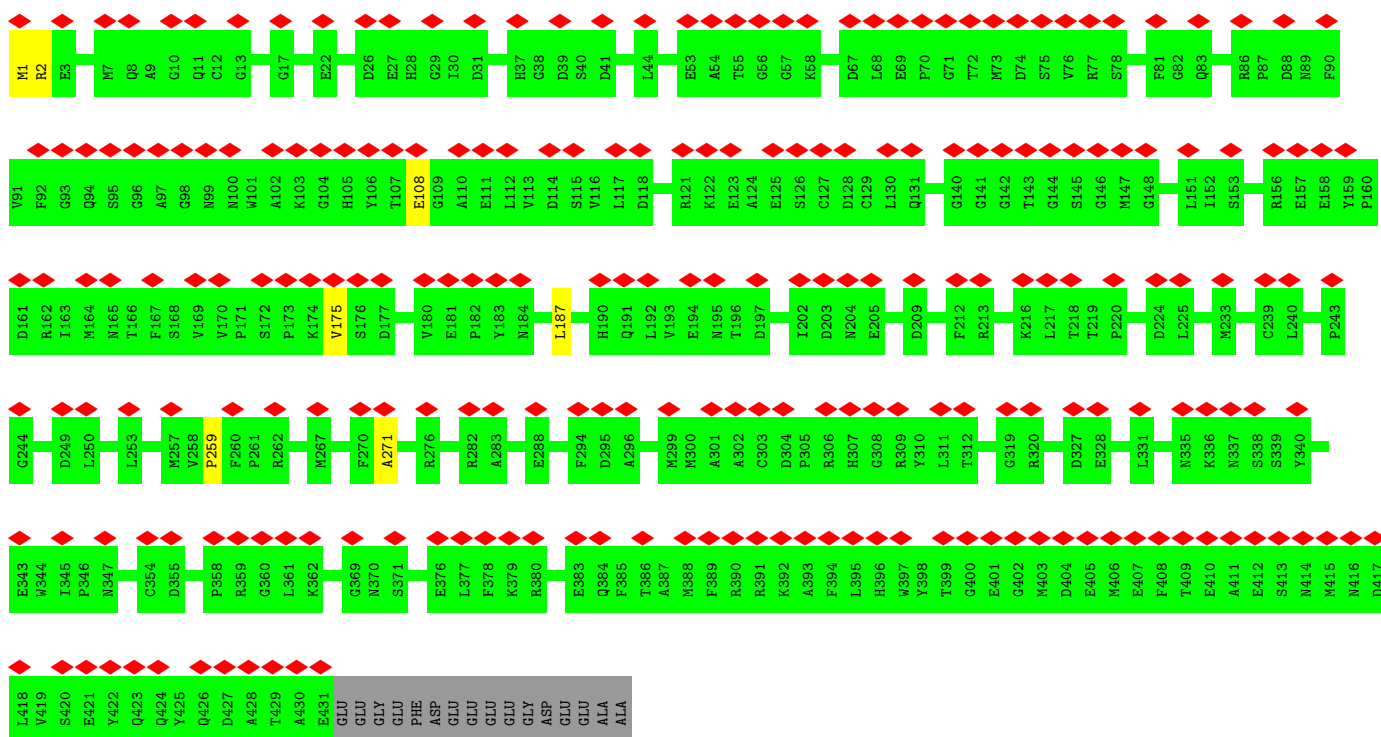


- Molecule 55: Tubulin beta chain

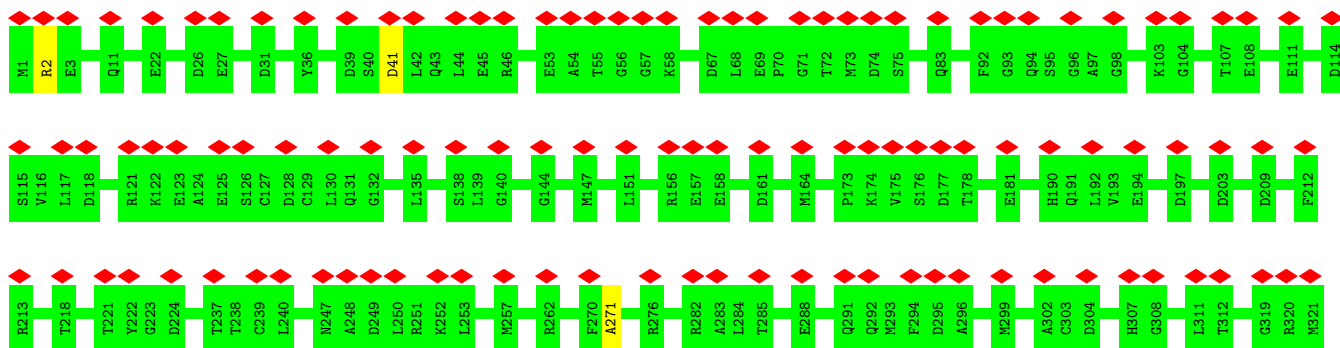


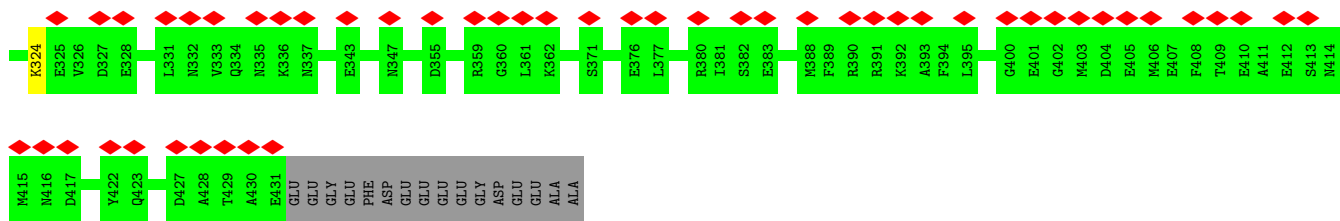


- Molecule 55: Tubulin beta chain

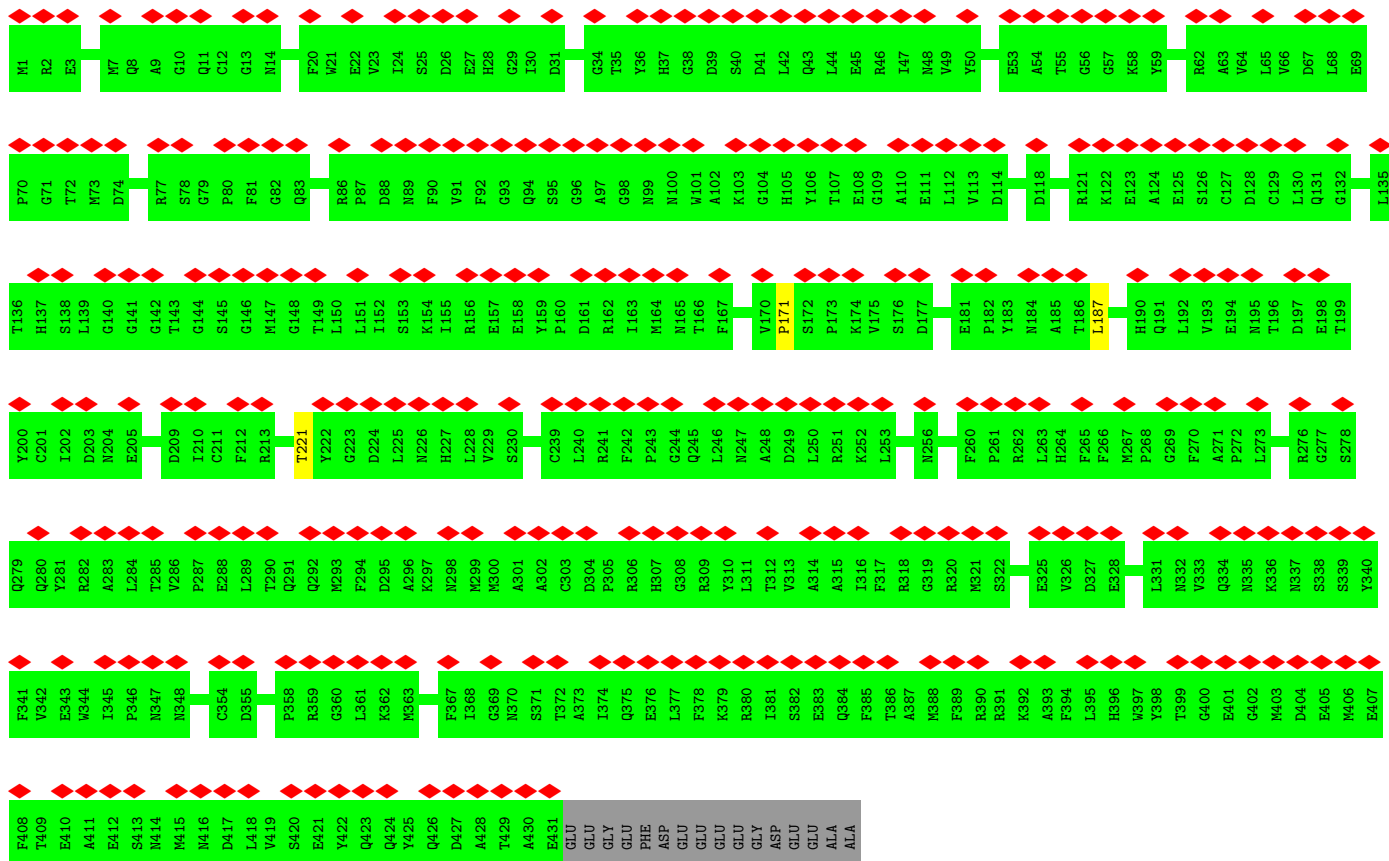


- Molecule 55: Tubulin beta chain

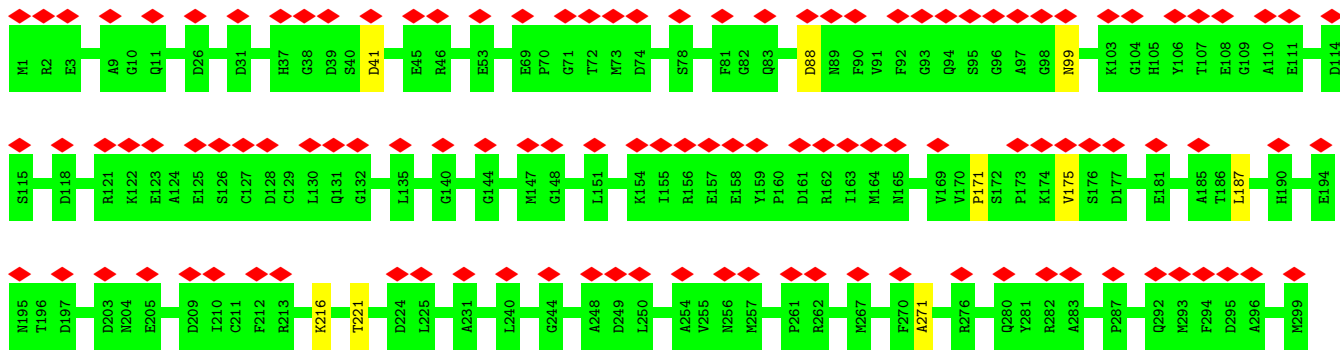
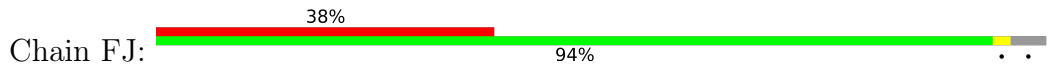


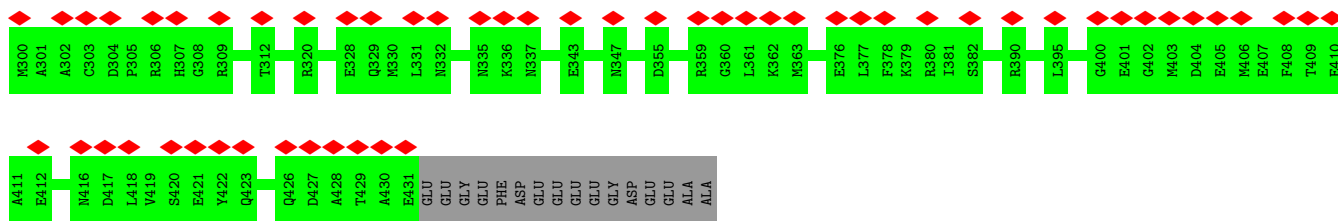


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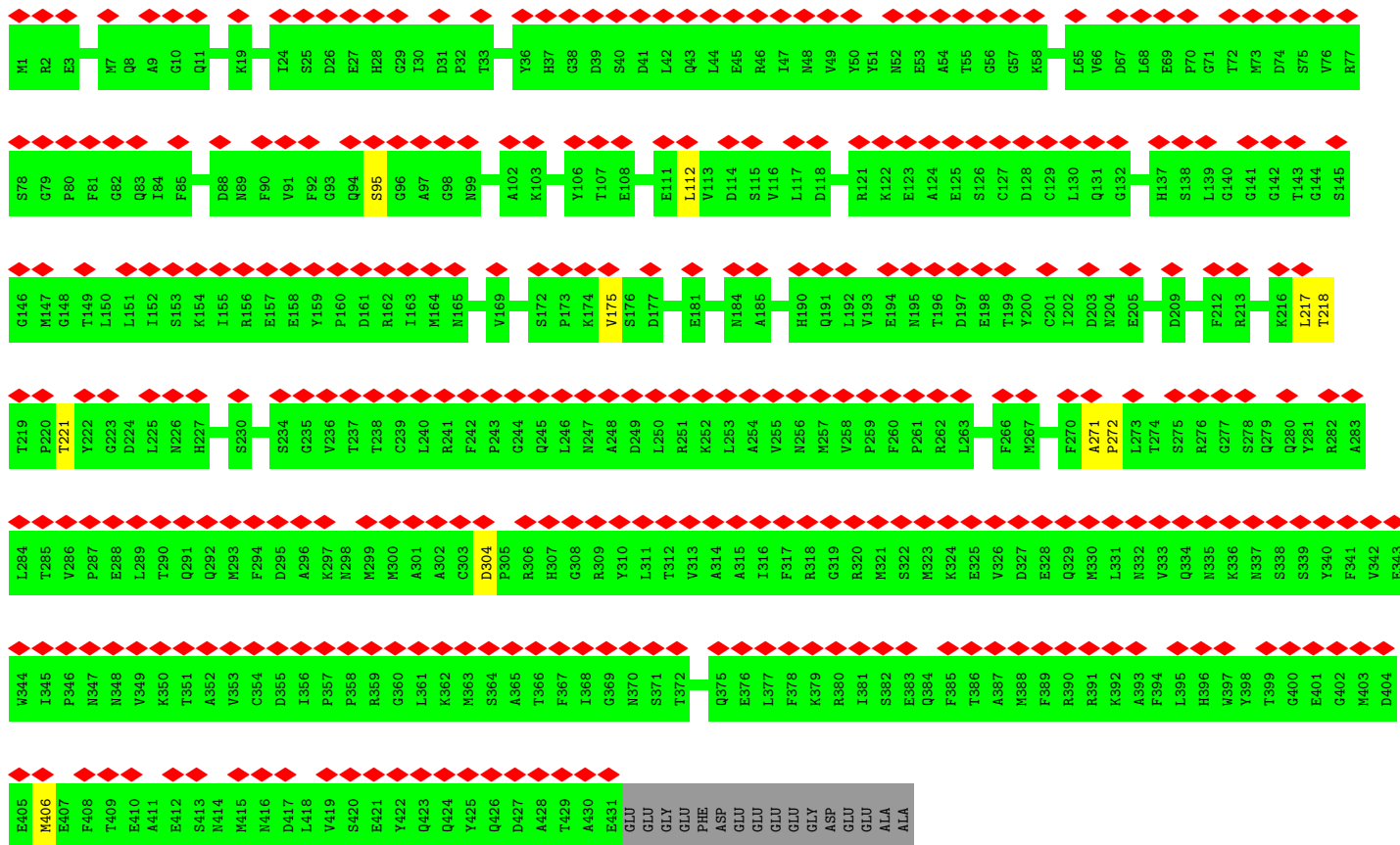
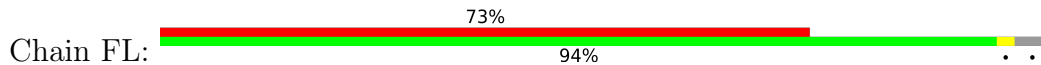


• Molecule 55: Tubulin beta chain

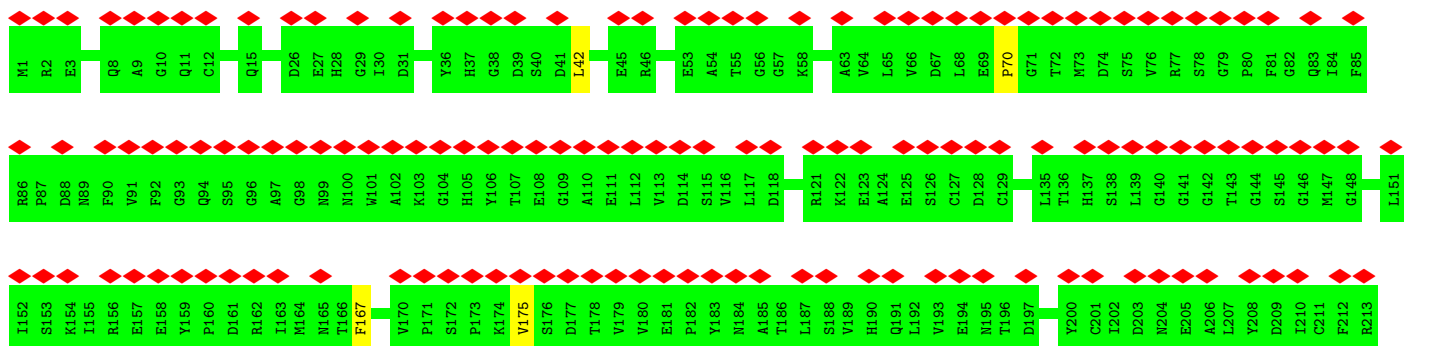


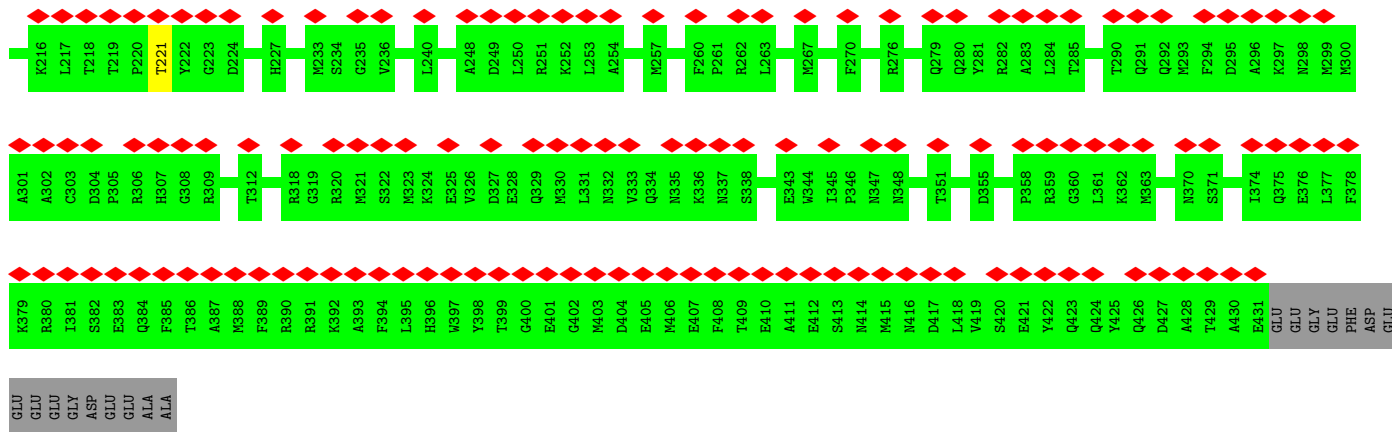


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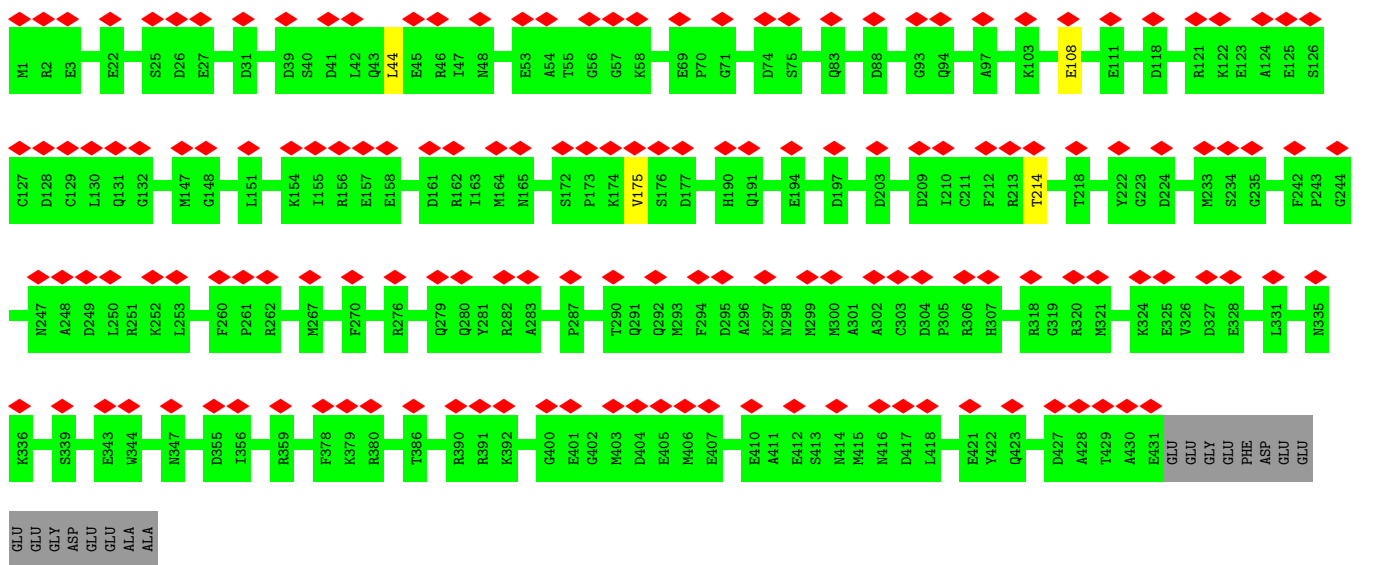


• Molecule 55: Tubulin beta chain

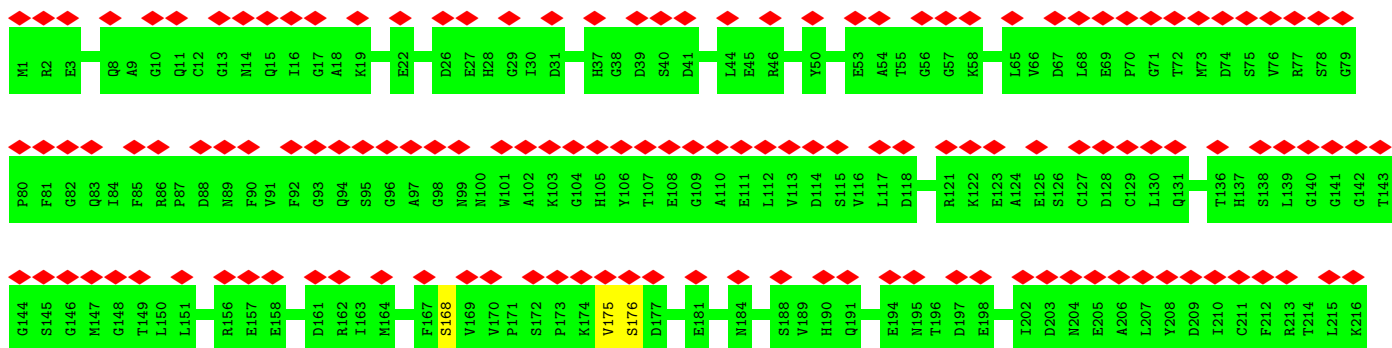


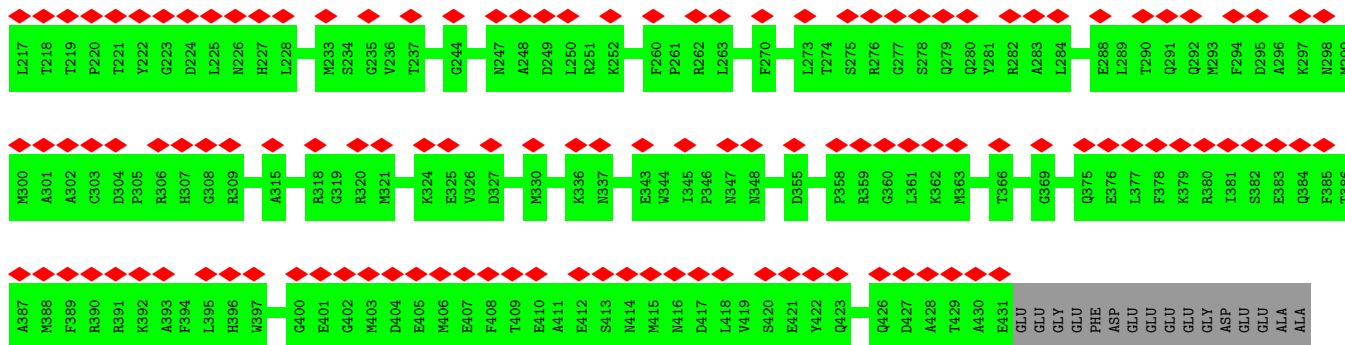


• Molecule 55: Tubulin beta chain

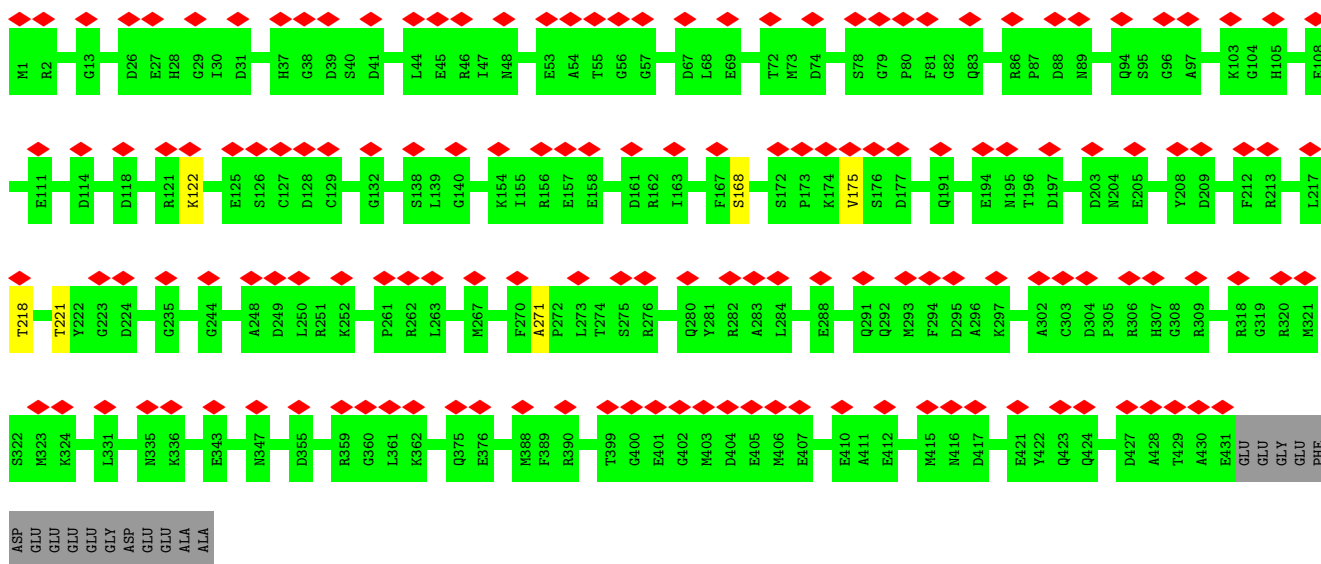


• Molecule 55: Tubulin beta chain

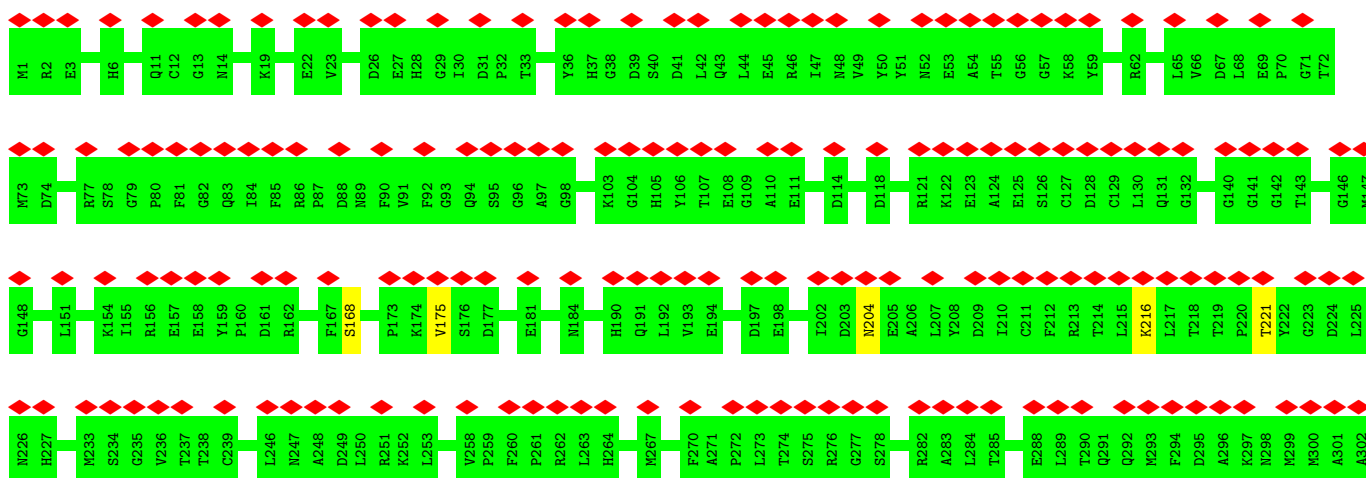




• Molecule 55: Tubulin beta chain



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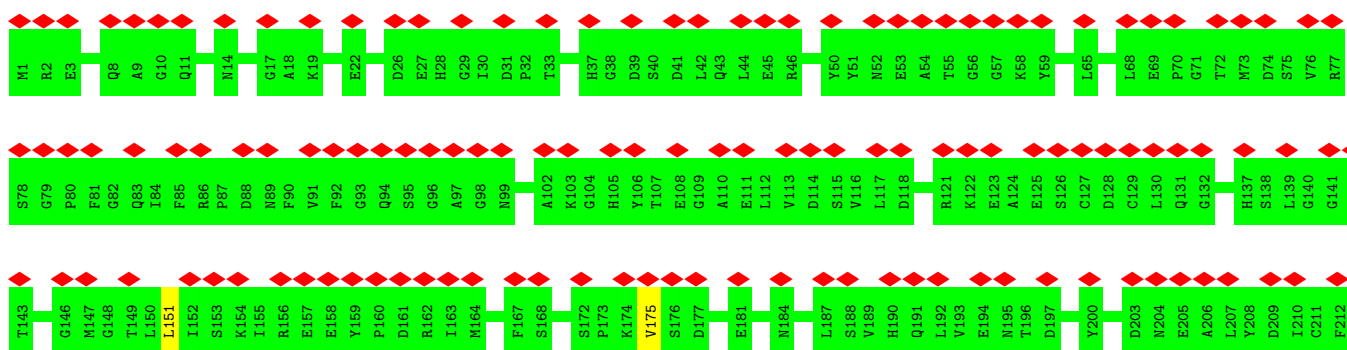


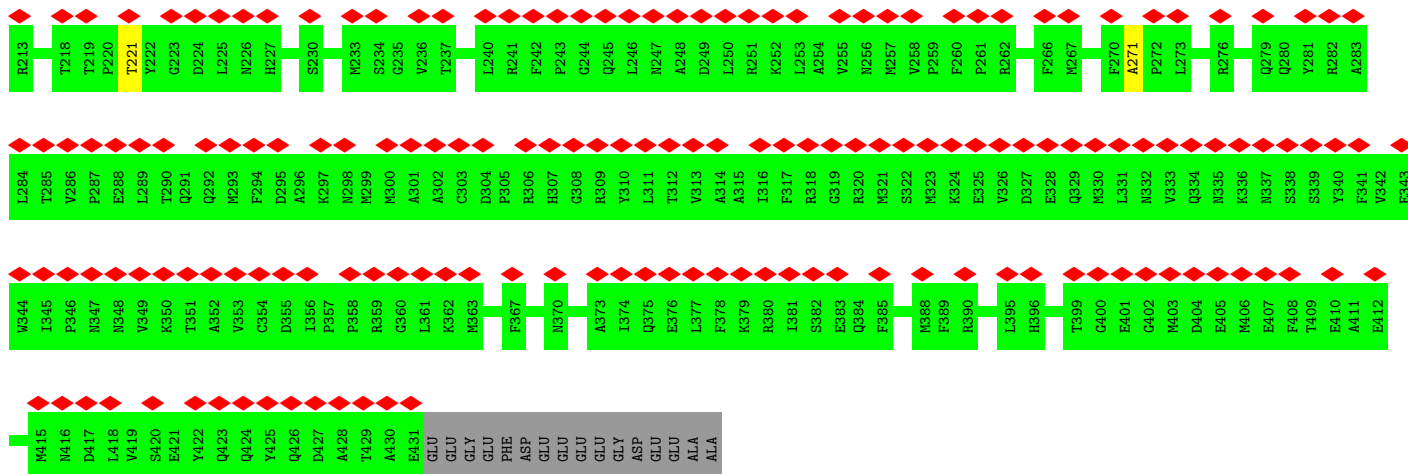


• Molecule 55: Tubulin beta chain

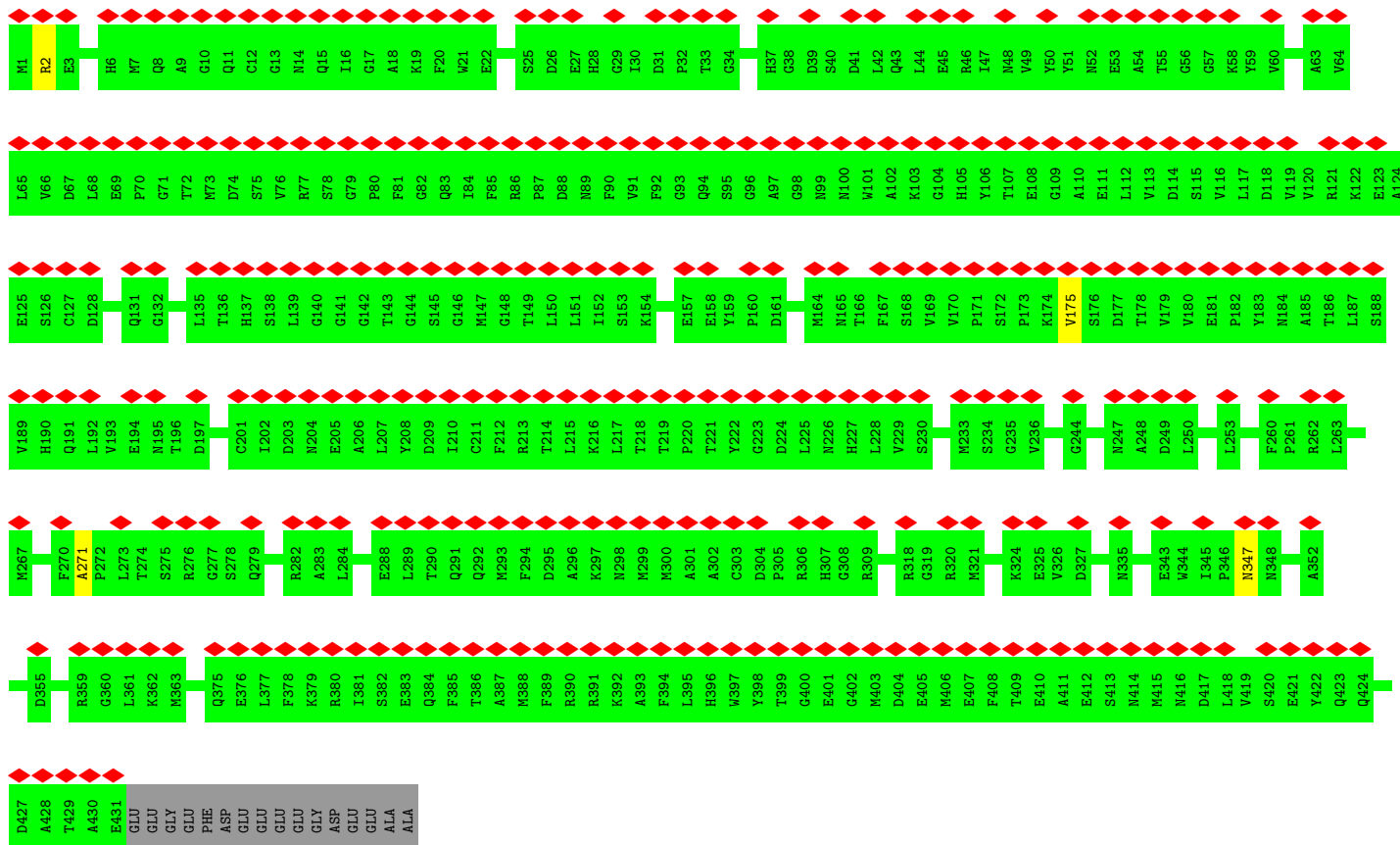


• Molecule 55: Tubulin beta chain



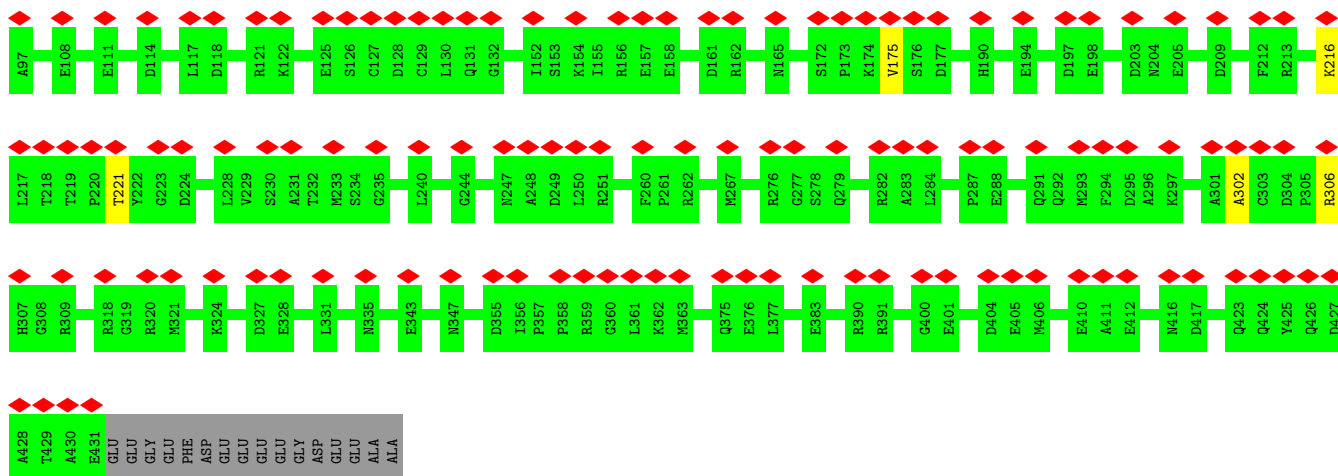


• Molecule 55: Tubulin beta chain

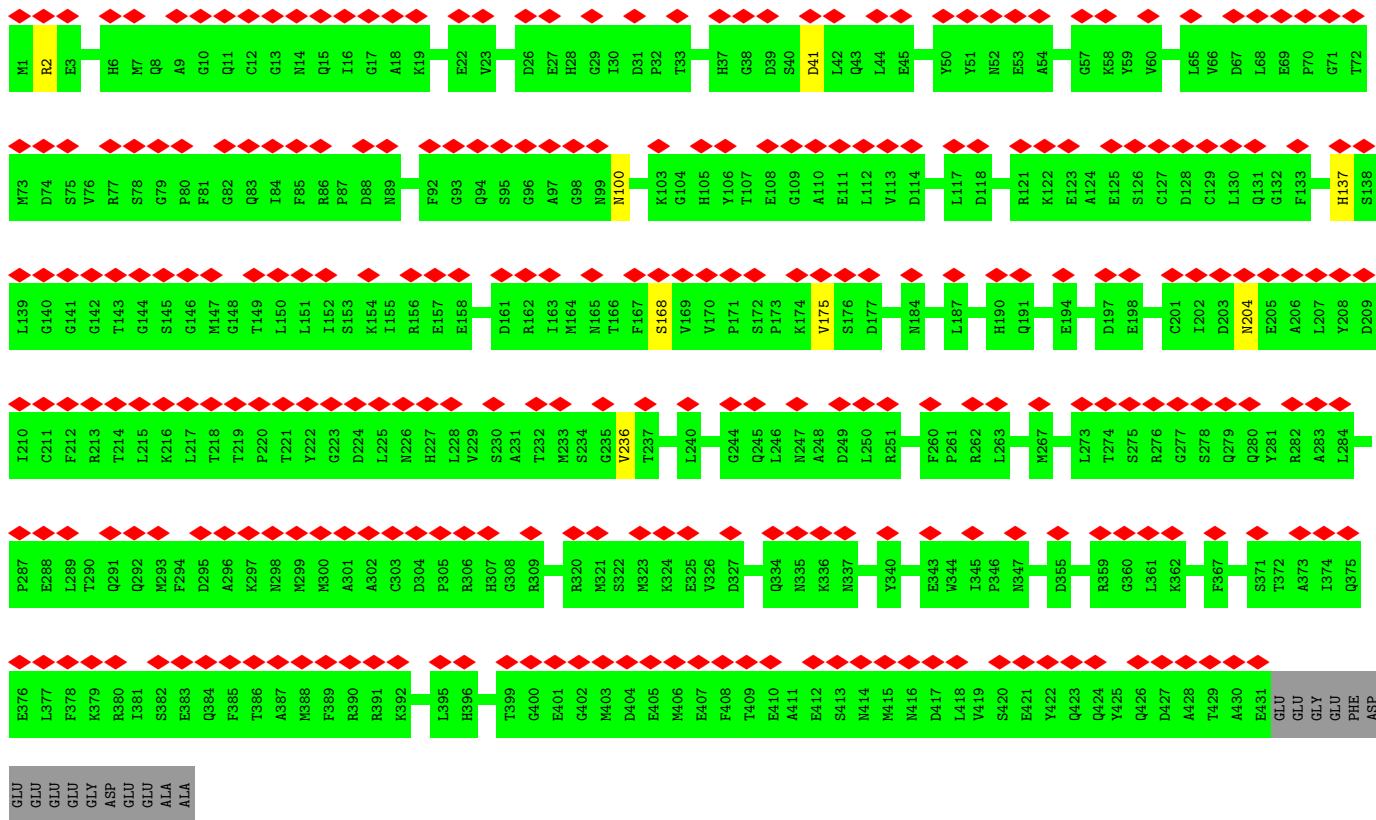


• Molecule 55: Tubulin beta chain

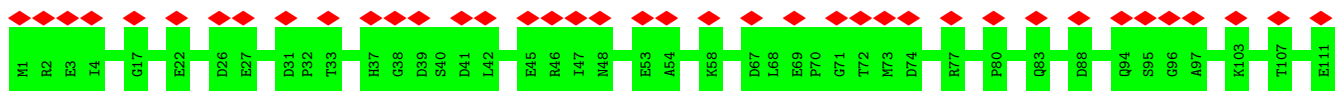


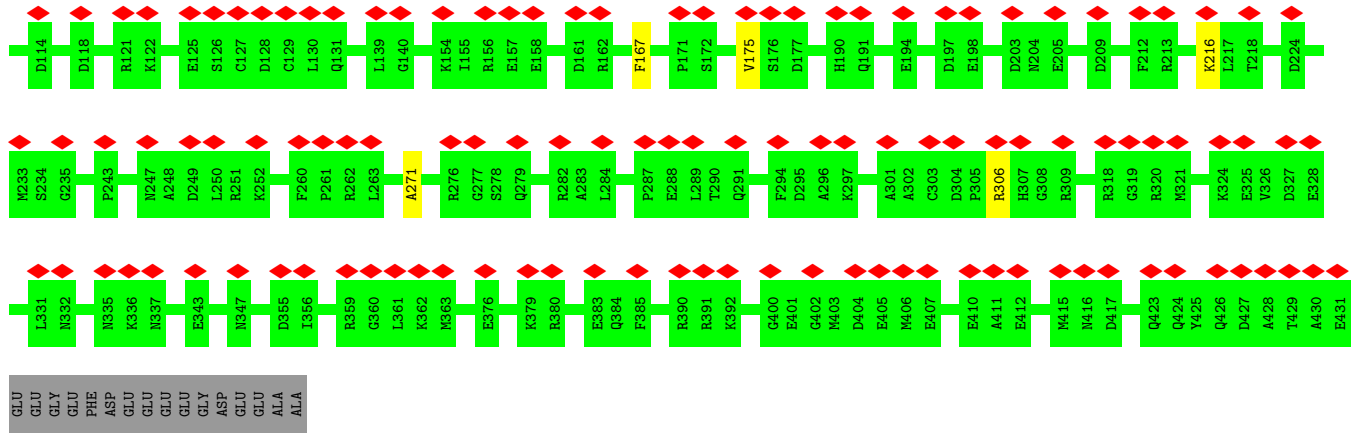


• Molecule 55: Tubulin beta chain

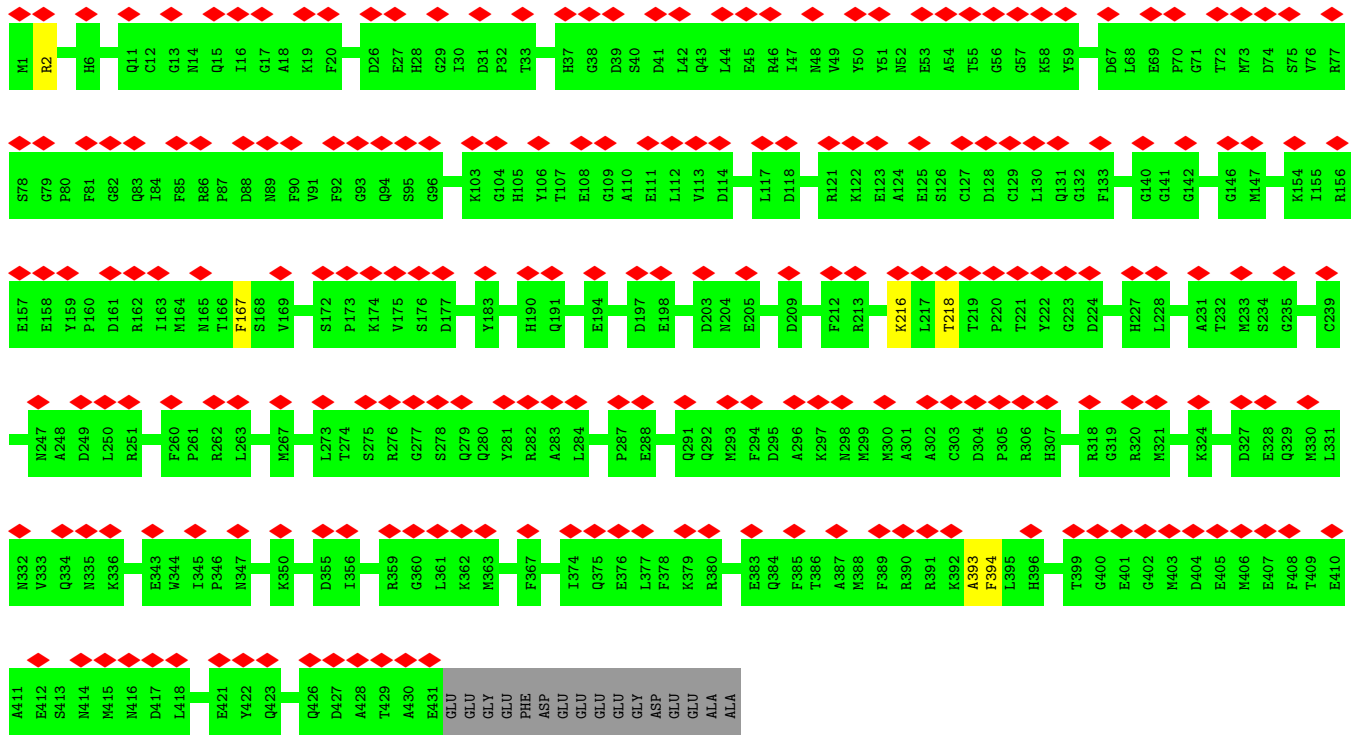


• Molecule 55: Tubulin beta chain

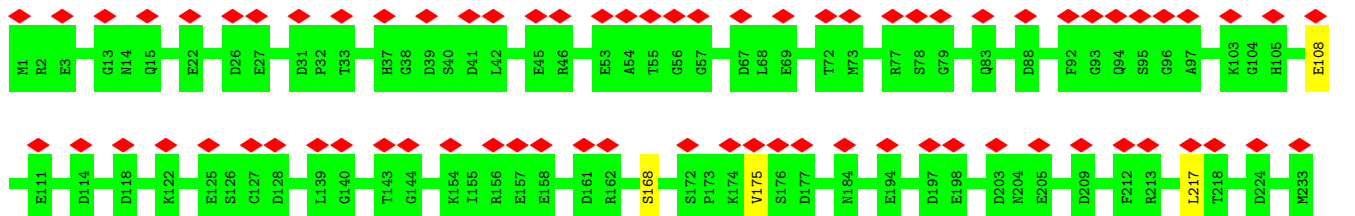


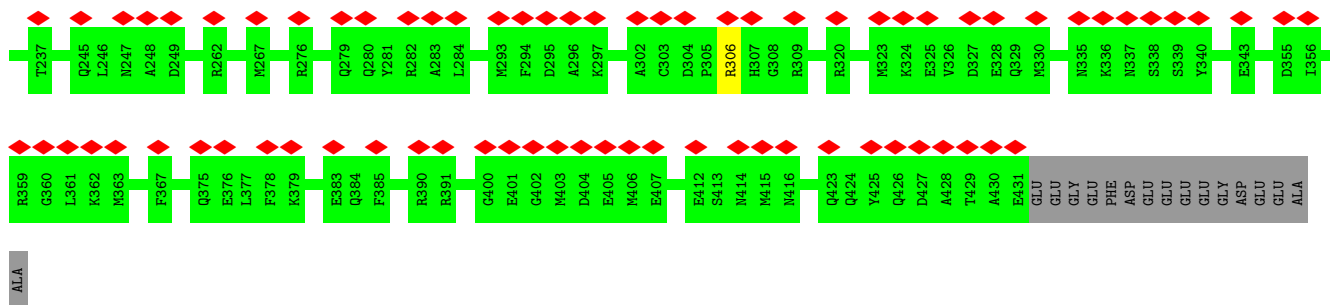


• Molecule 55: Tubulin beta chain

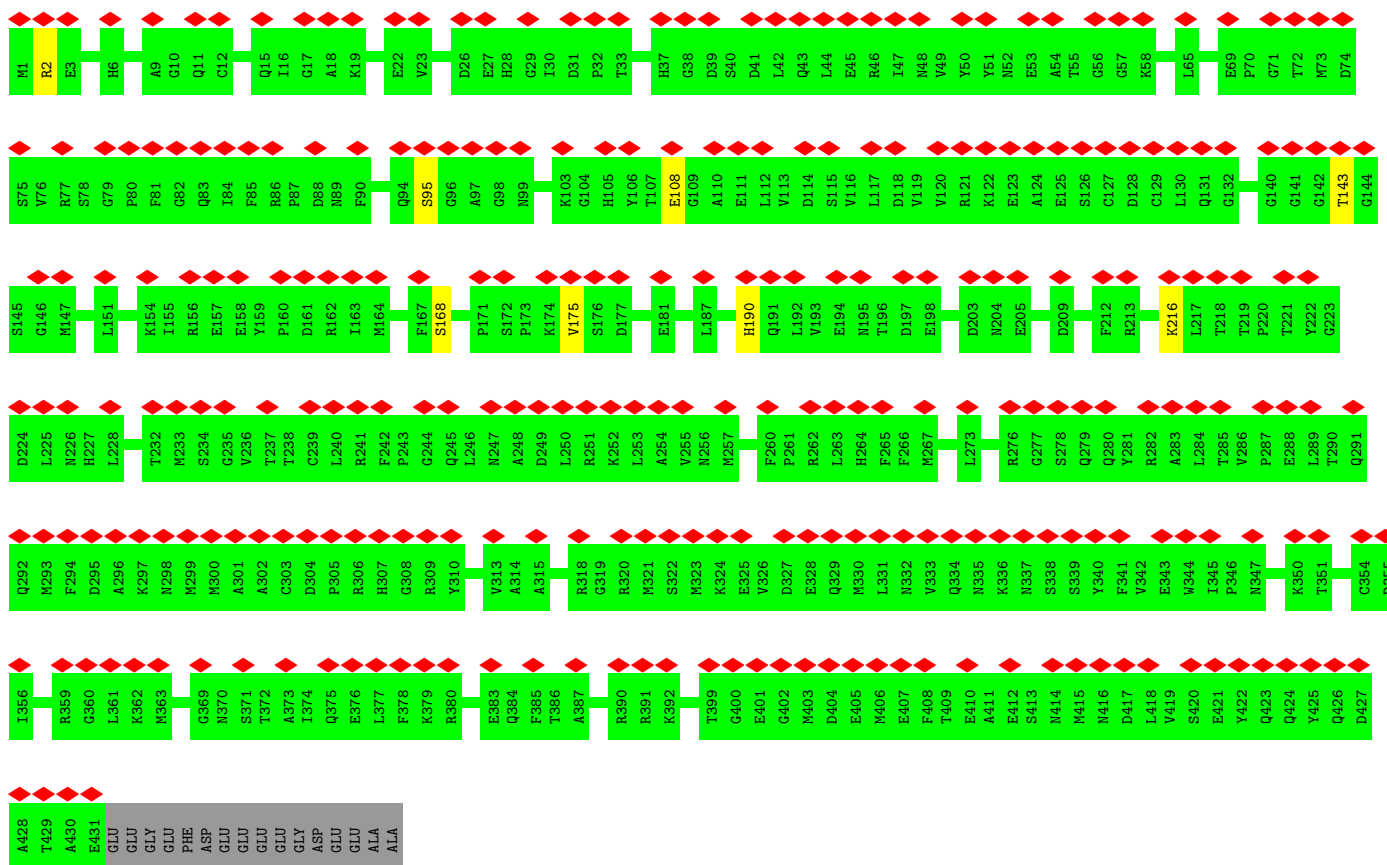


• Molecule 55: Tubulin beta chain

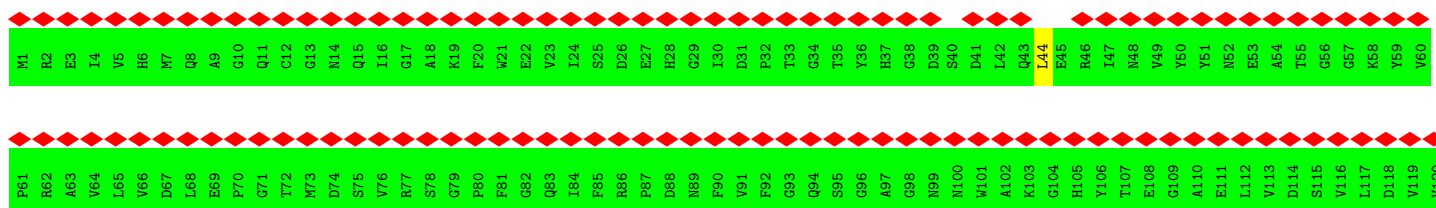
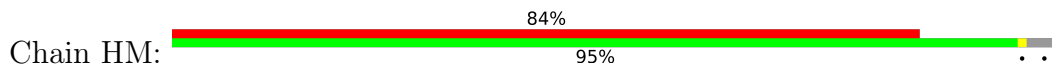




- Molecule 55: Tubulin beta chain

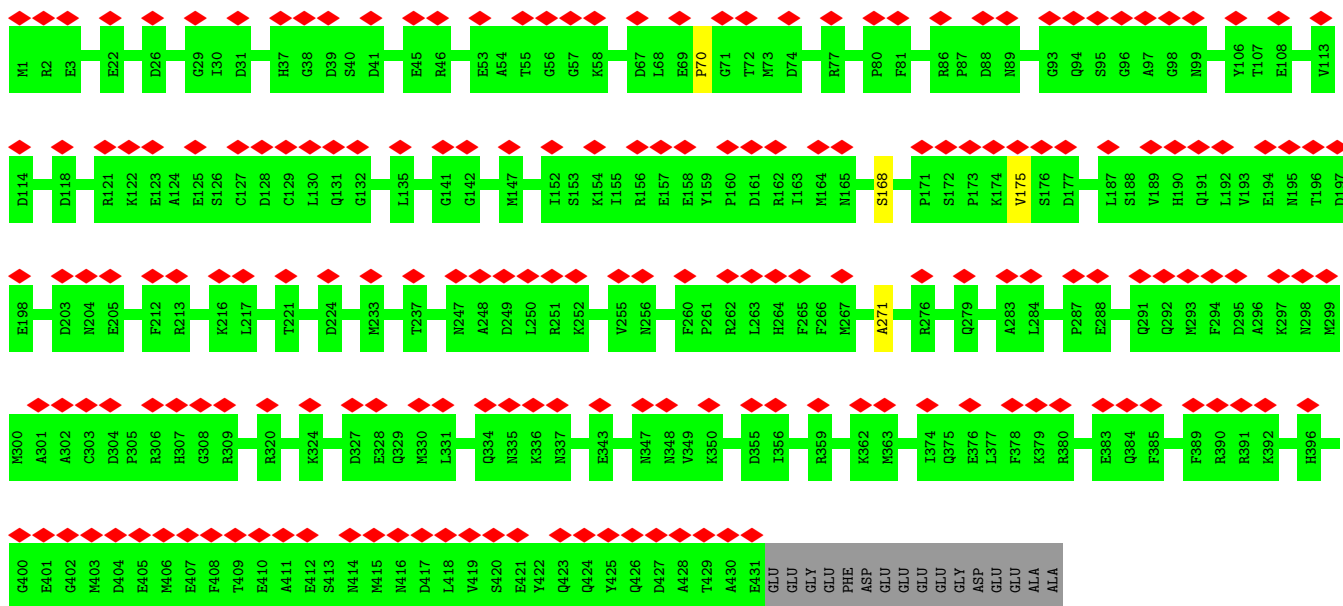
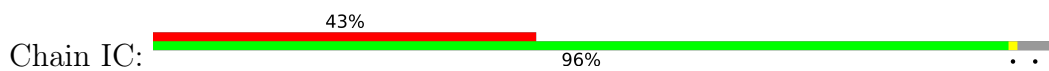


- Molecule 55: Tubulin beta chain

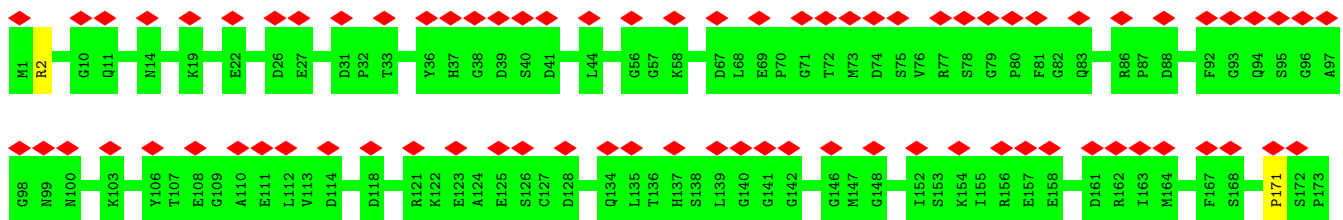
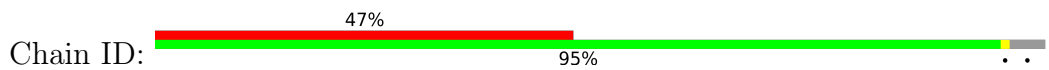


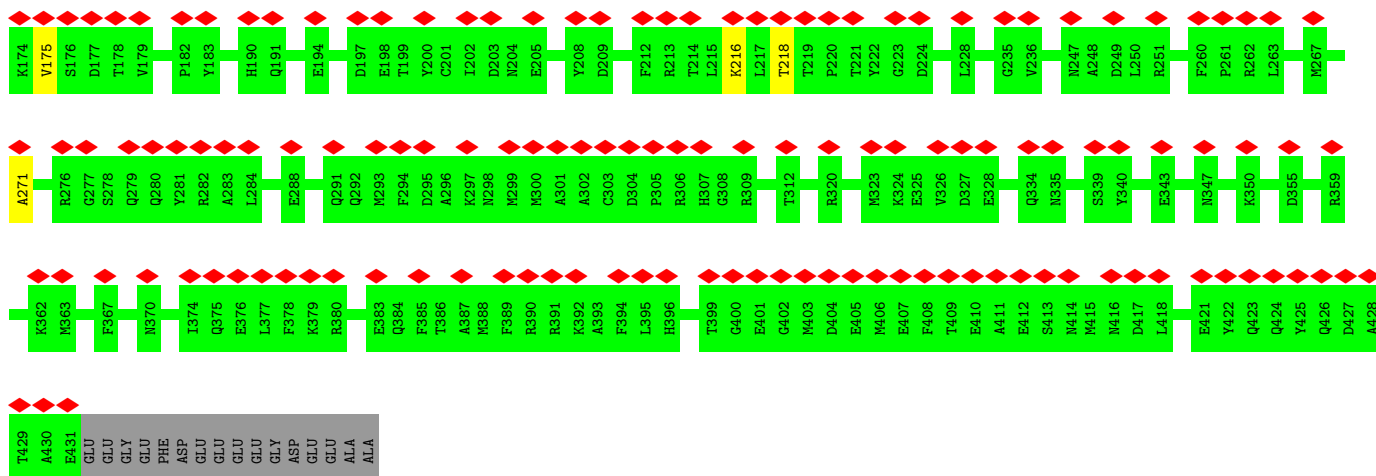


• Molecule 55: Tubulin beta chain



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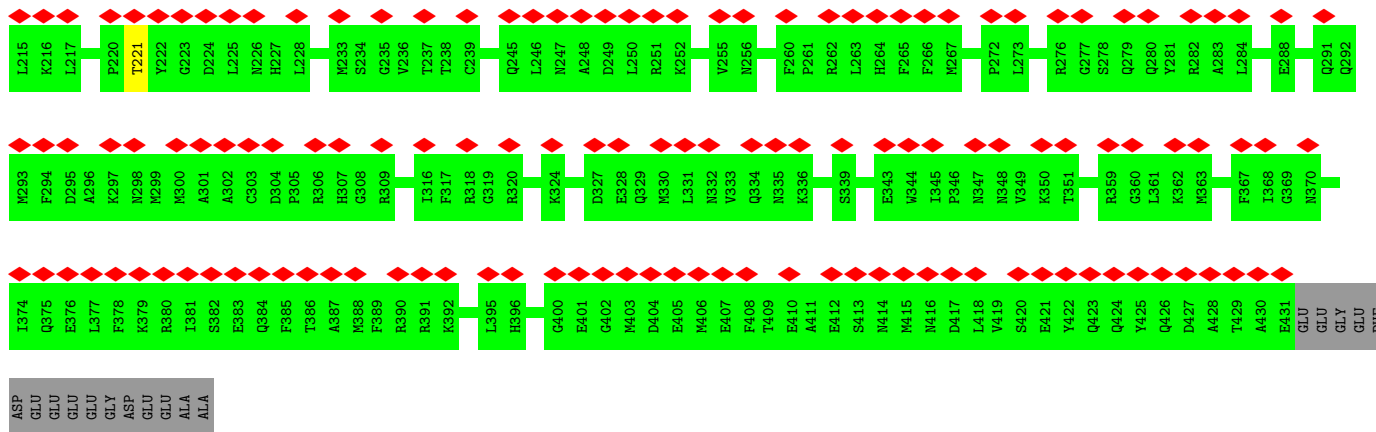


• Molecule 55: Tubulin beta chain

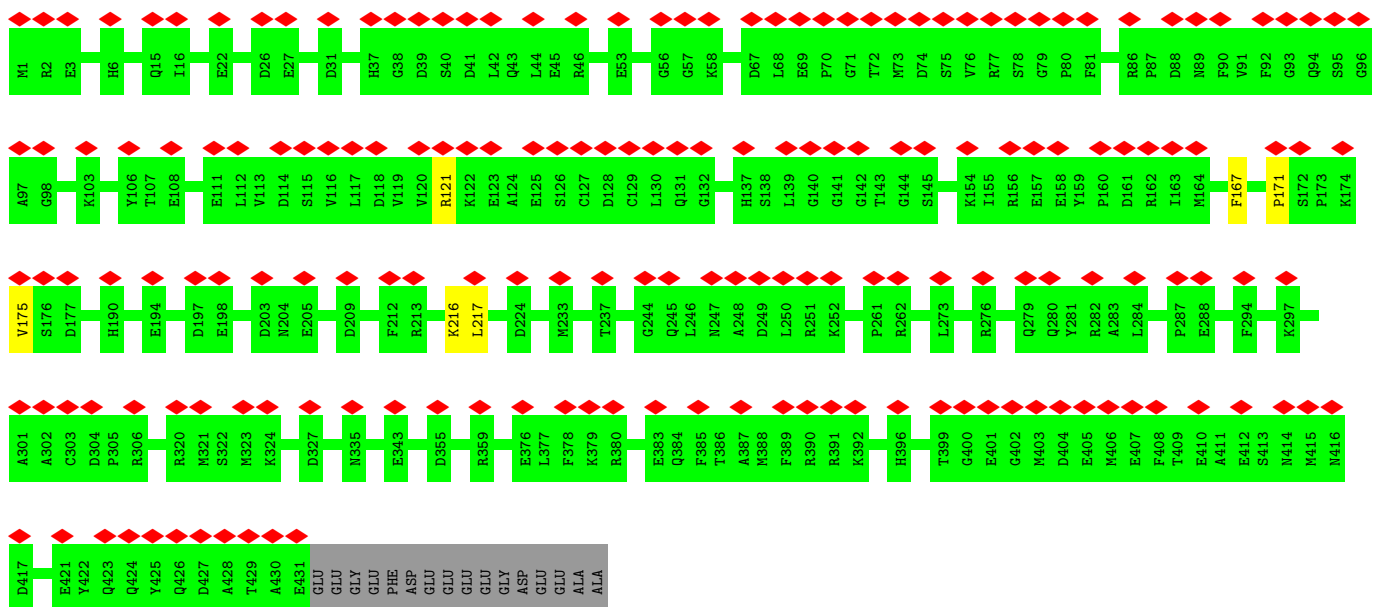
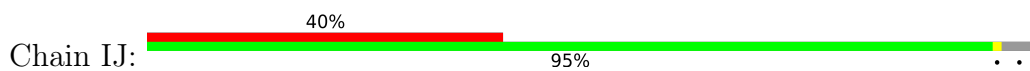


• Molecule 55: Tubulin beta chain





• Molecule 55: Tubulin beta chain

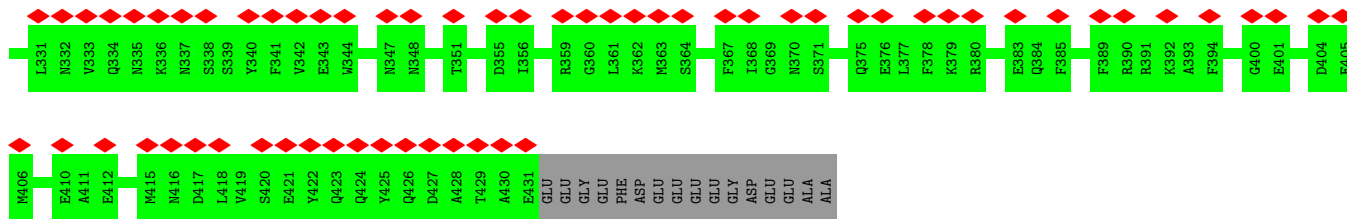


• Molecule 55: Tubulin beta chain

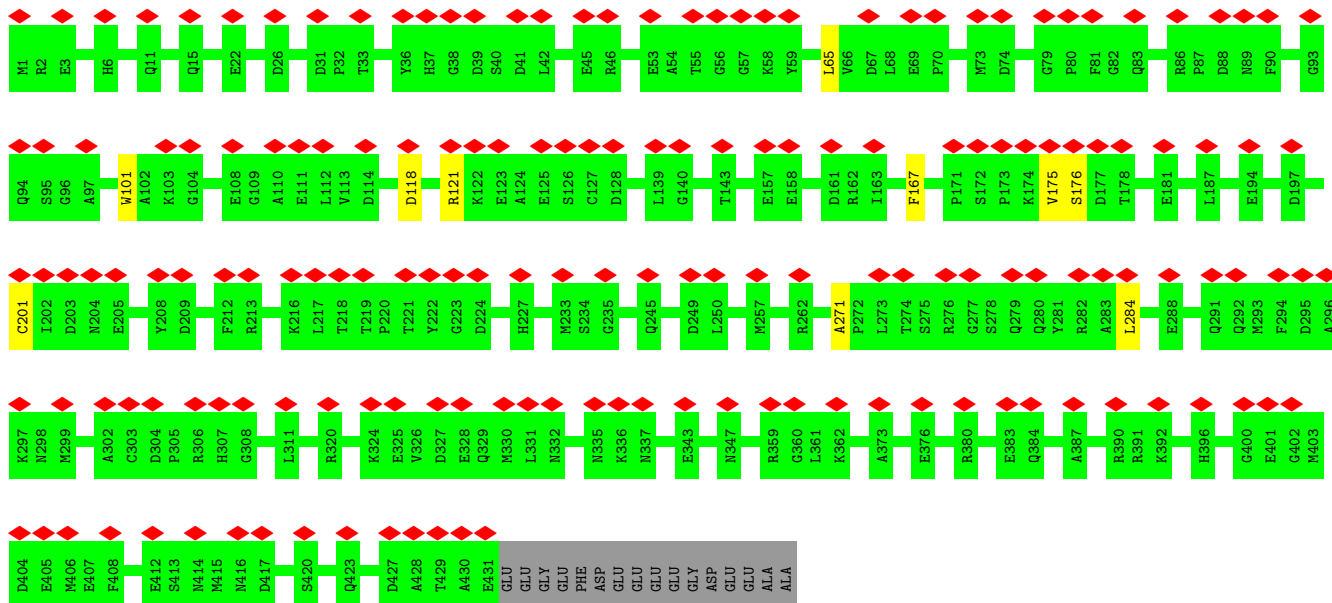




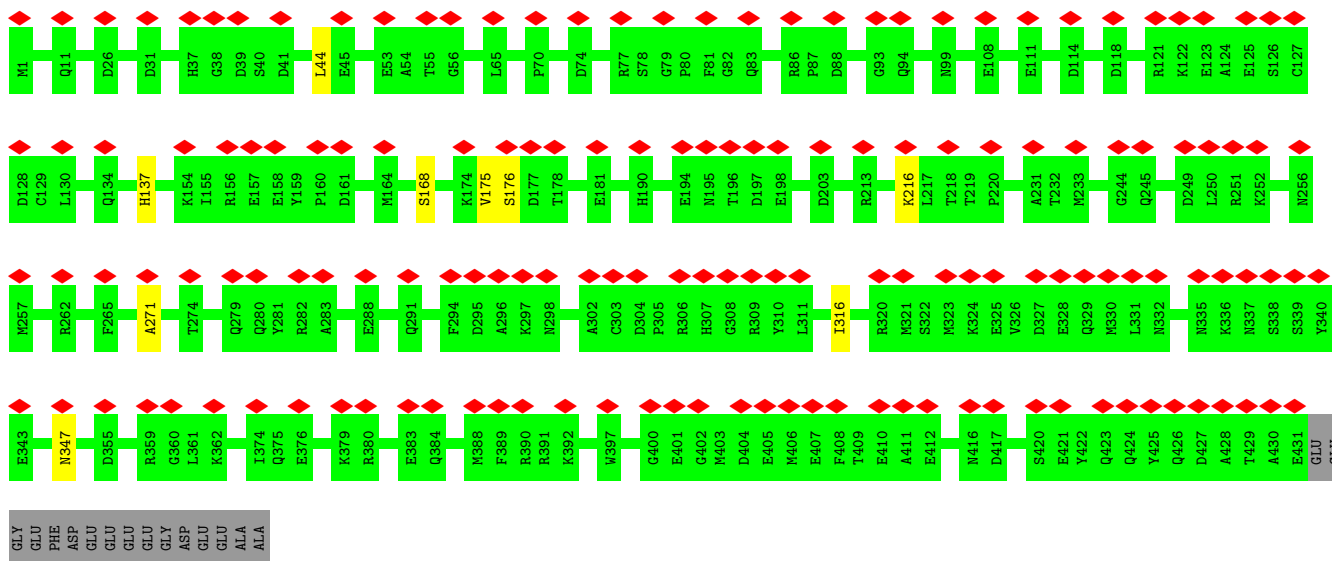




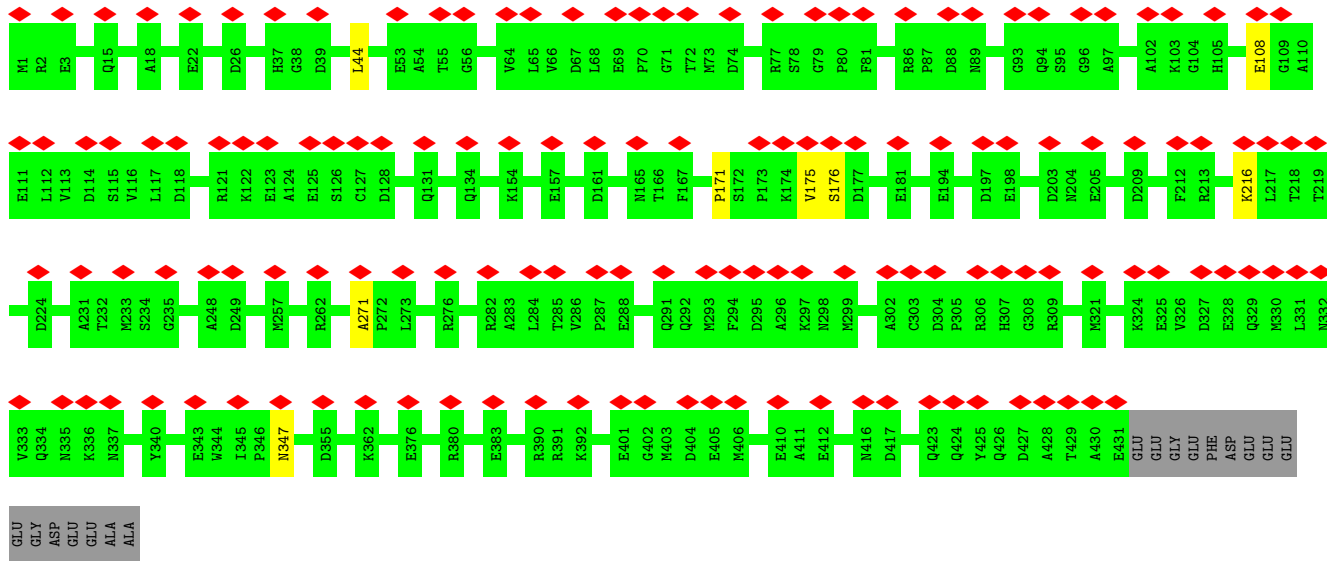
• Molecule 55: Tubulin beta chain



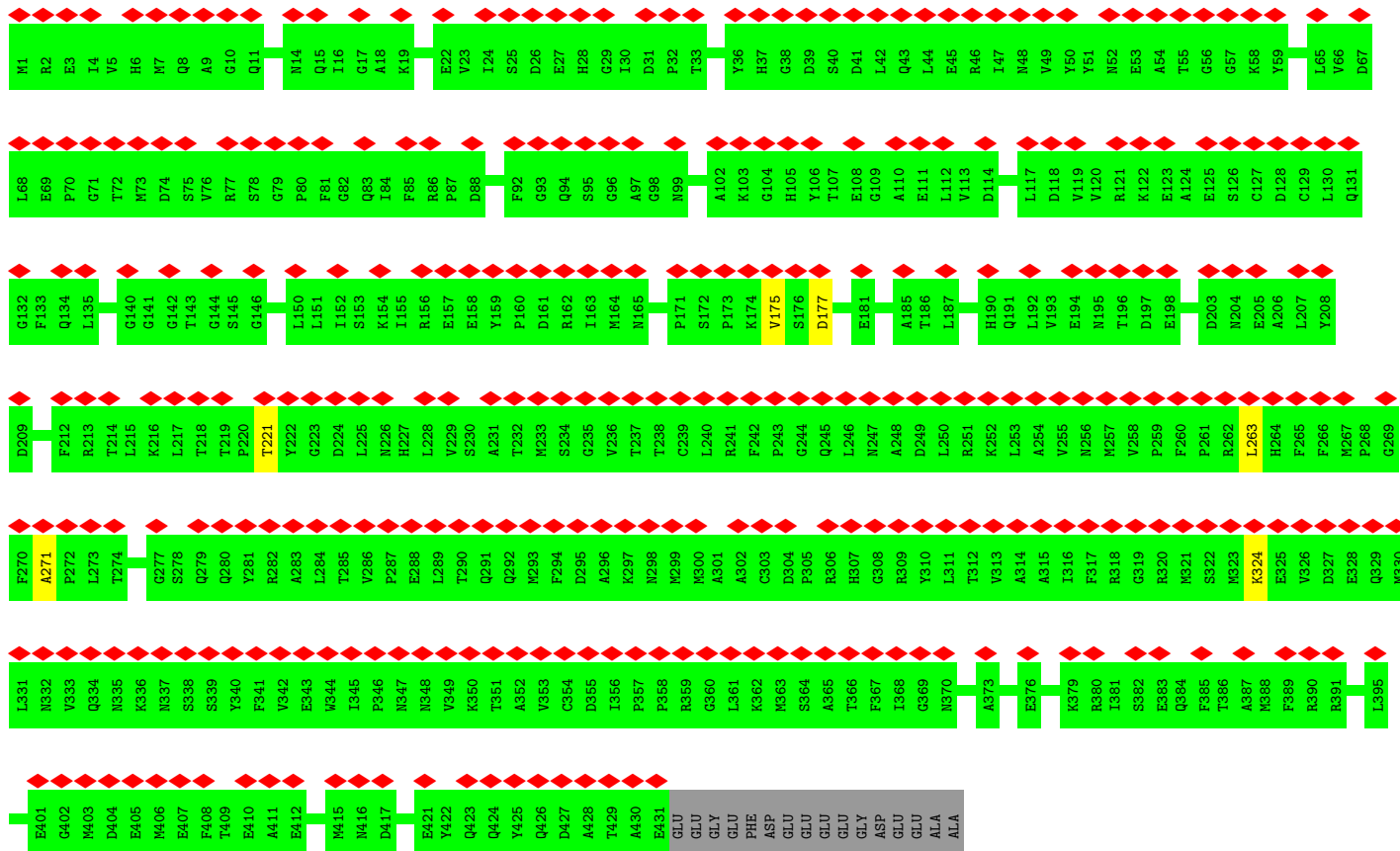
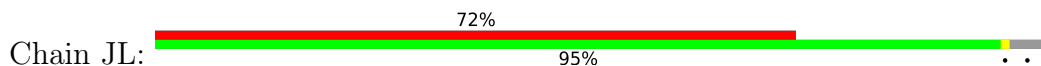
• Molecule 55: Tubulin beta chain



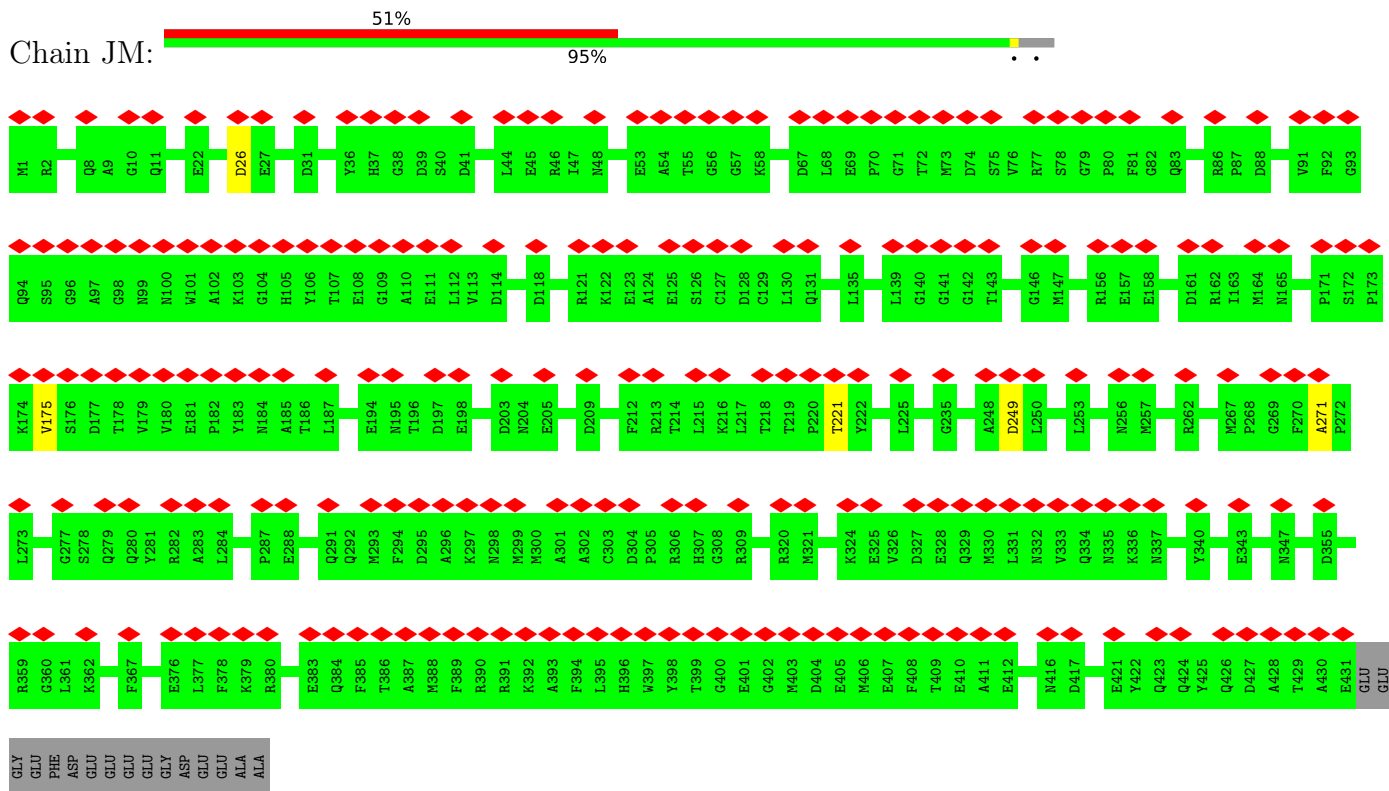
• Molecule 55: Tubulin beta chain



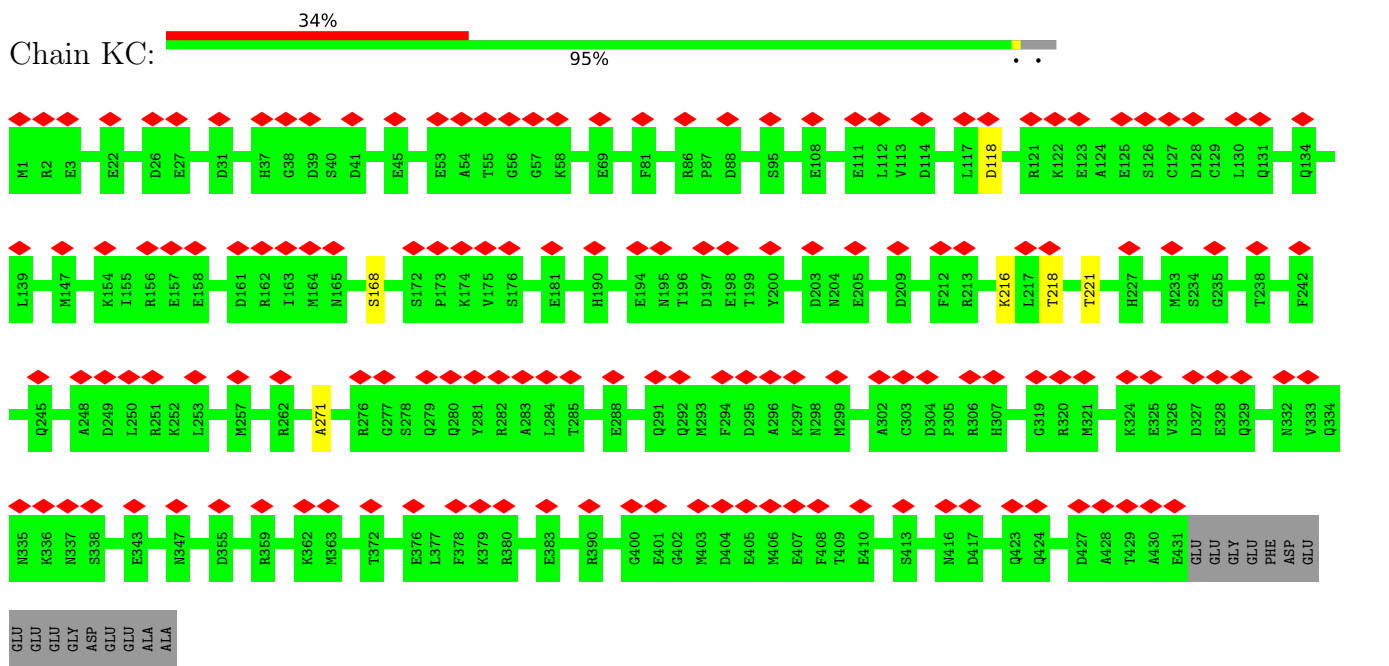
• Molecule 55: Tubulin beta chain



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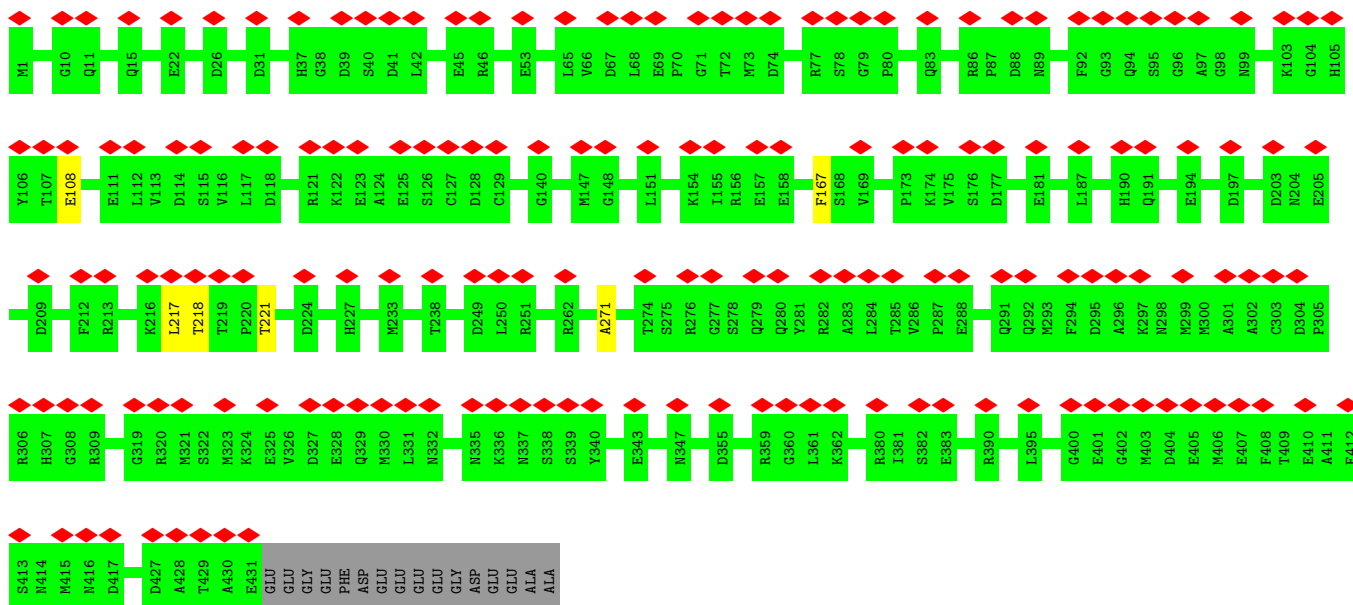


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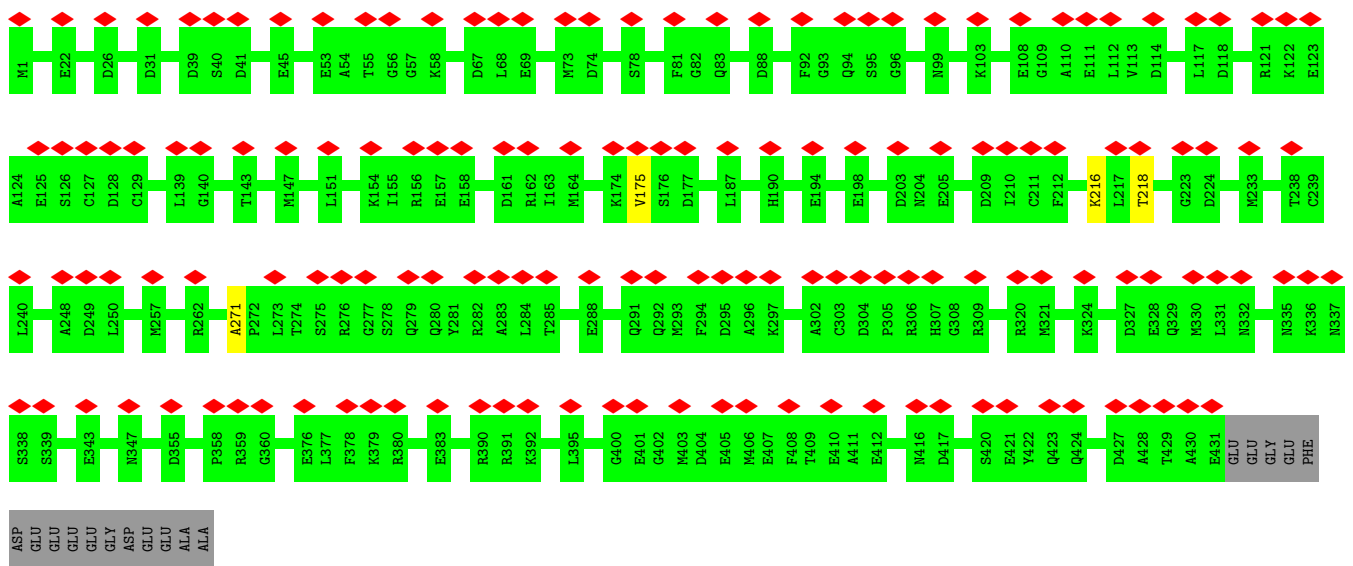


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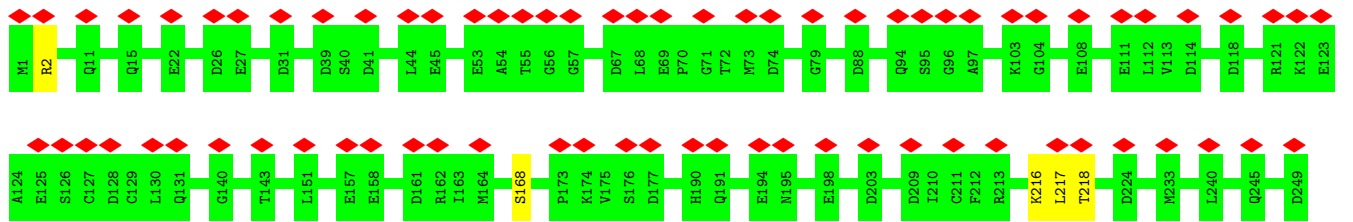


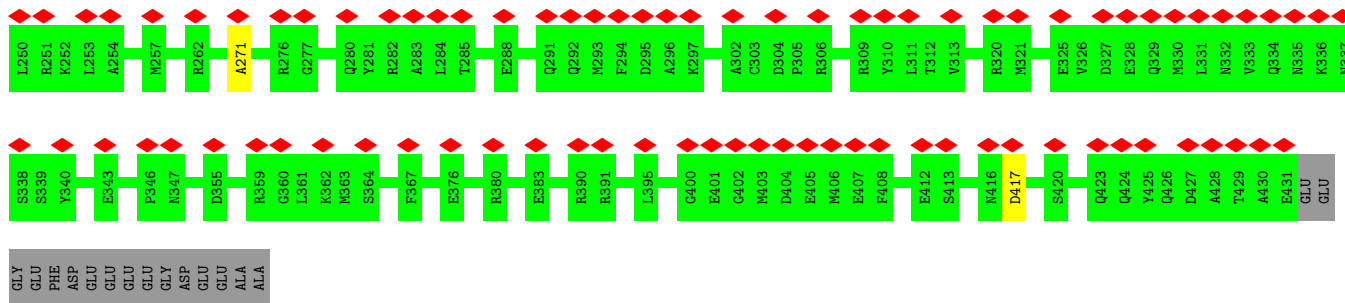


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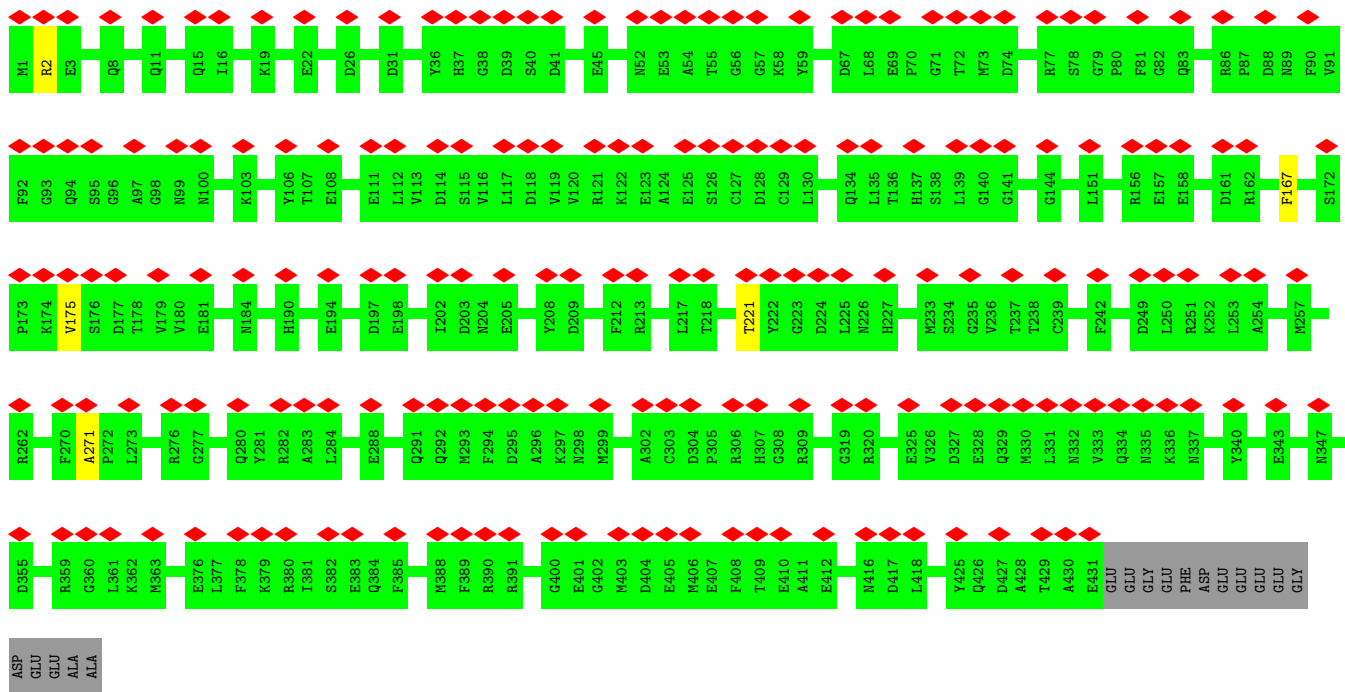
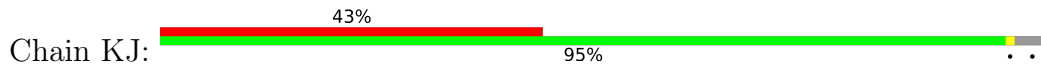


• Molecule 55: Tubulin beta chain

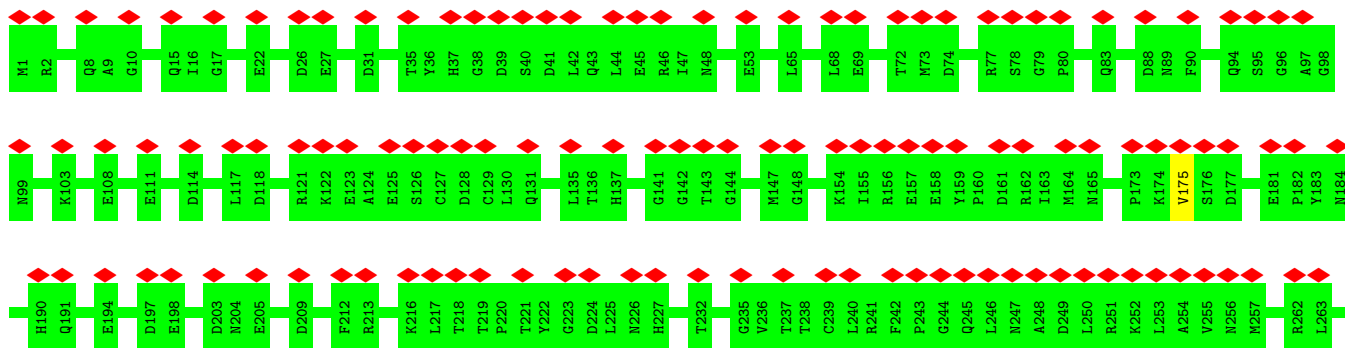


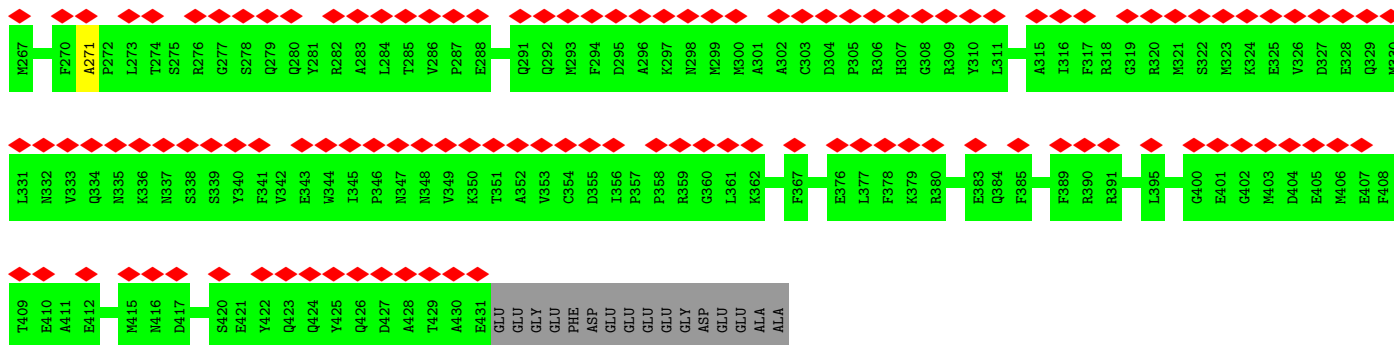


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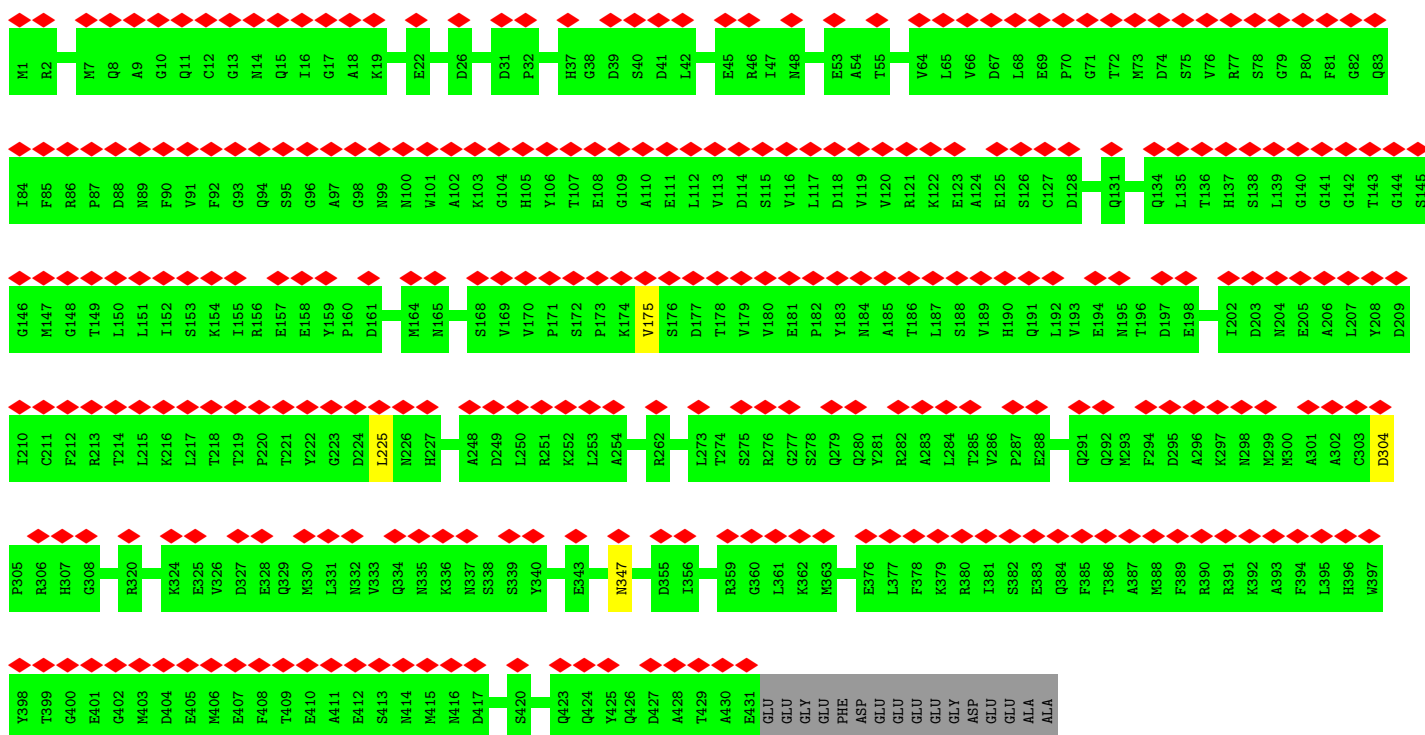


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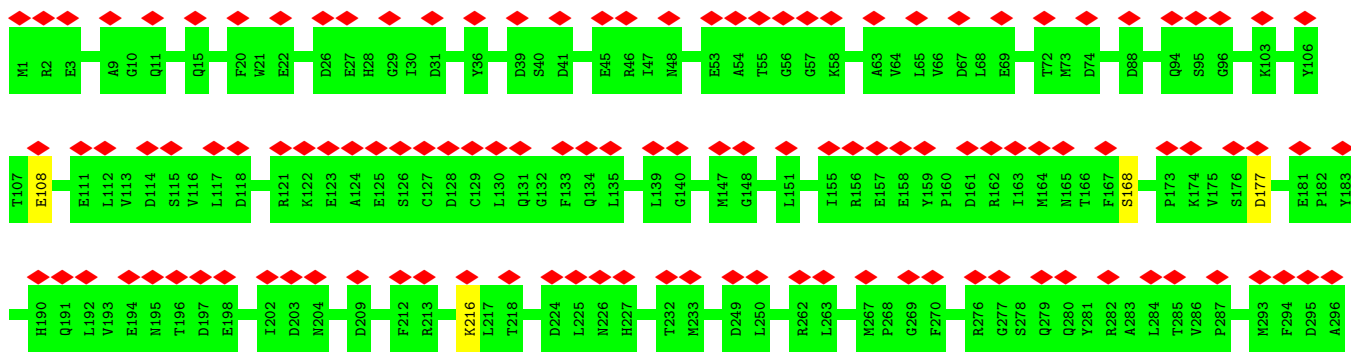
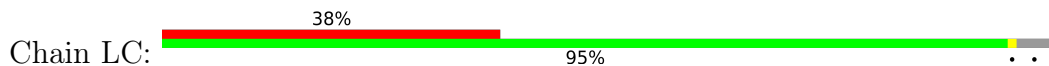


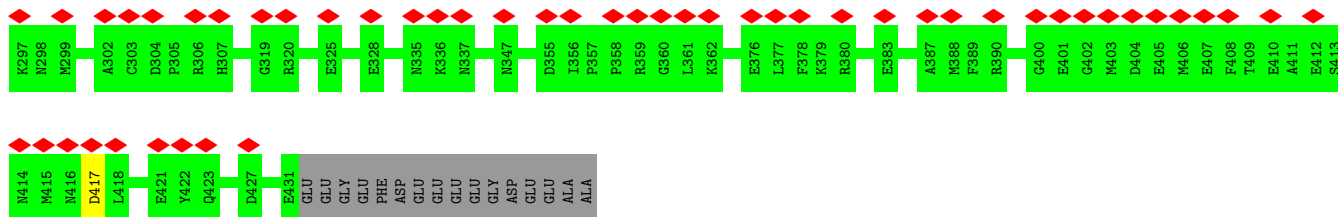


• Molecule 55: Tubulin beta chain



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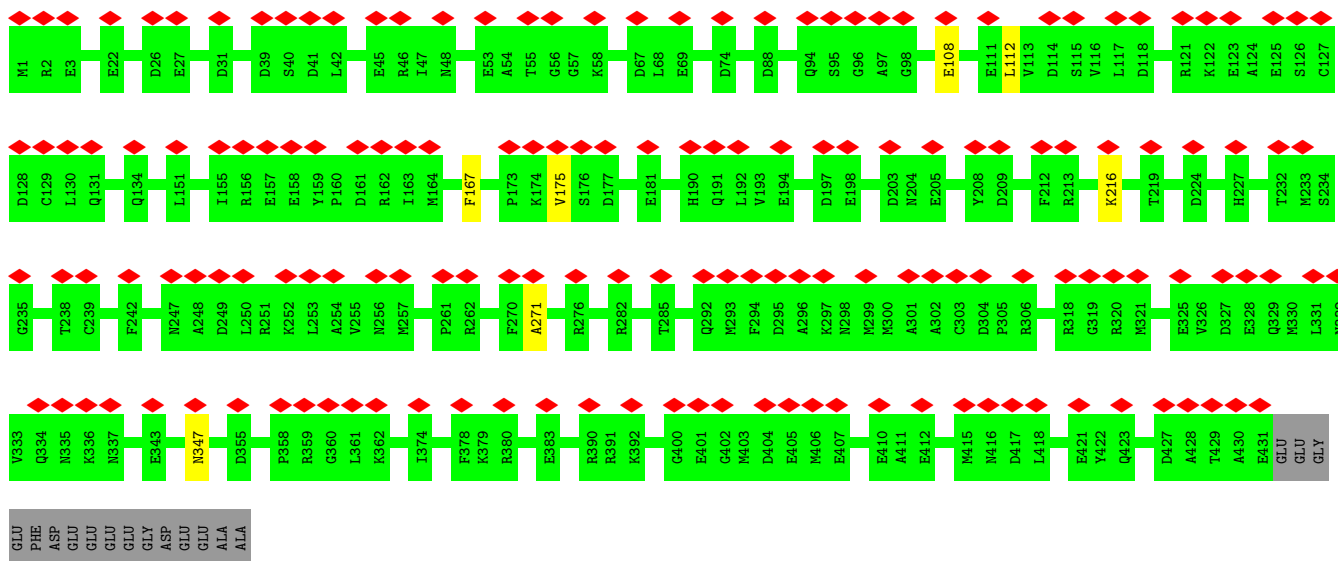




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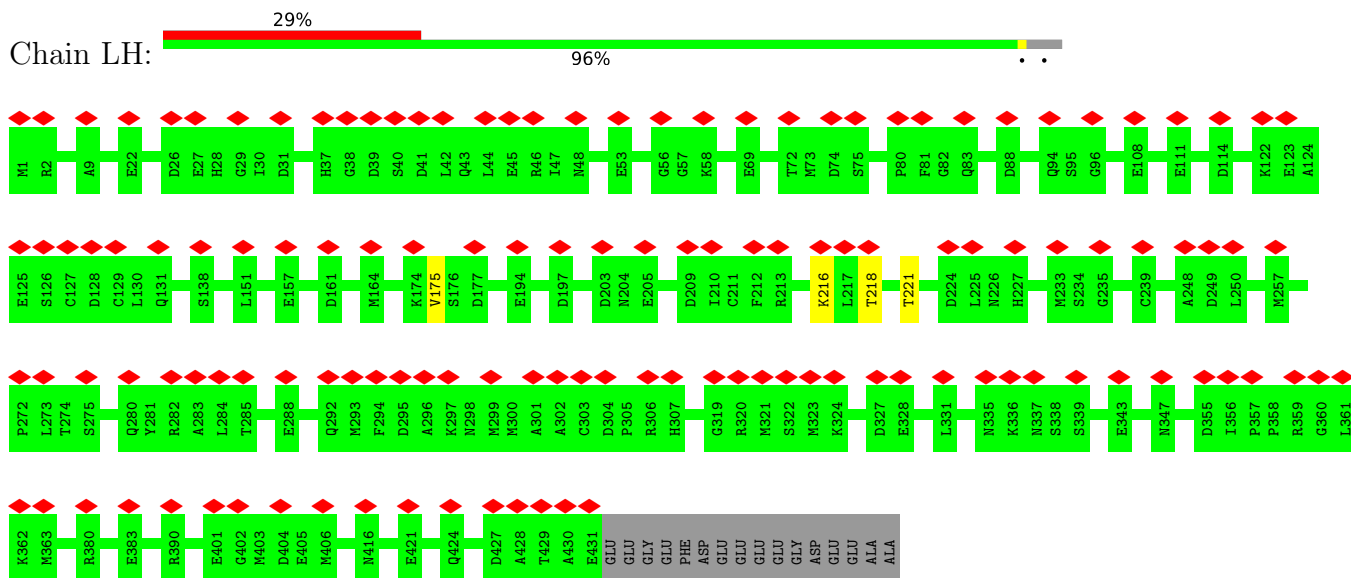


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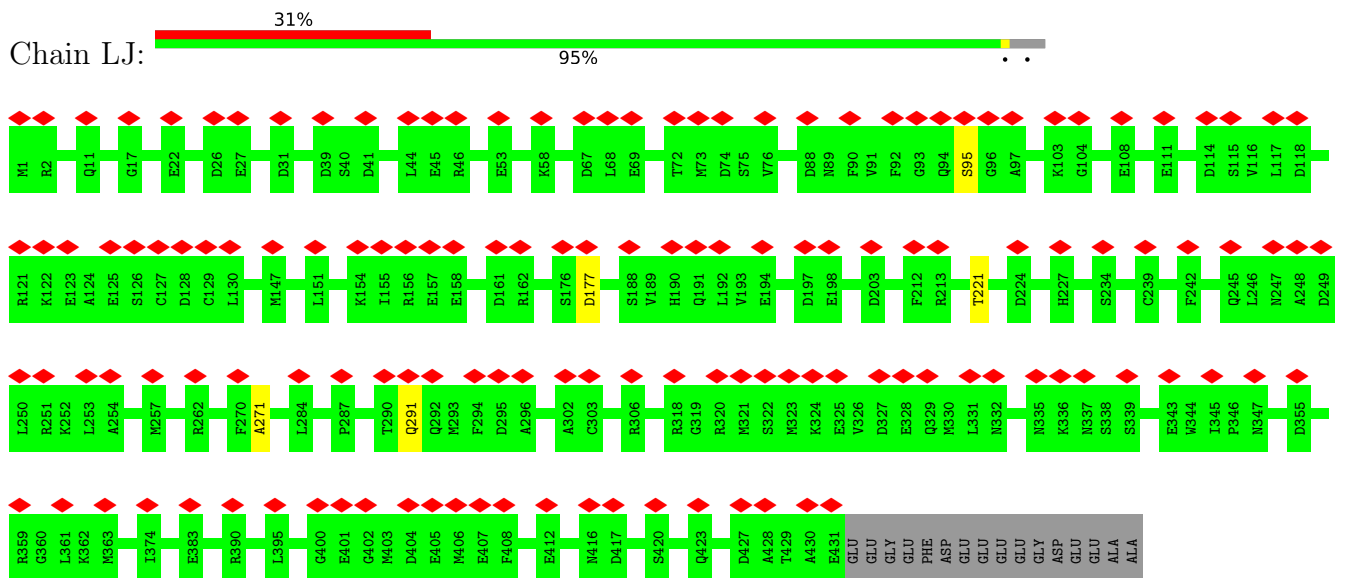


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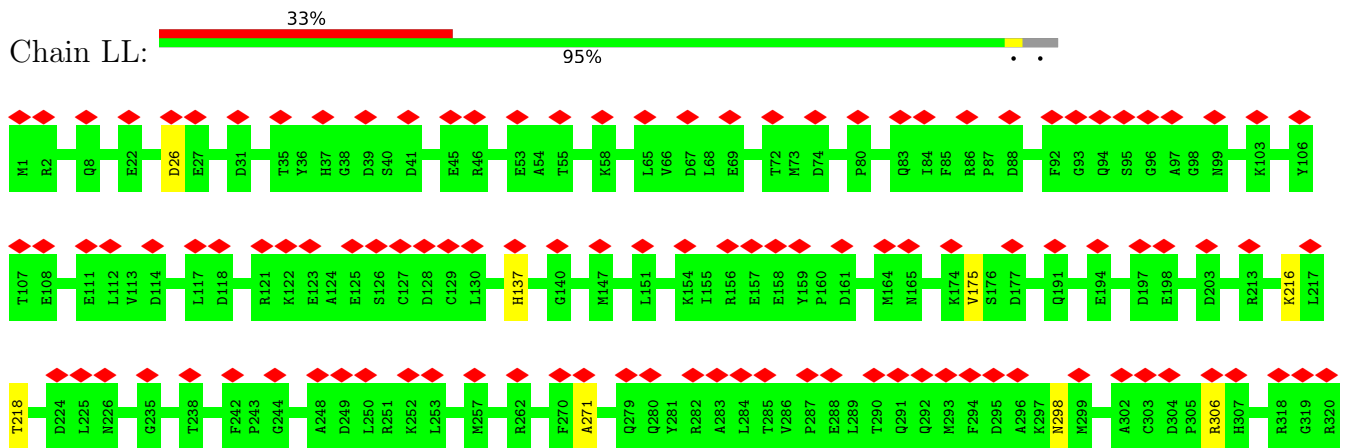


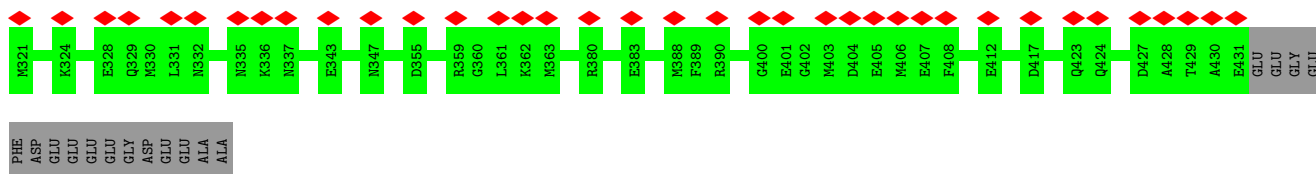


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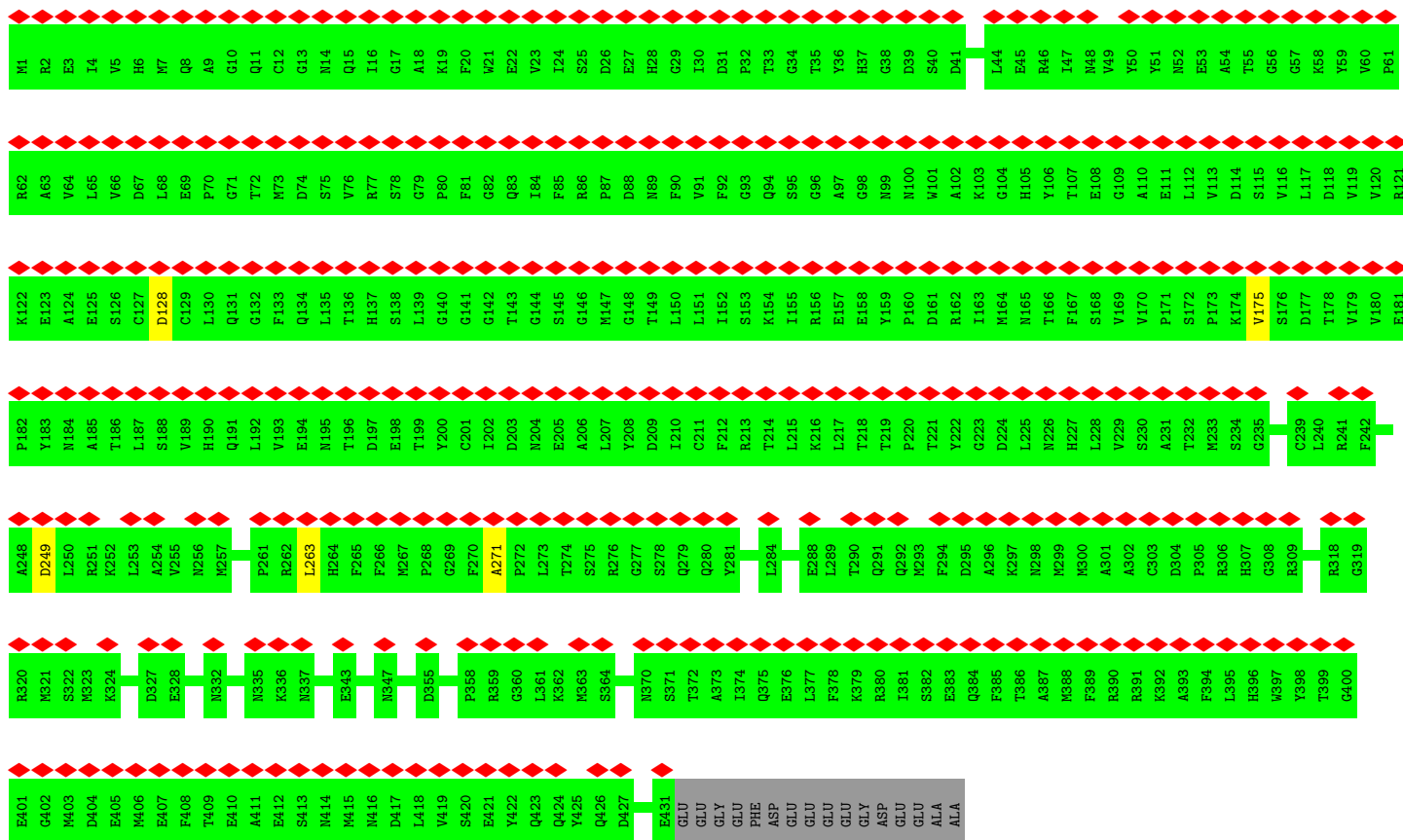
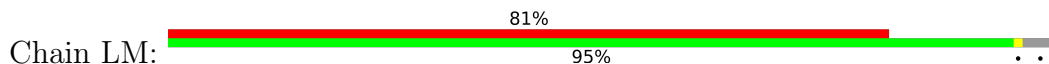


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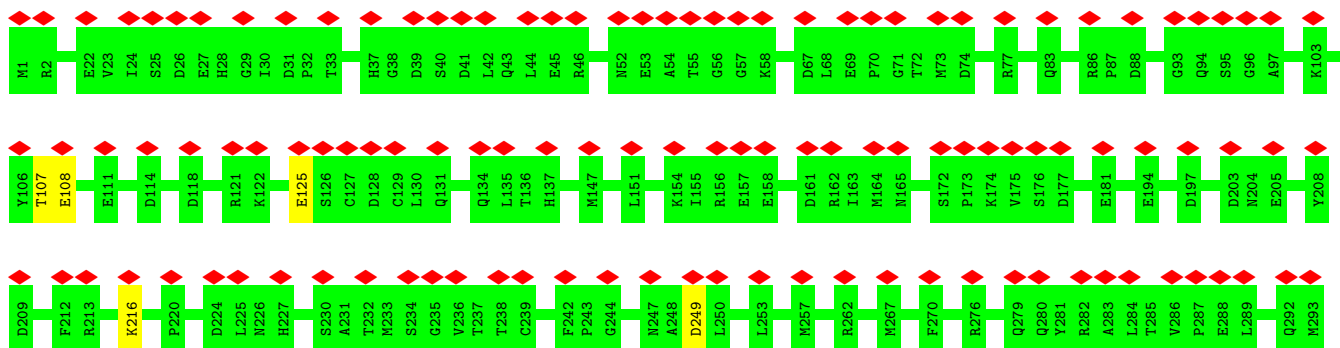


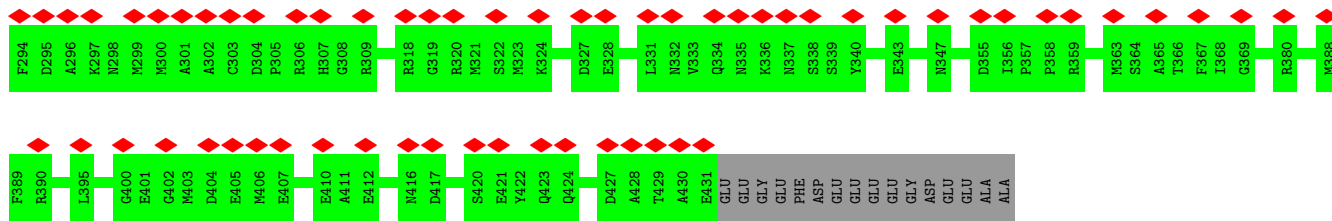


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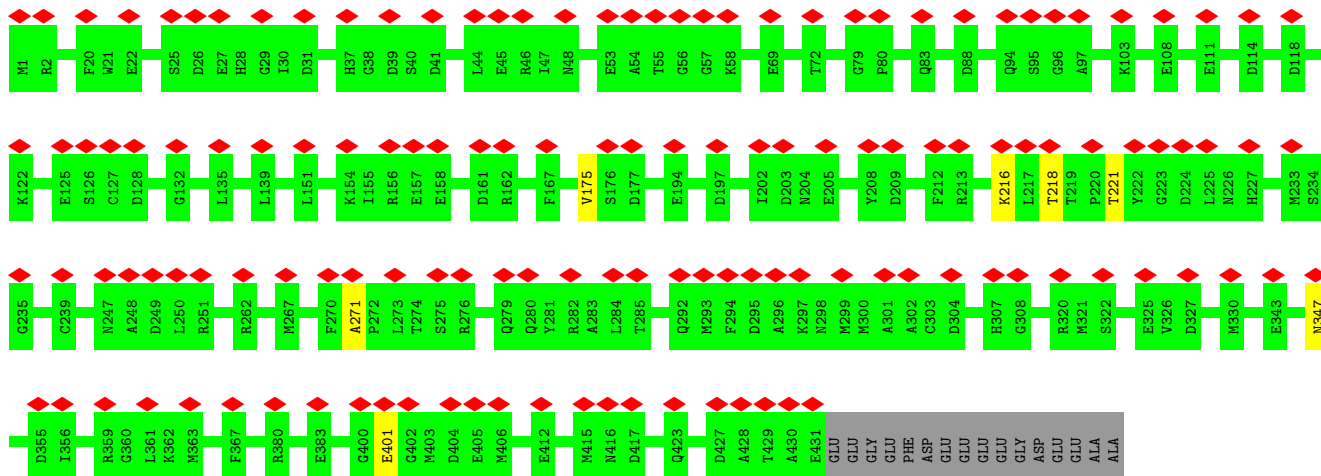


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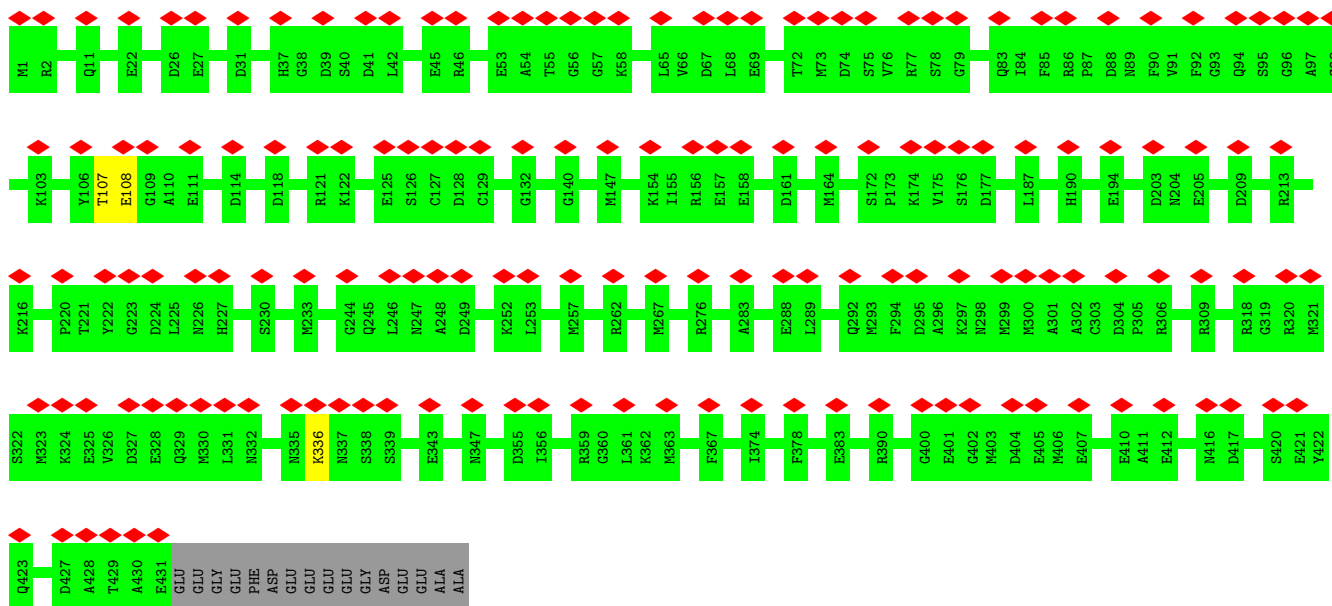




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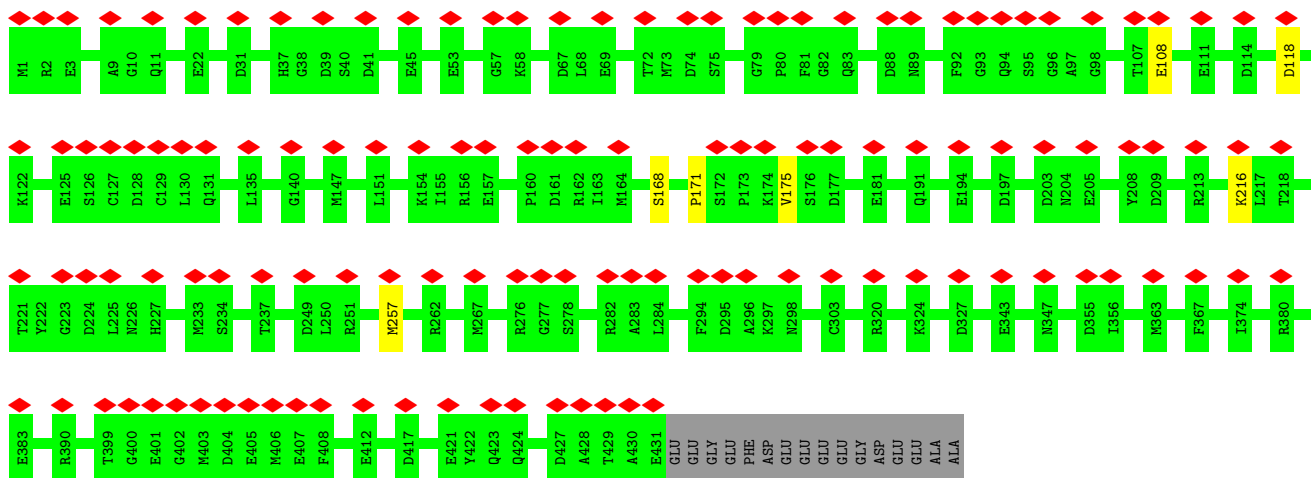


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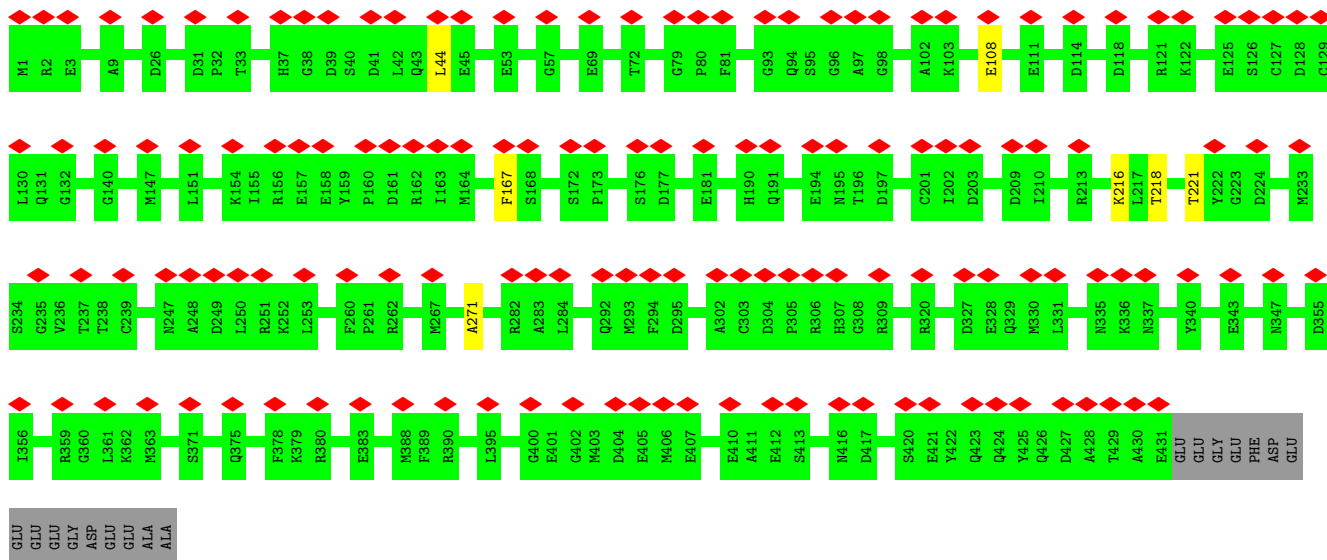


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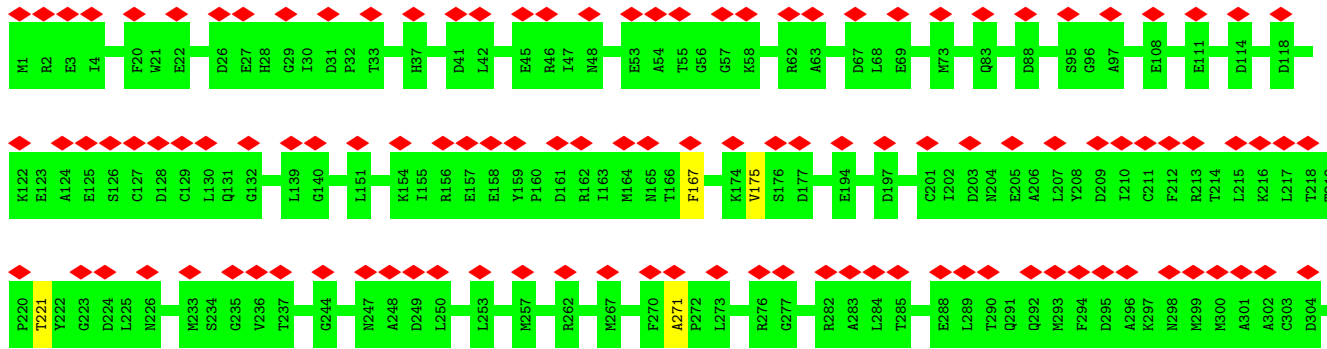


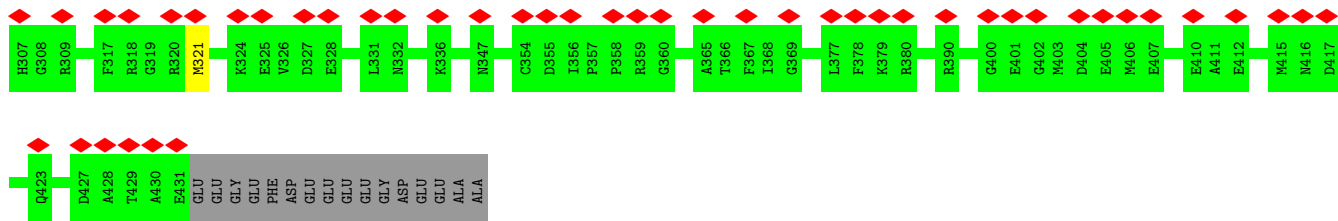


• Molecule 55: Tubulin beta chain



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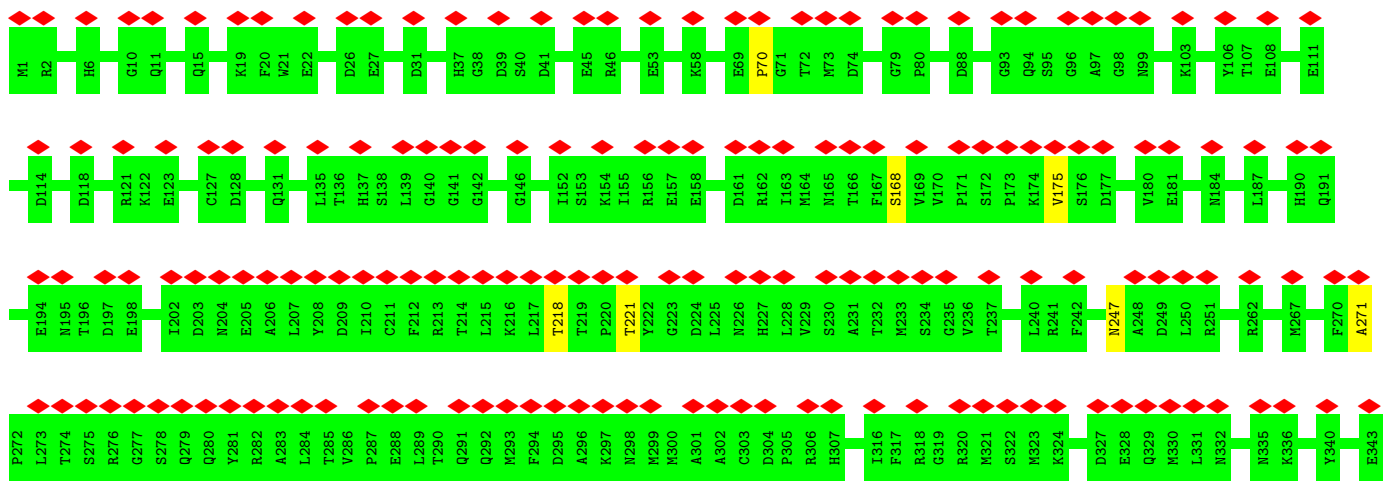


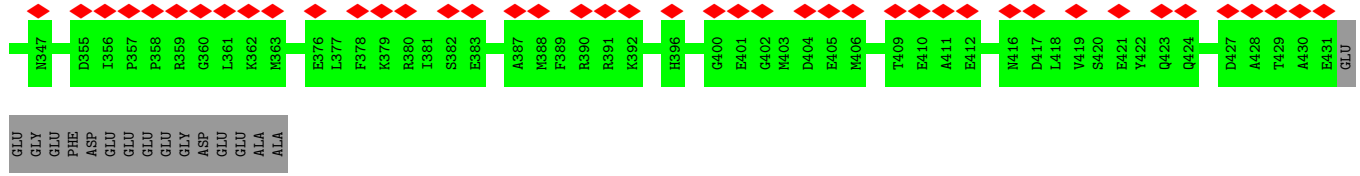


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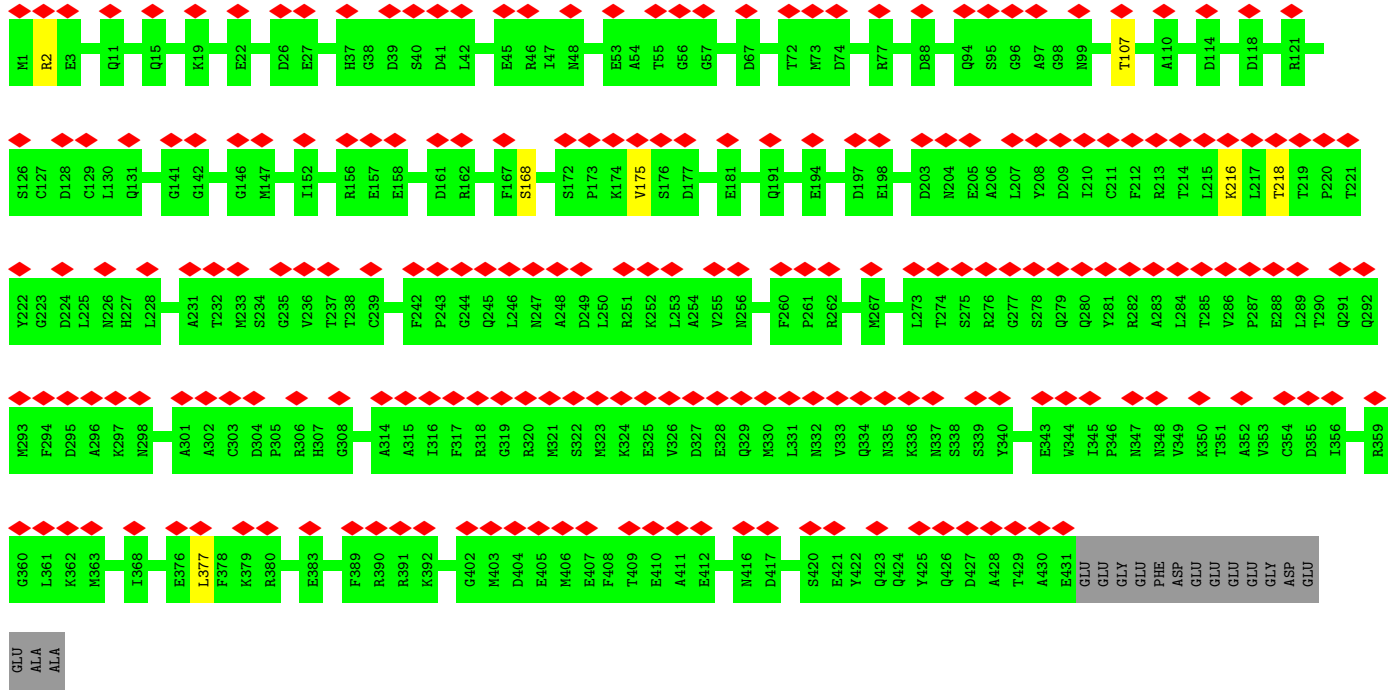


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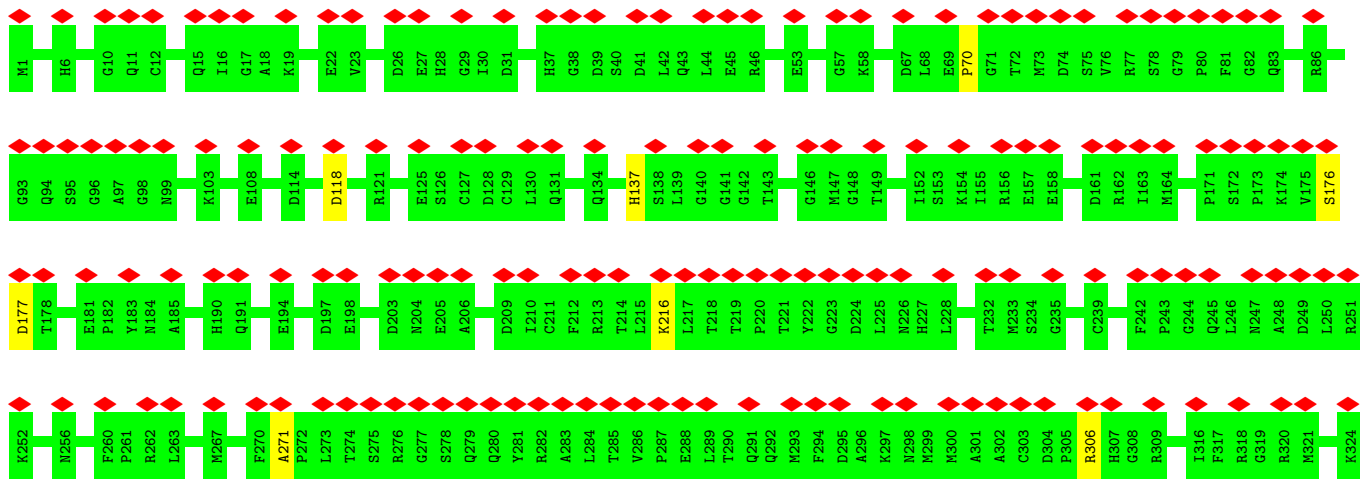


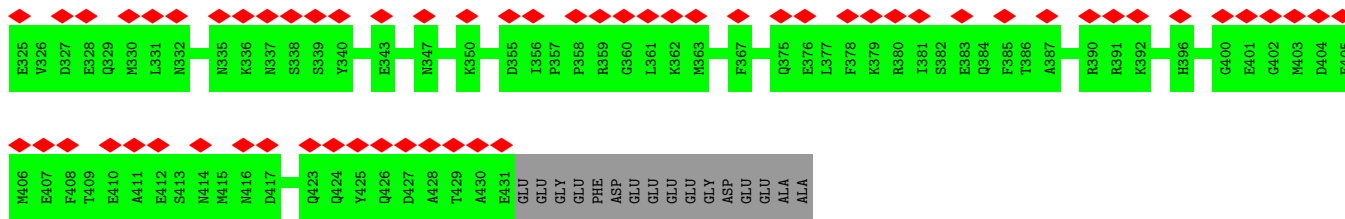


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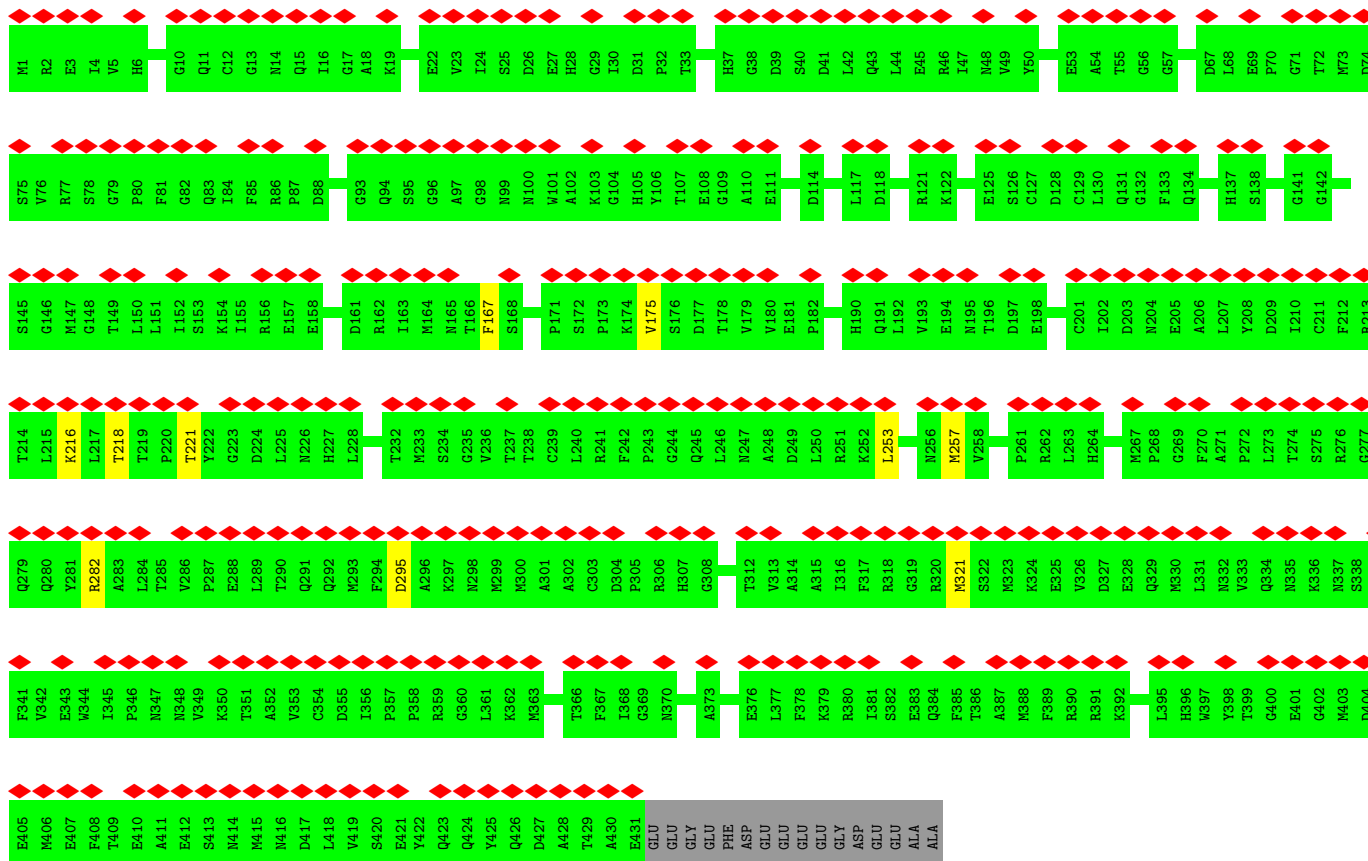


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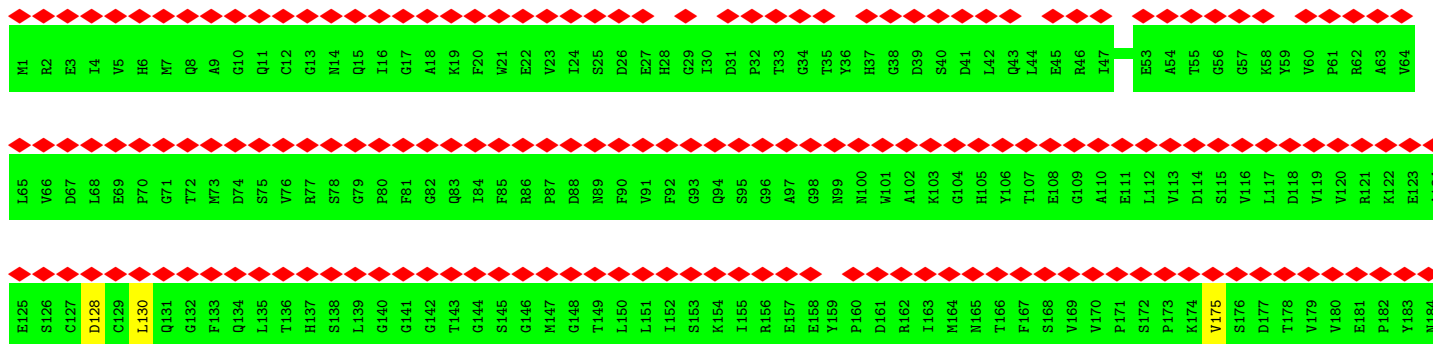
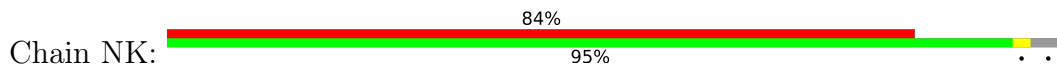


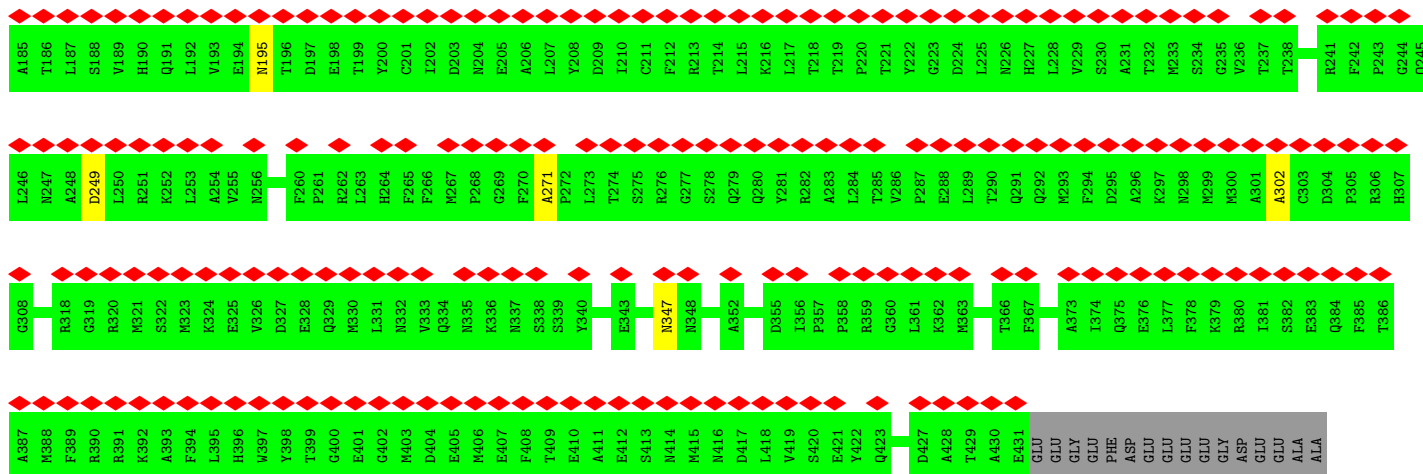


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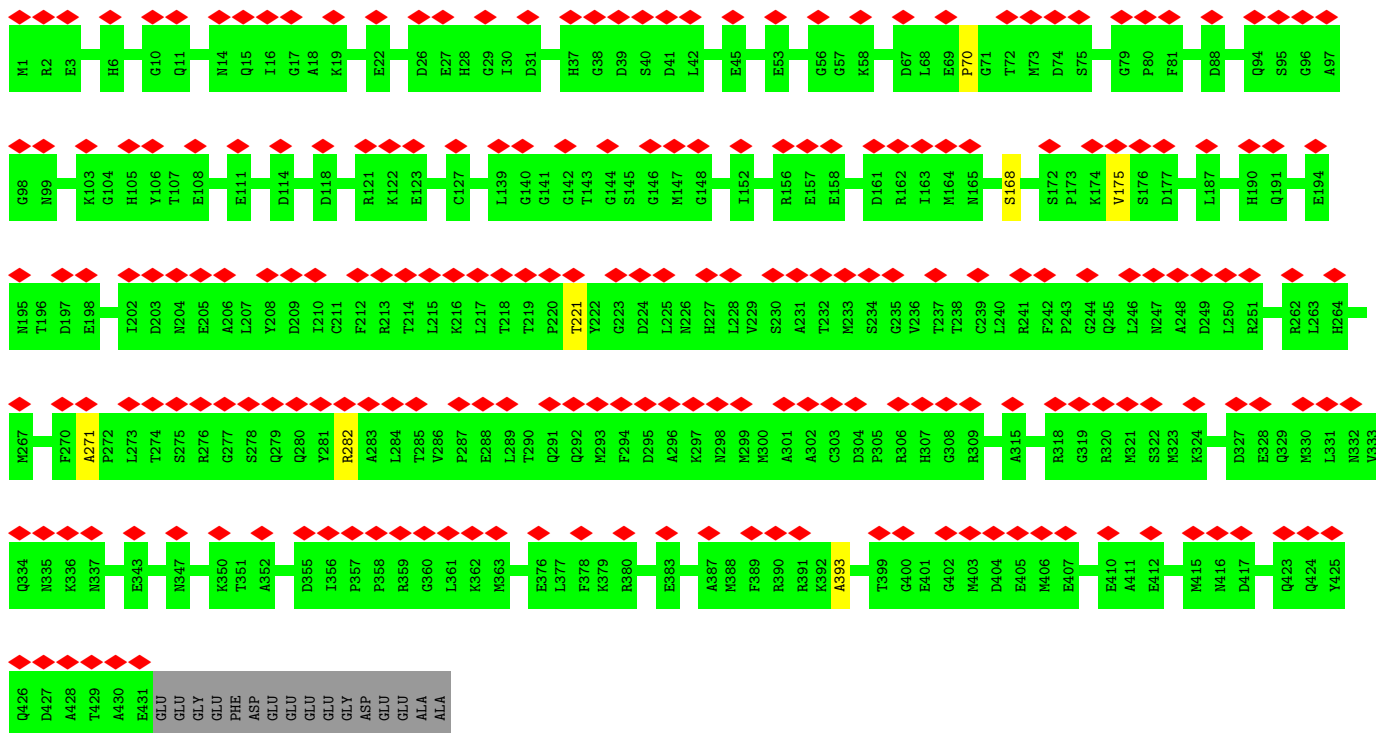


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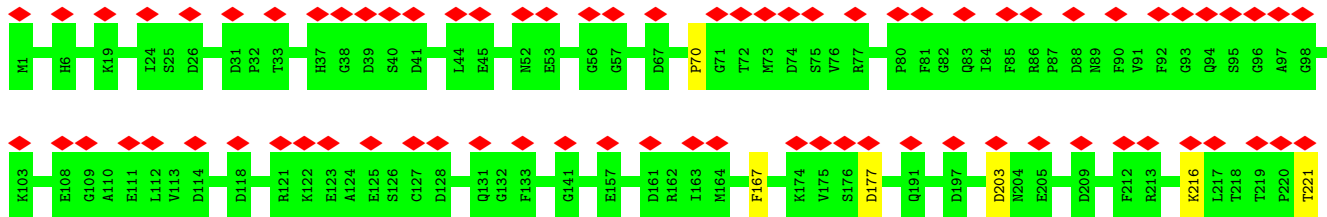




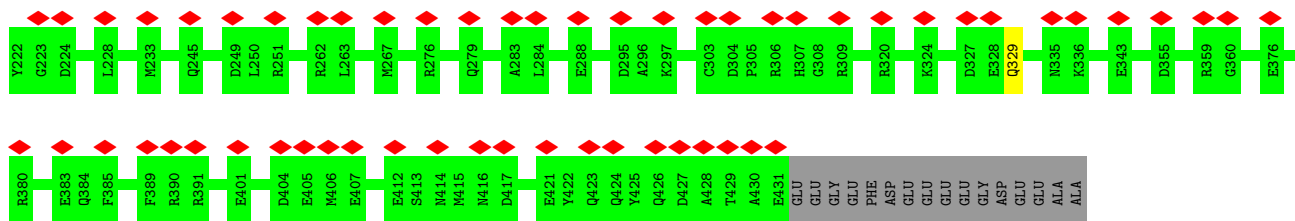
• Molecule 55: Tubulin beta chain



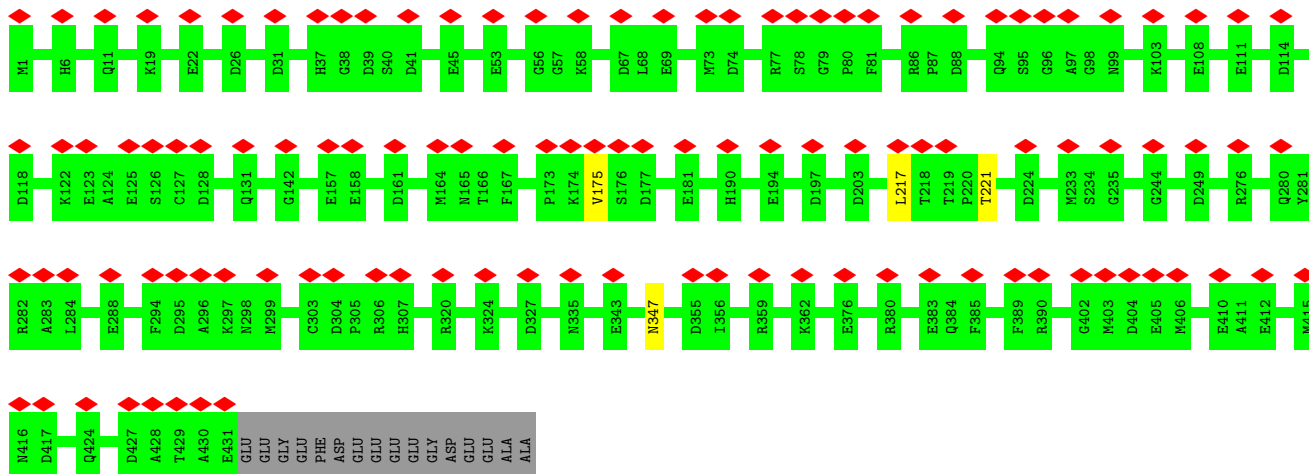
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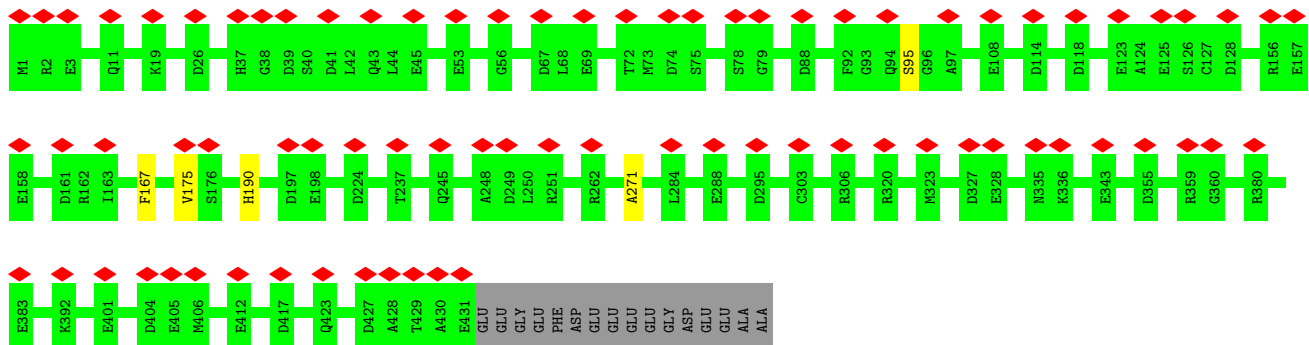




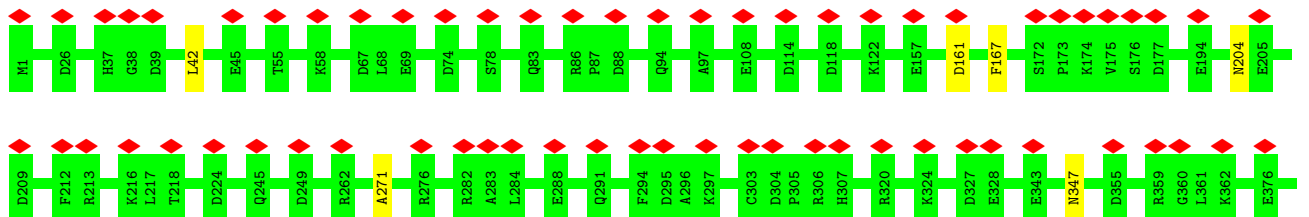
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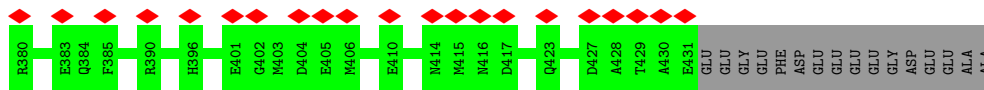


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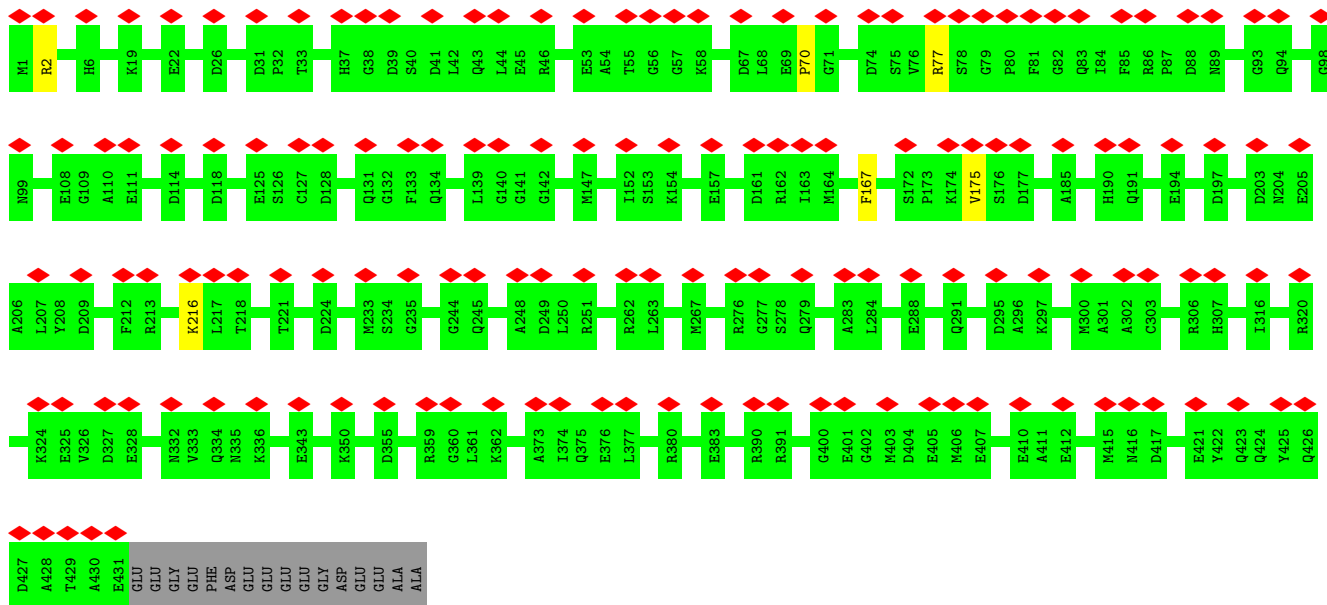


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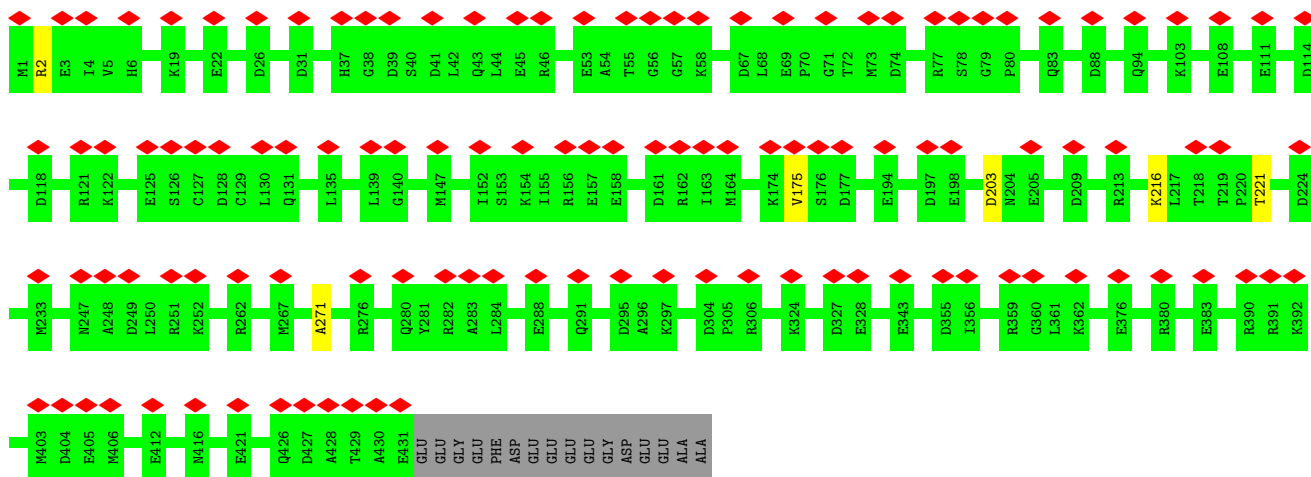




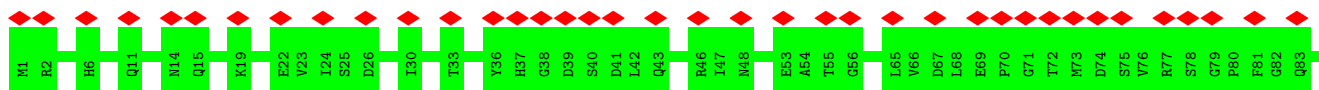
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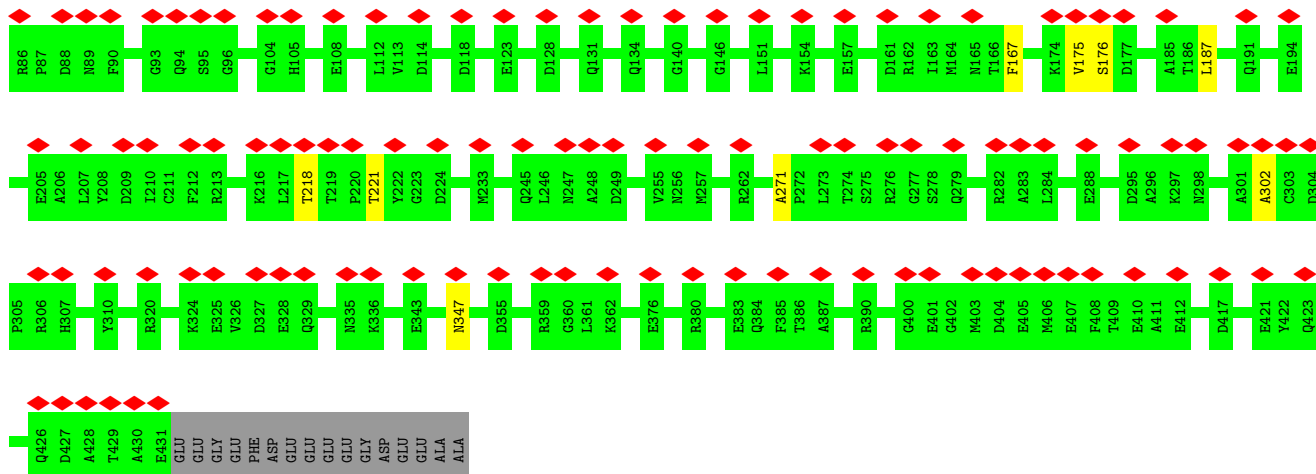


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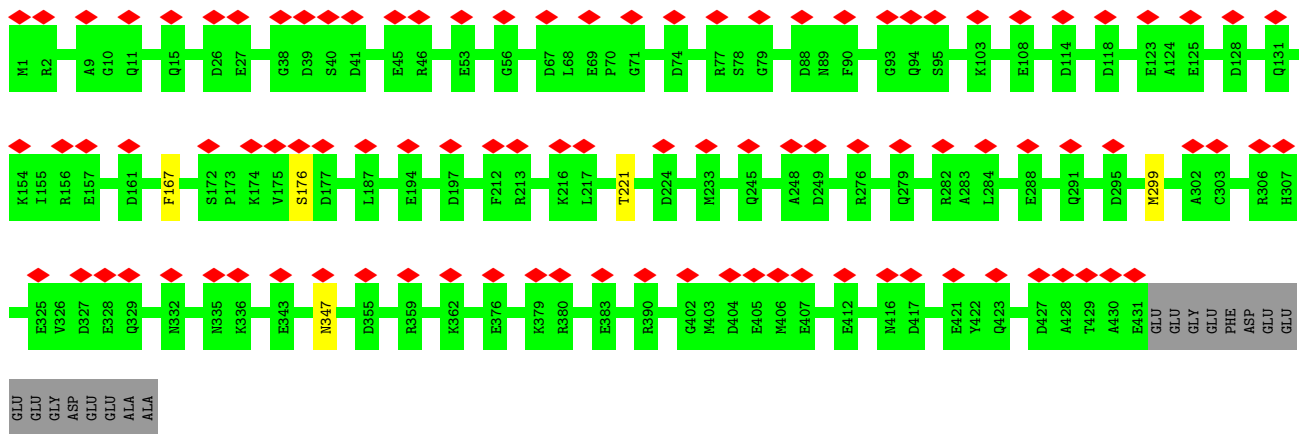


• Molecule 55: Tubulin beta chain

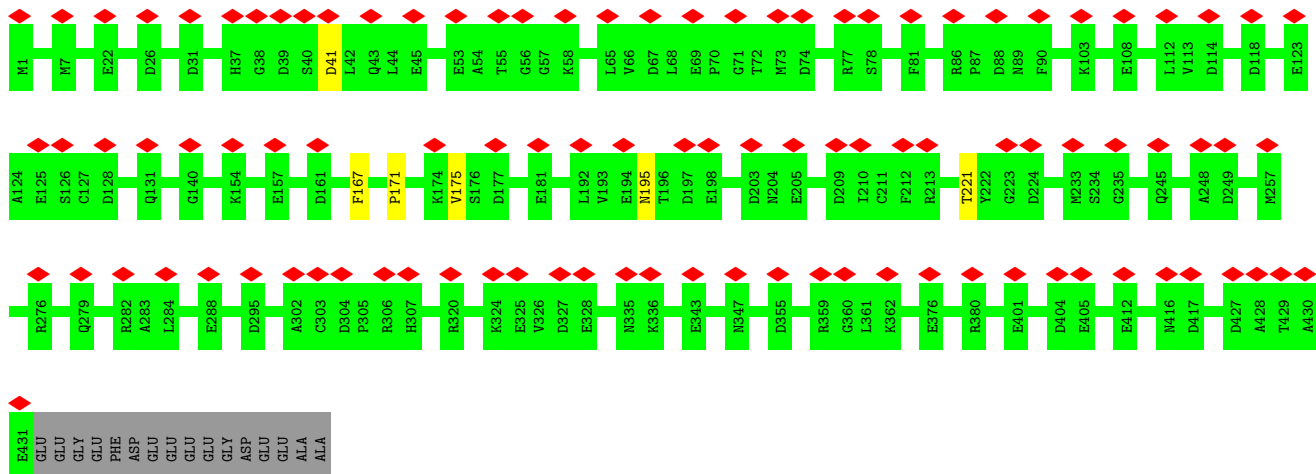




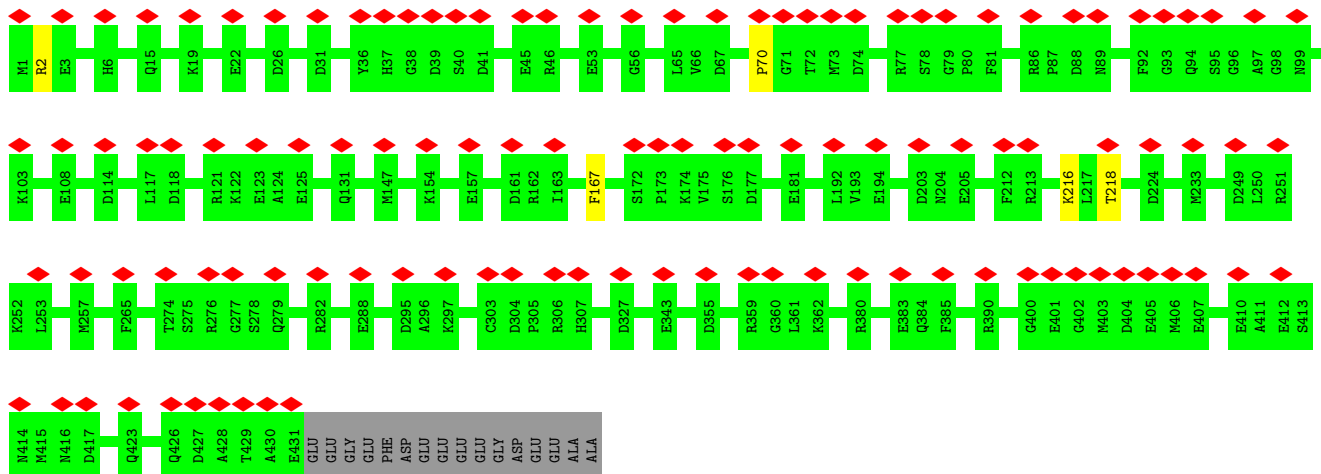
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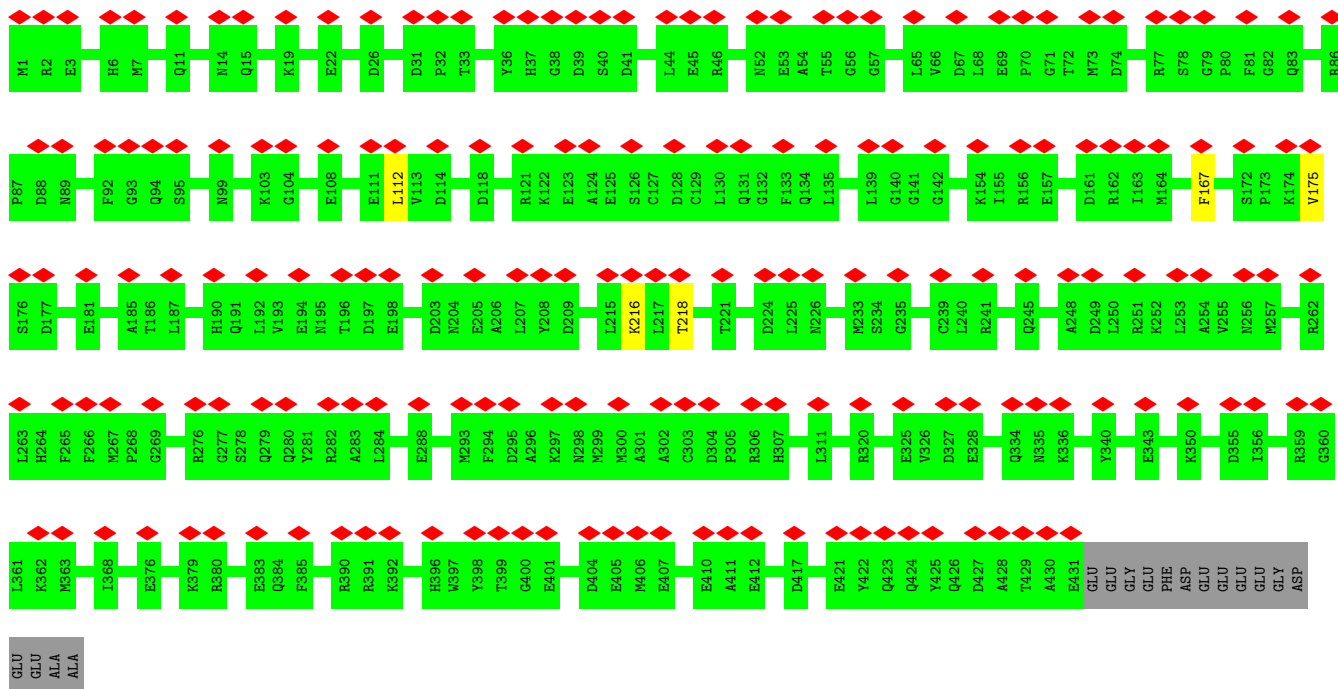
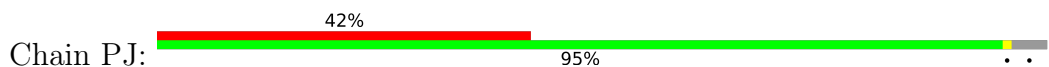
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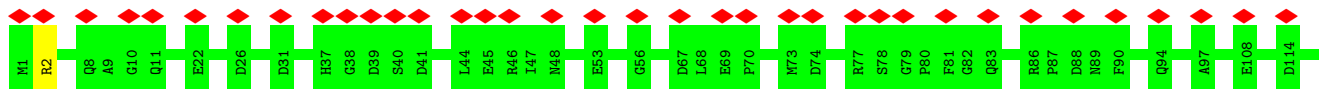
• Molecule 55: Tubulin beta chain

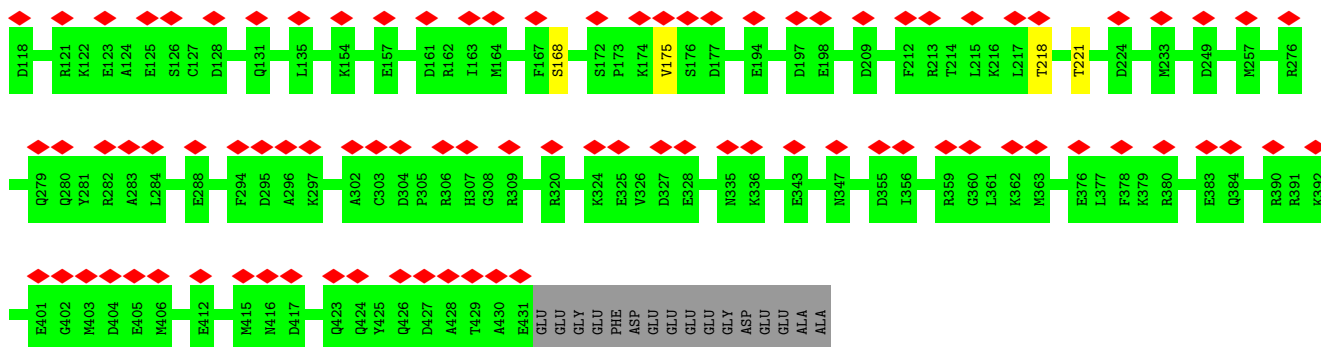


• Molecule 55: Tubulin beta chain

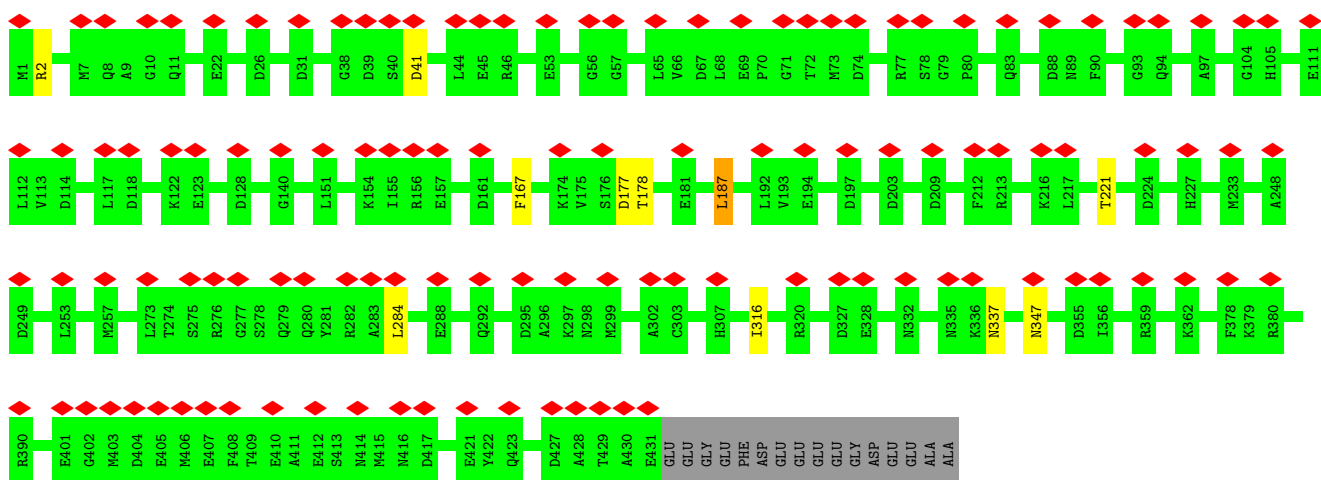


• Molecule 55: Tubulin beta chain

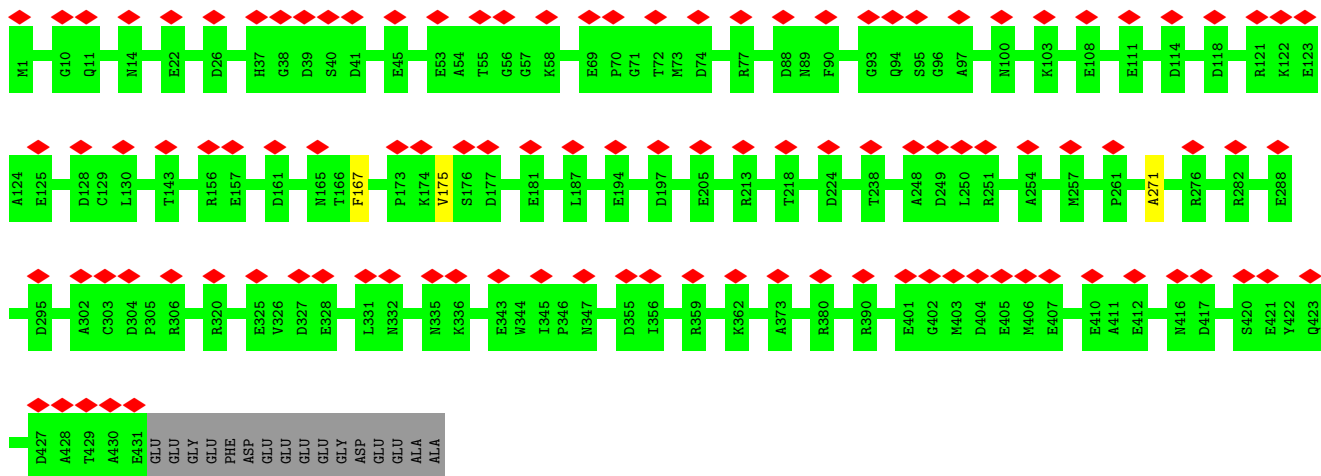




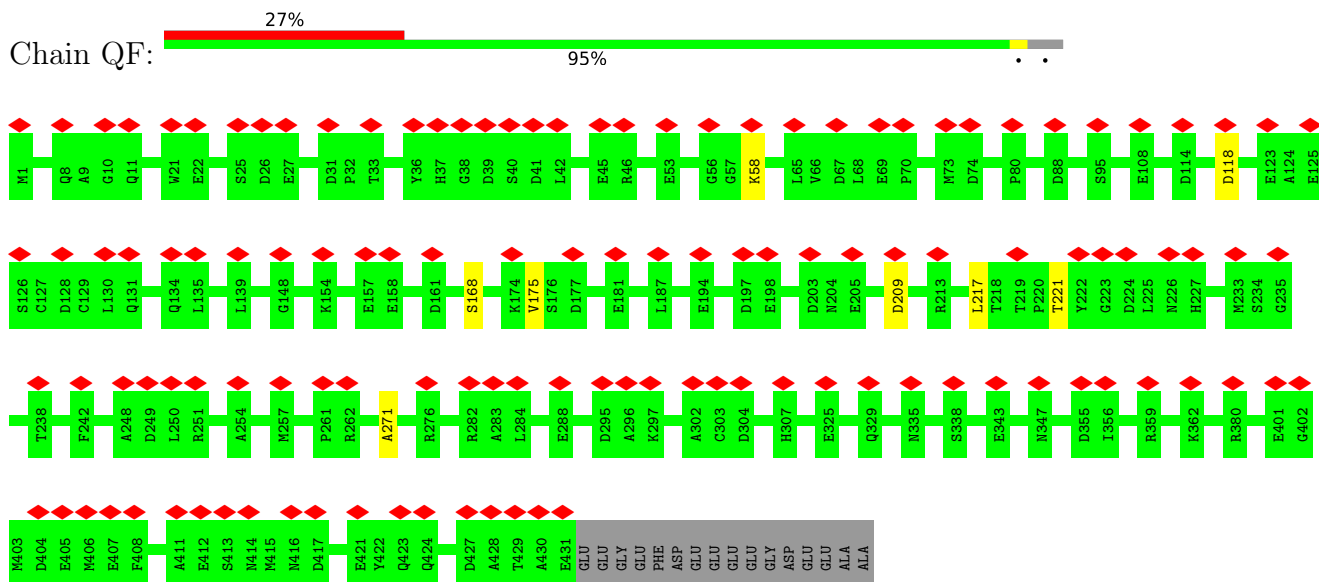
• Molecule 55: Tubulin beta chain



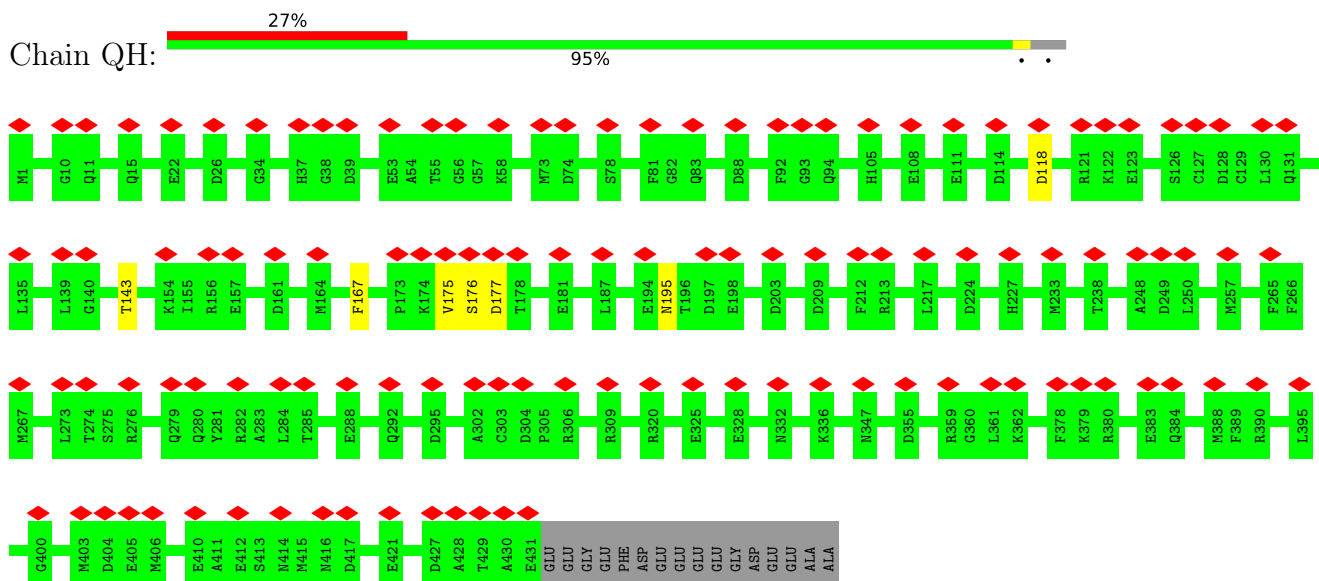
• Molecule 55: Tubulin beta chain



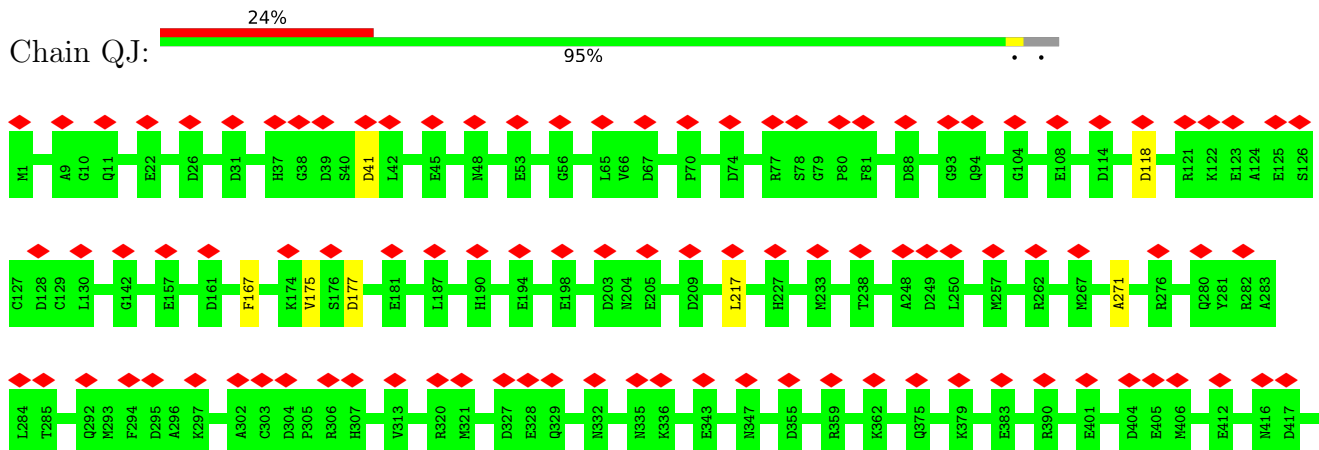
• Molecule 55: Tubulin beta chain

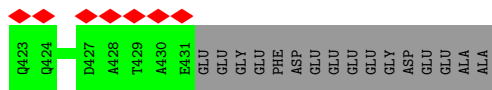


• Molecule 55: Tubulin beta chain

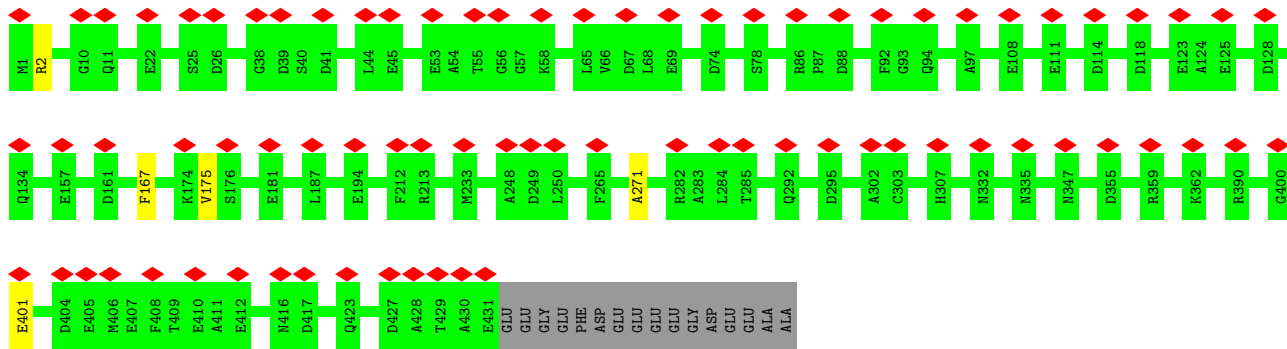


• Molecule 55: Tubulin beta chain

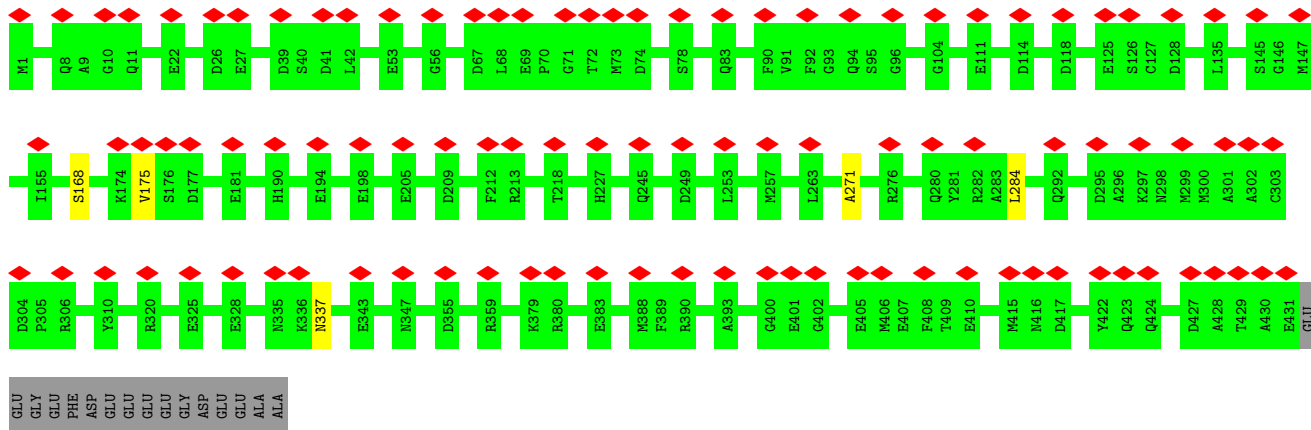




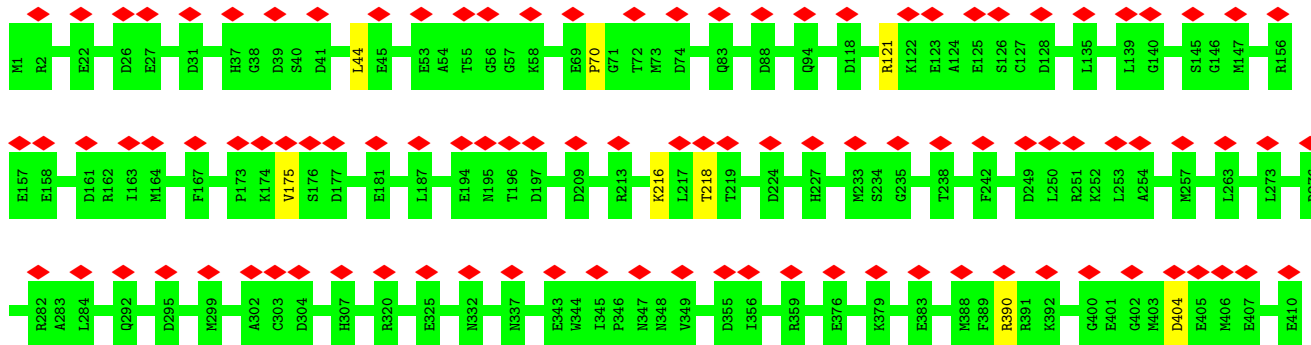
• Molecule 55: Tubulin beta chain

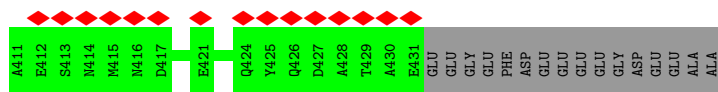


• Molecule 55: Tubulin beta chain

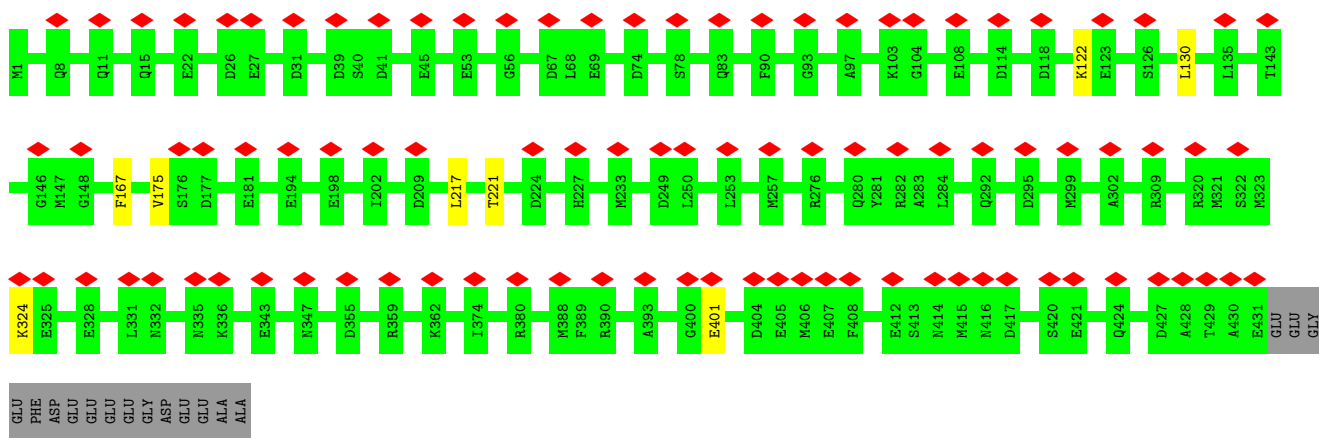


• Molecule 55: Tubulin beta chain

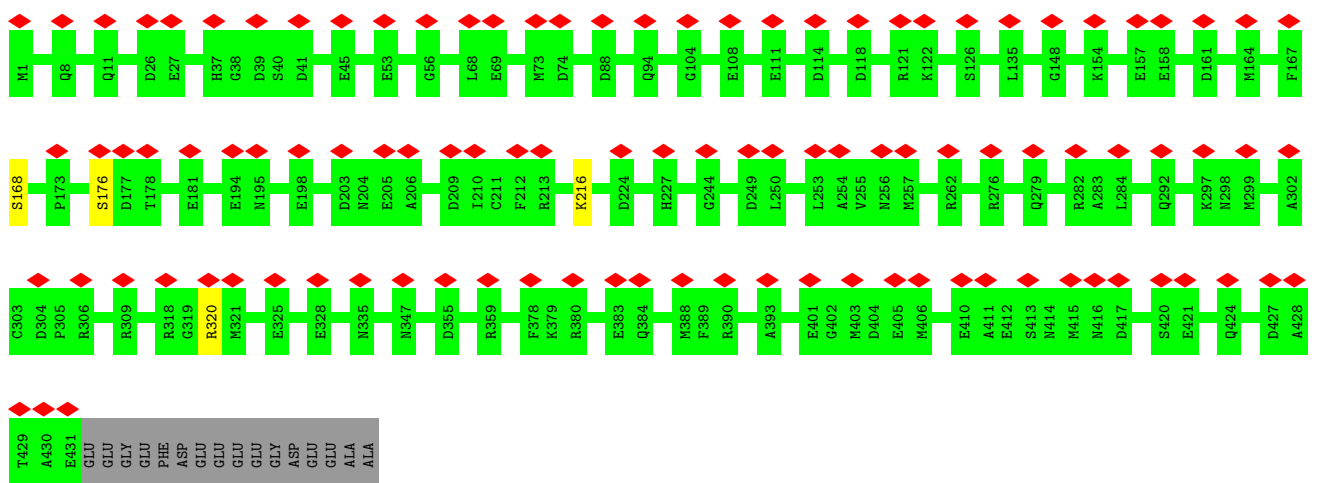




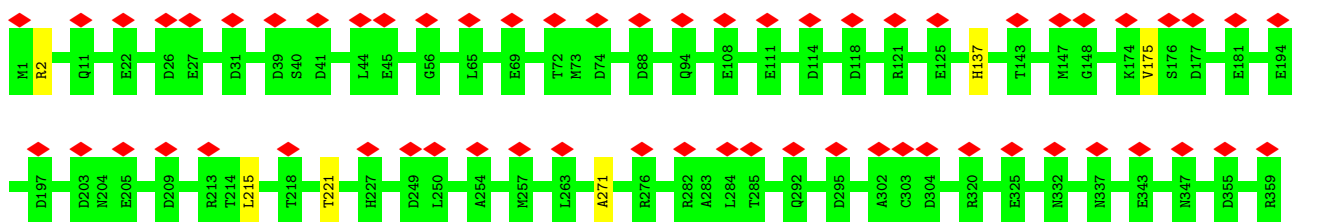
• Molecule 55: Tubulin beta chain



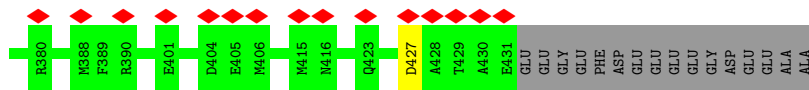
• Molecule 55: Tubulin beta chain



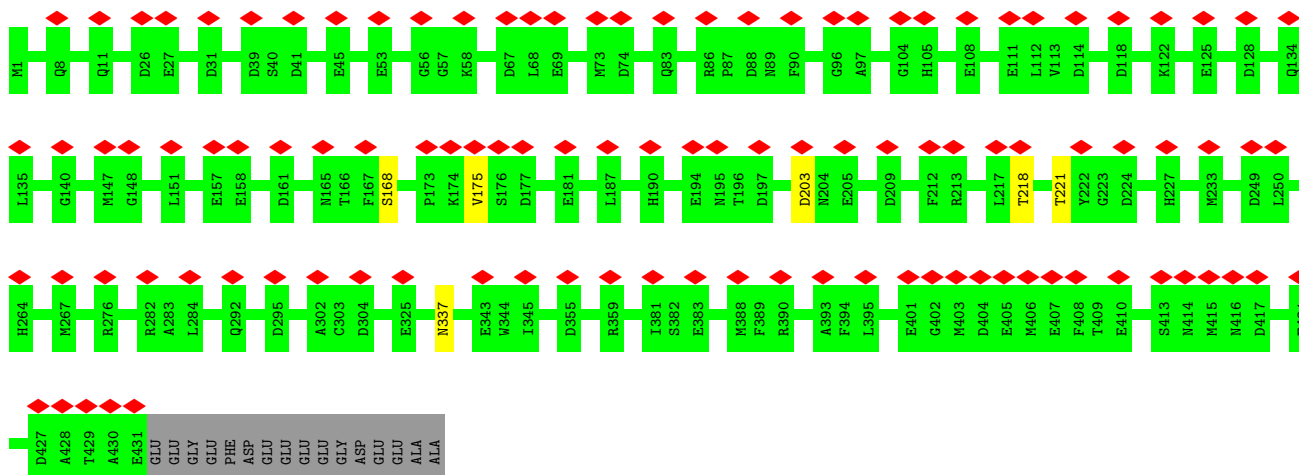
• Molecule 55: Tubulin beta chain



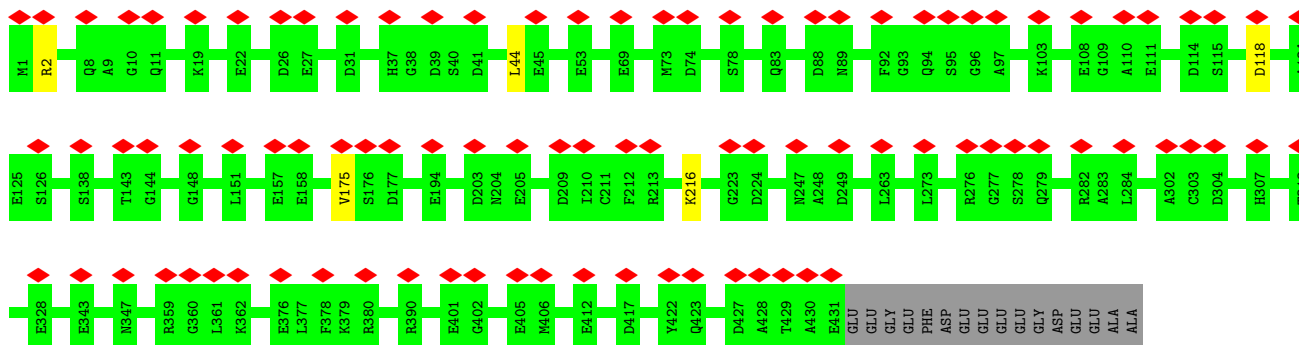




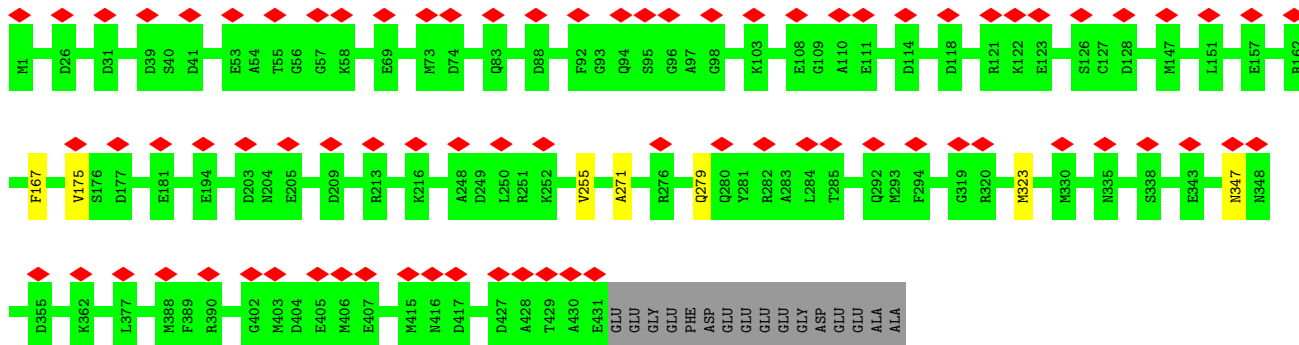
• Molecule 55: Tubulin beta chain



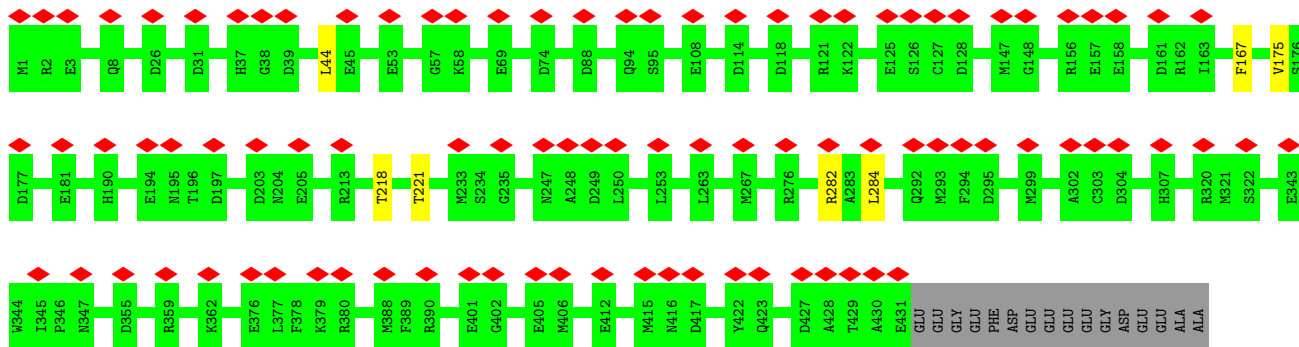
• Molecule 55: Tubulin beta chain



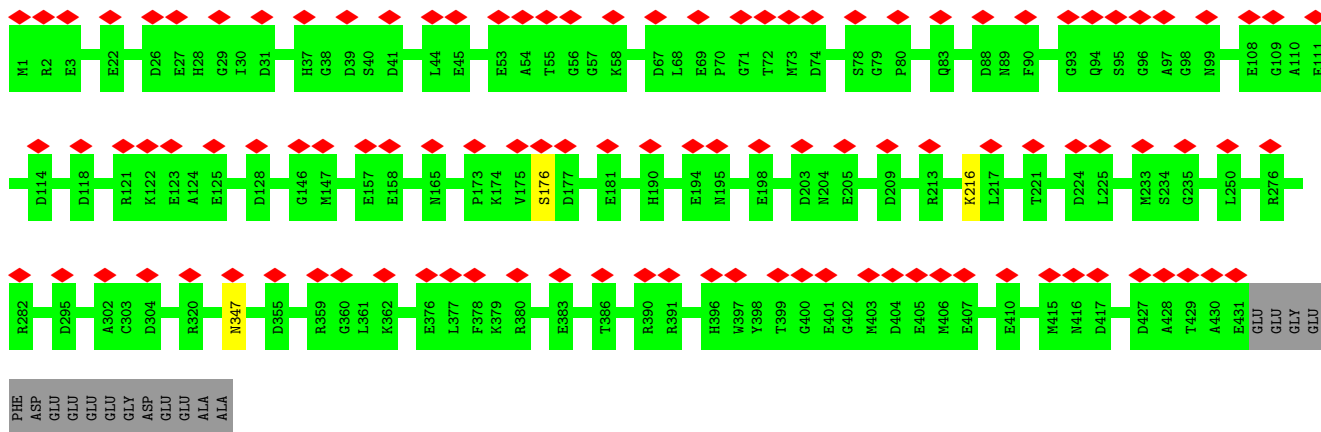
• Molecule 55: Tubulin beta chain



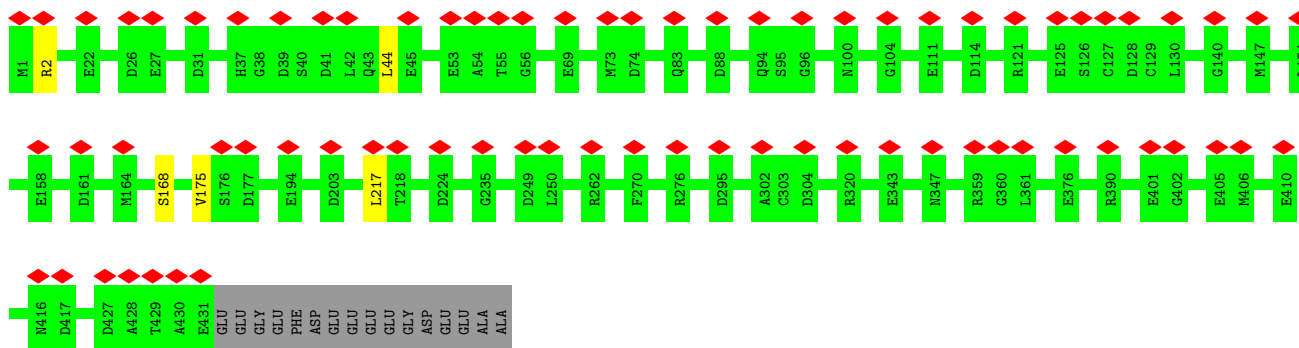
• Molecule 55: Tubulin beta chain



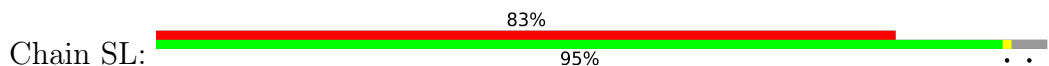
• Molecule 55: Tubulin beta chain

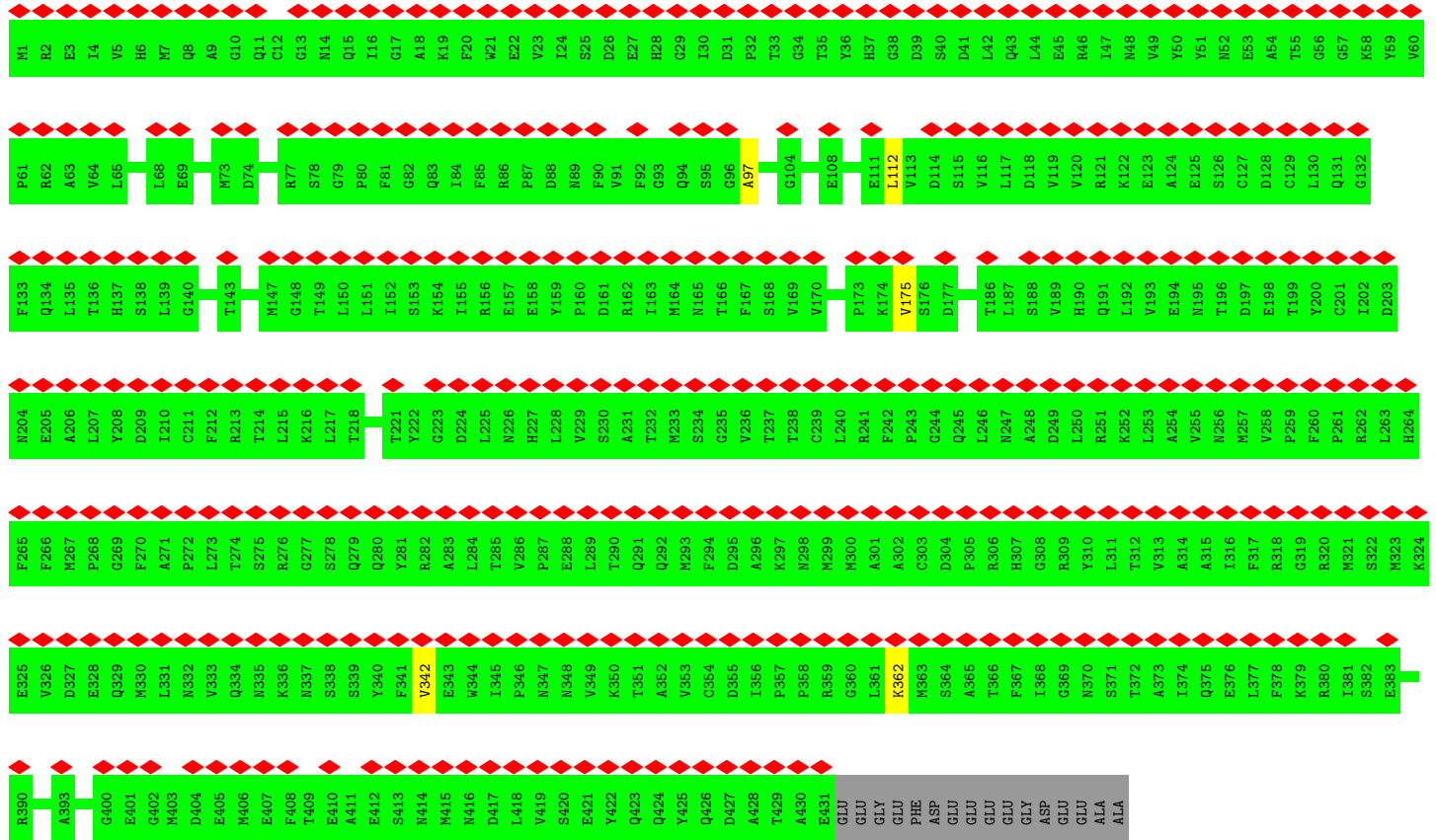


• Molecule 55: Tubulin beta chain

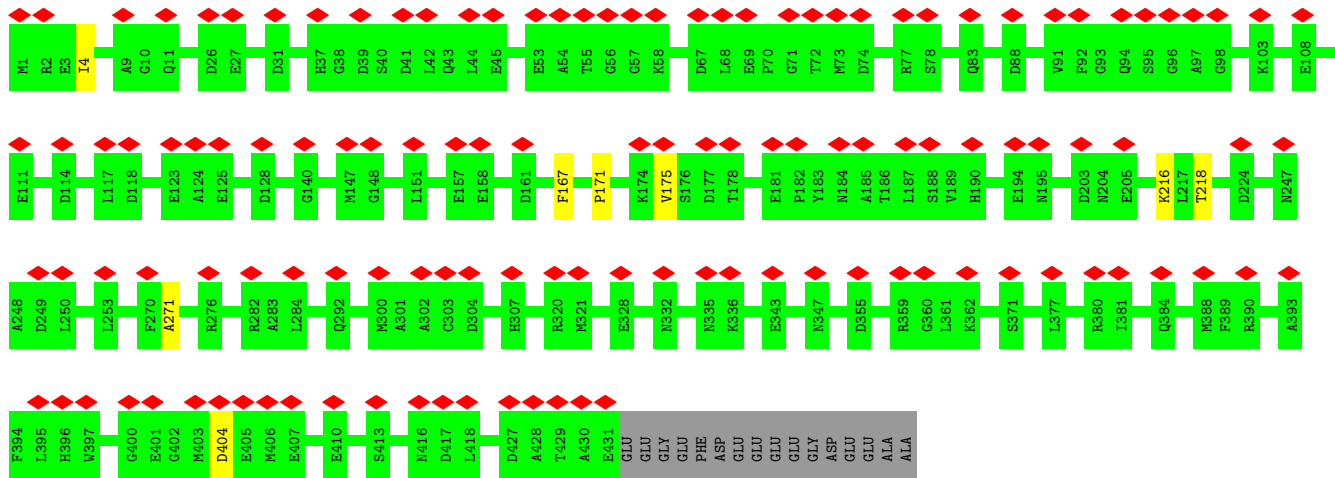


• Molecule 55: Tubulin beta chain

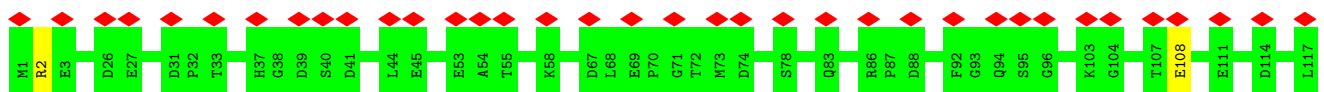


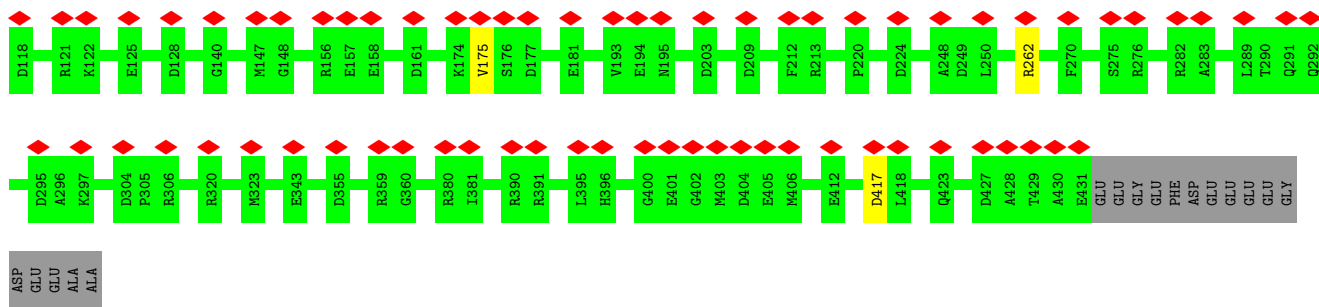


• Molecule 55: Tubulin beta chain

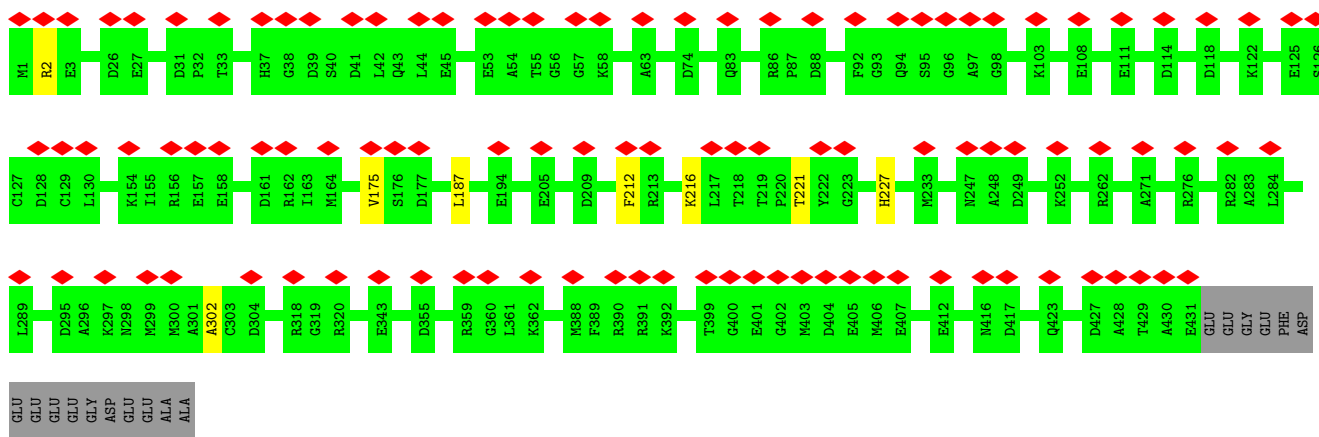


• Molecule 55: Tubulin beta chain

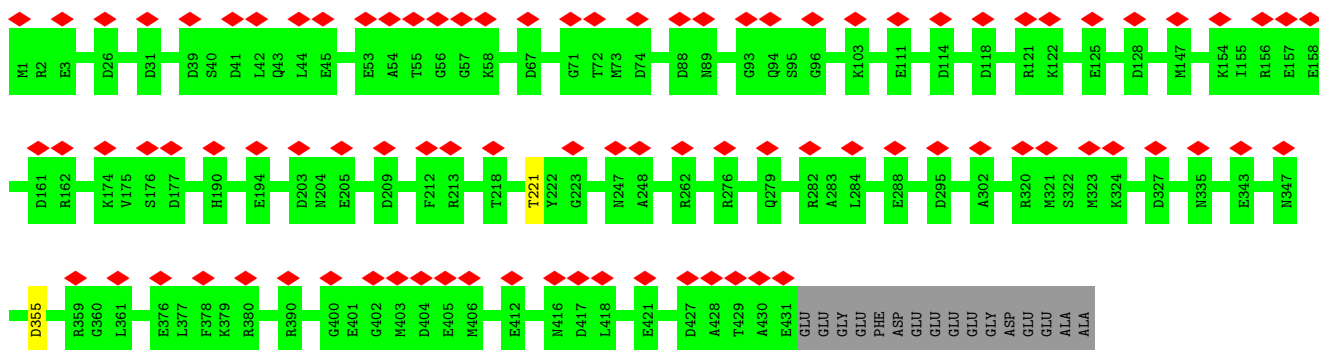




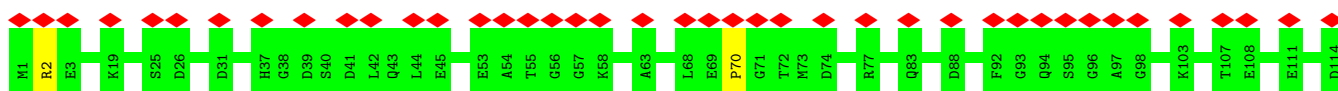
• Molecule 55: Tubulin beta chain

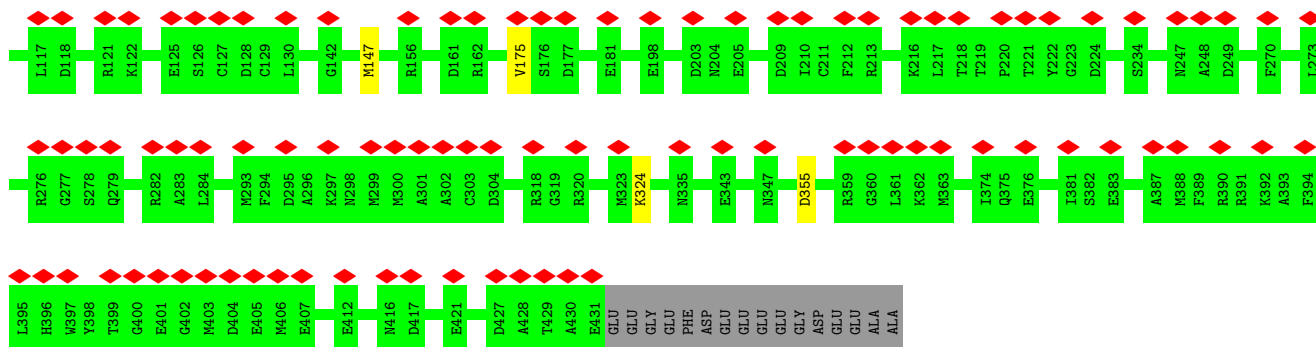


• Molecule 55: Tubulin beta chain

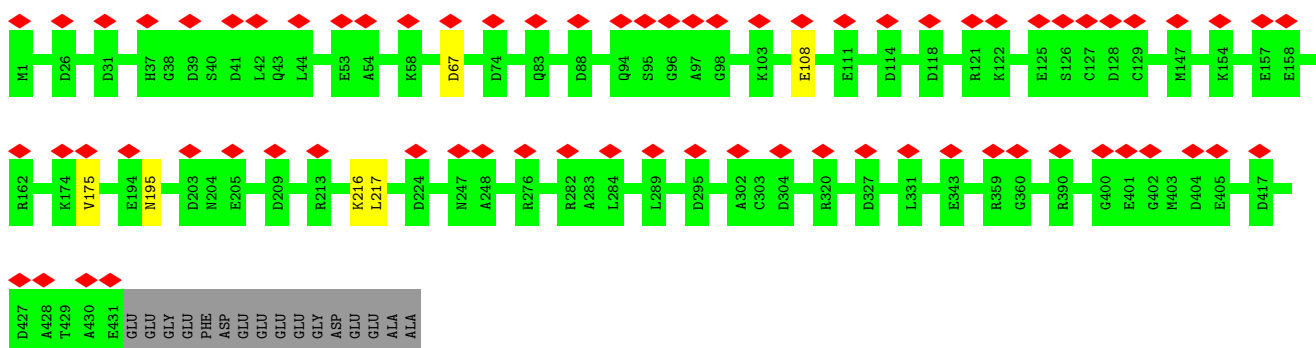


• Molecule 55: Tubulin beta chain

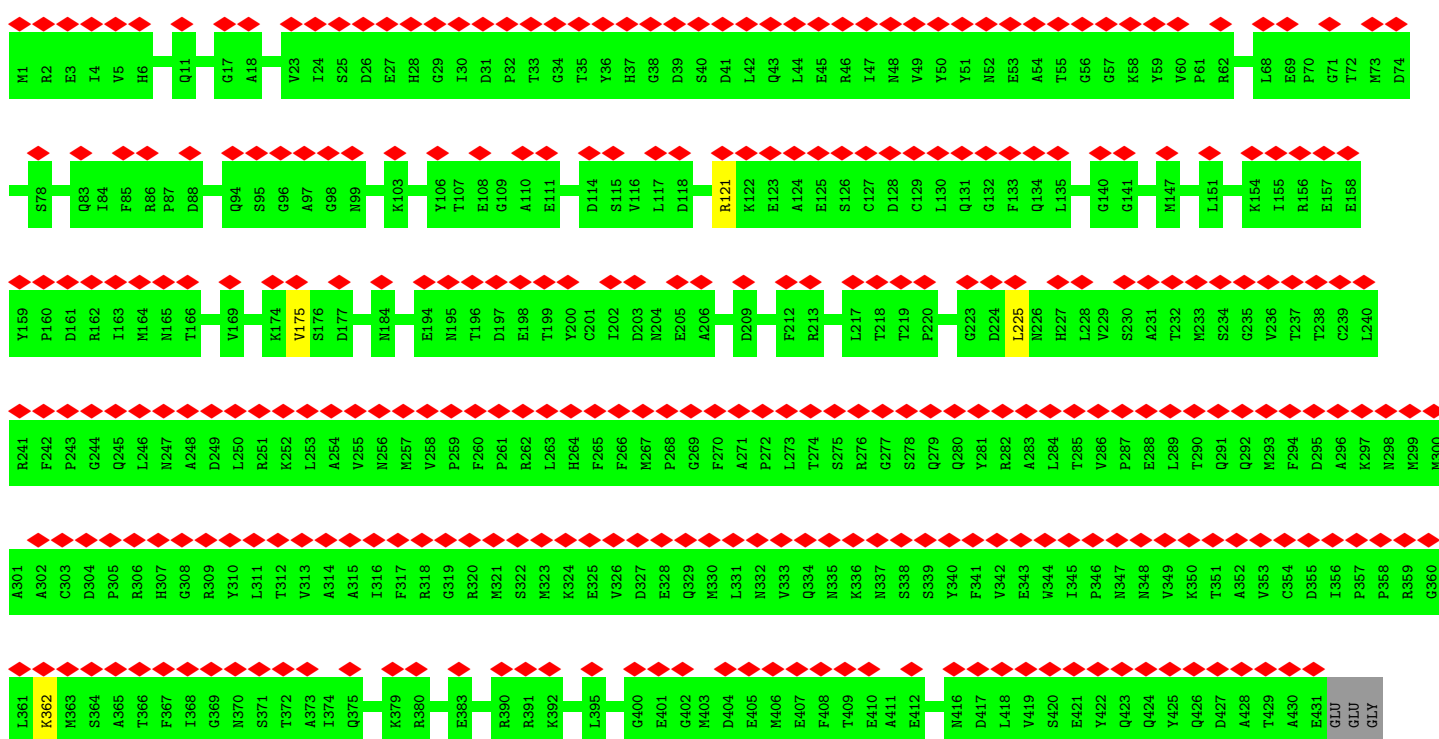




• Molecule 55: Tubulin beta chain

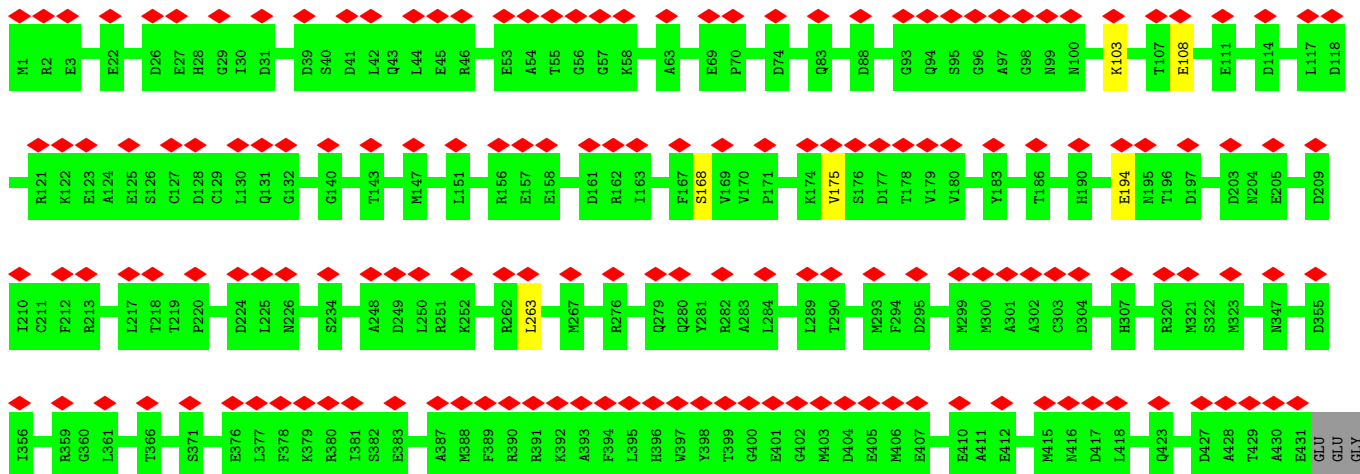


• Molecule 55: Tubulin beta chain



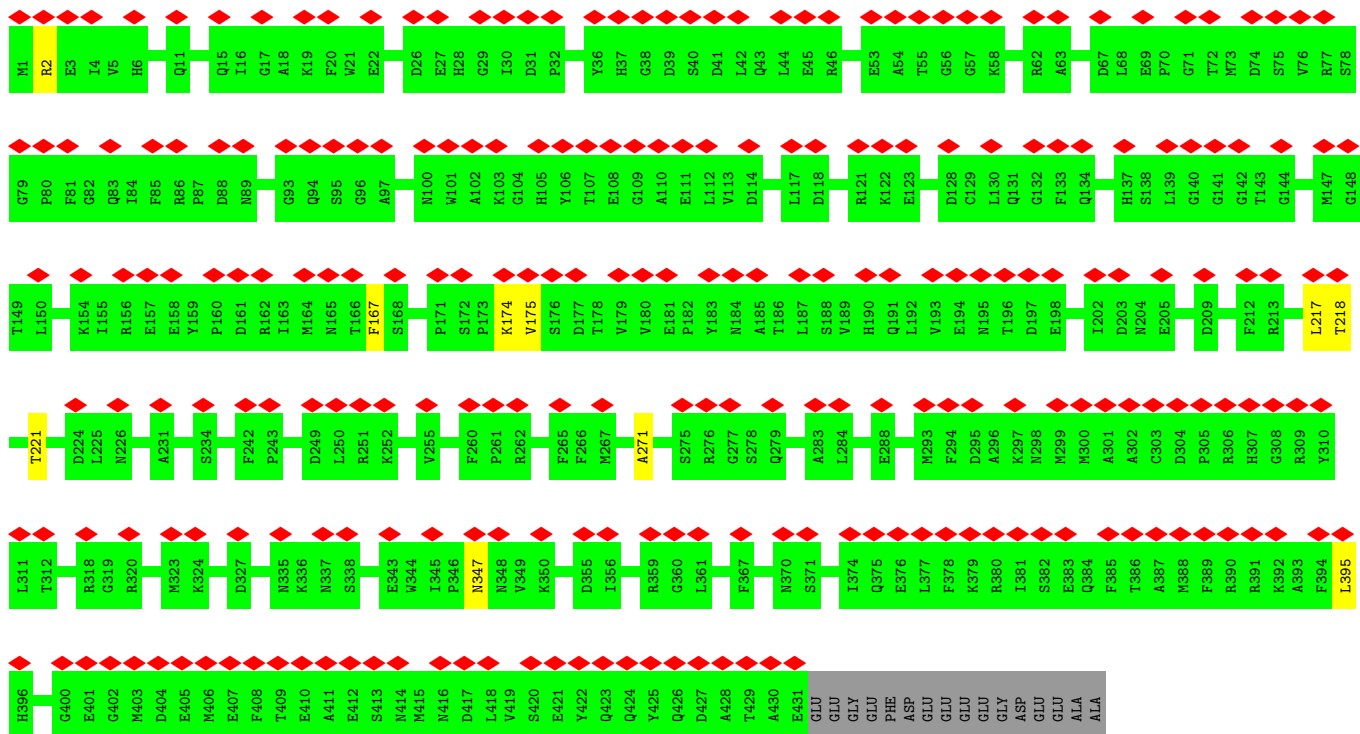
GLU  
PHE  
ASP  
GLU  
GLU  
GLU  
GLY  
ASP  
GLU  
GLU  
ALA  
ALA

• Molecule 55: Tubulin beta chain

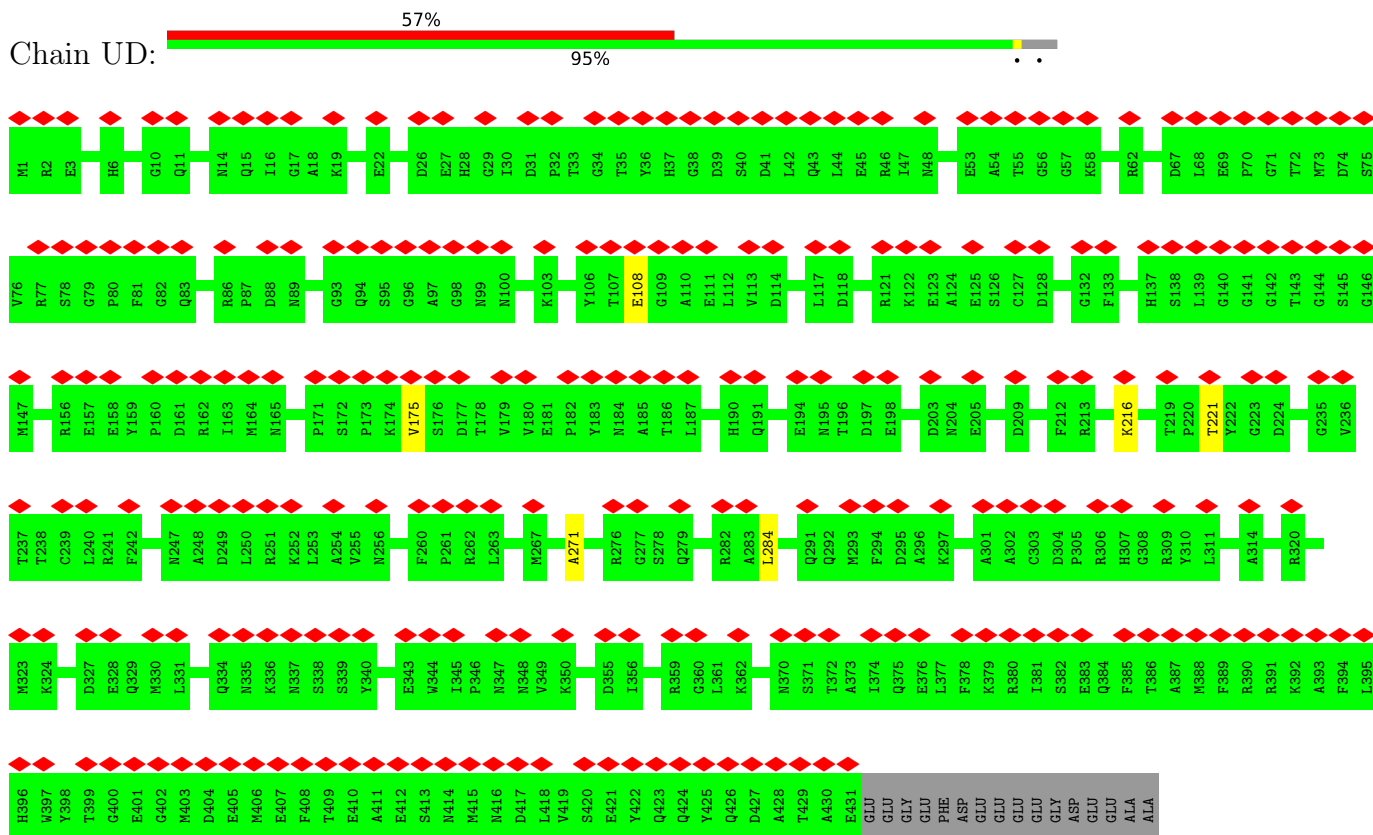


GLU  
PHE  
ASP  
GLU  
GLU  
GLU  
GLY  
ASP  
GLU  
GLU  
ALA  
ALA

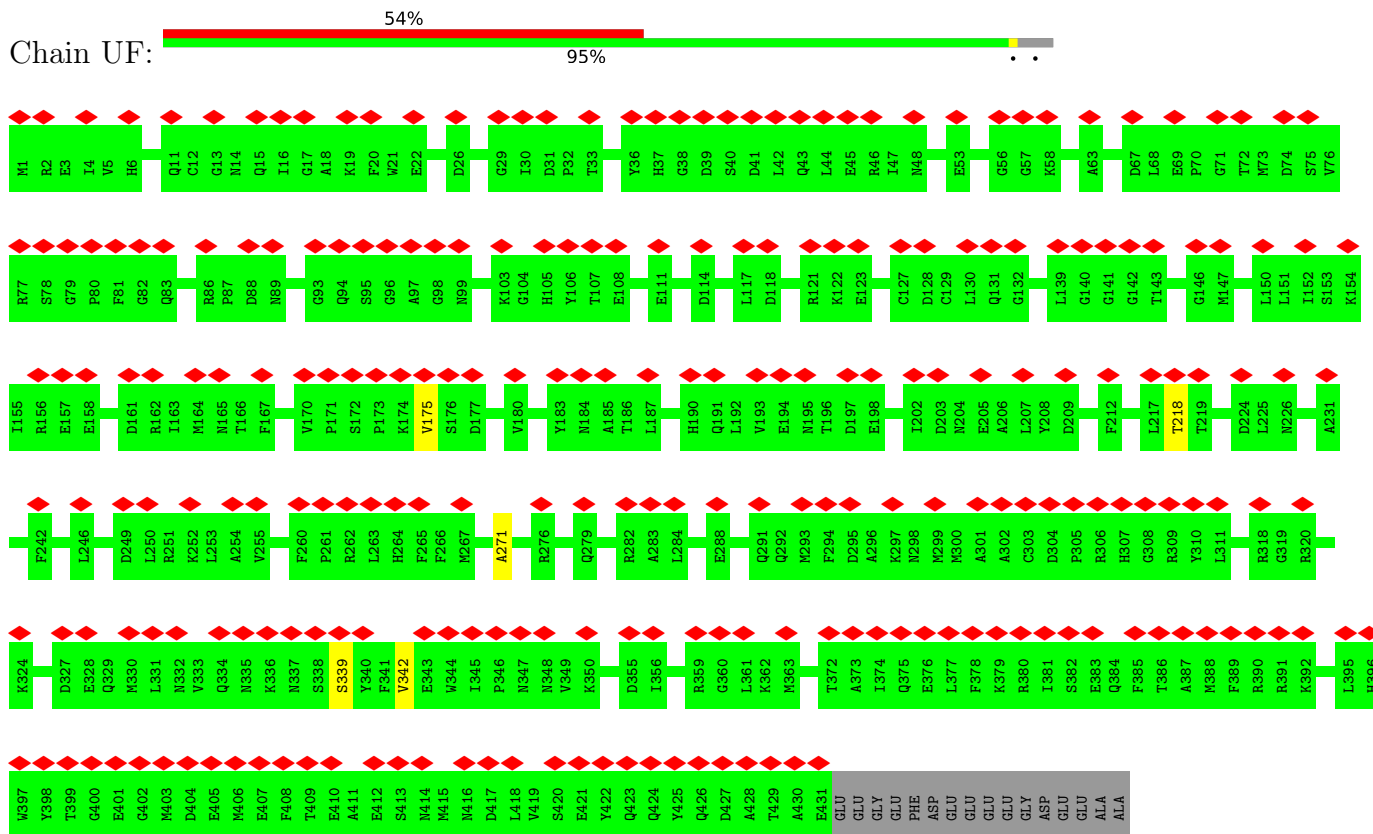
• Molecule 55: Tubulin beta chain



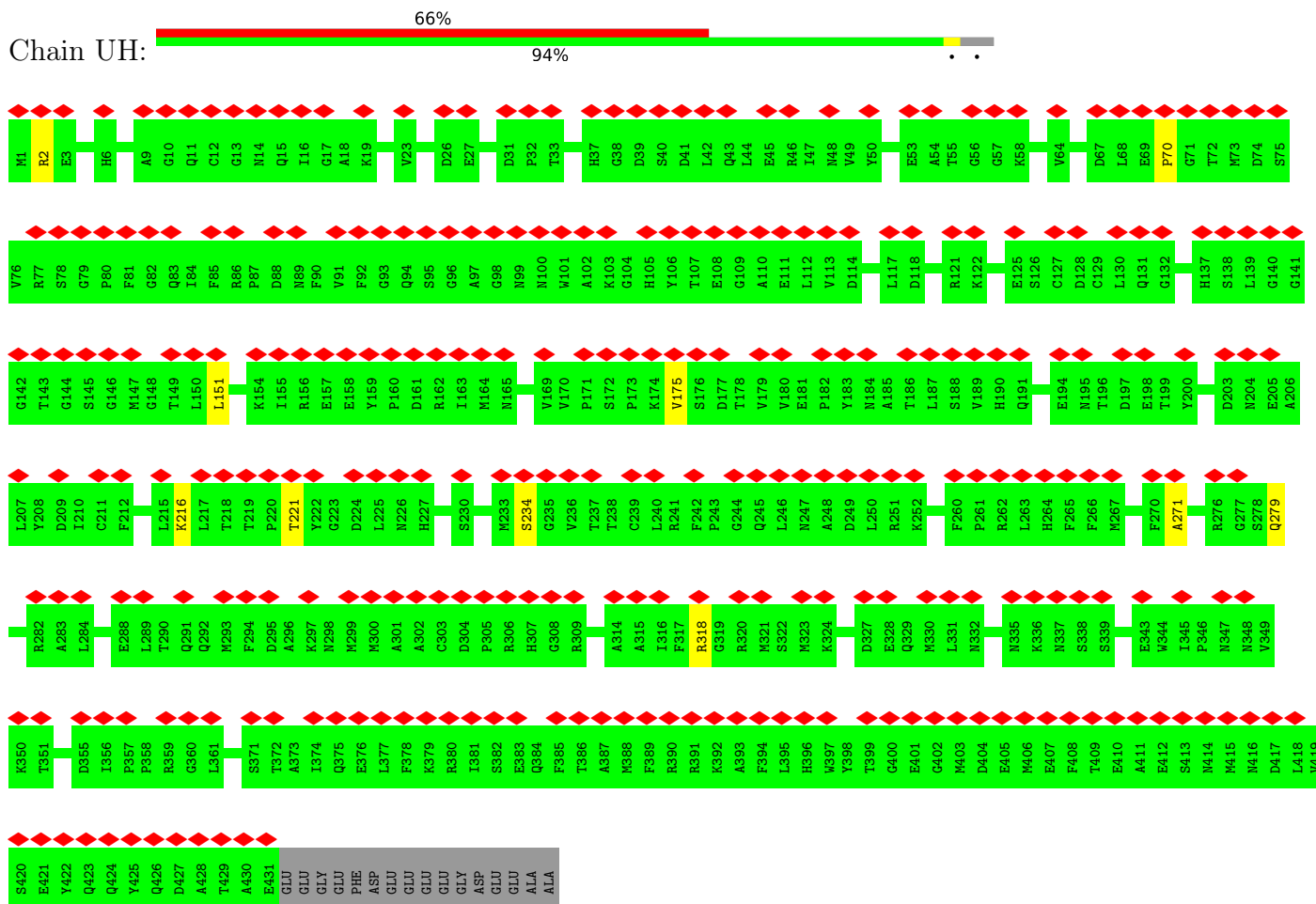
• Molecule 55: Tubulin beta chain



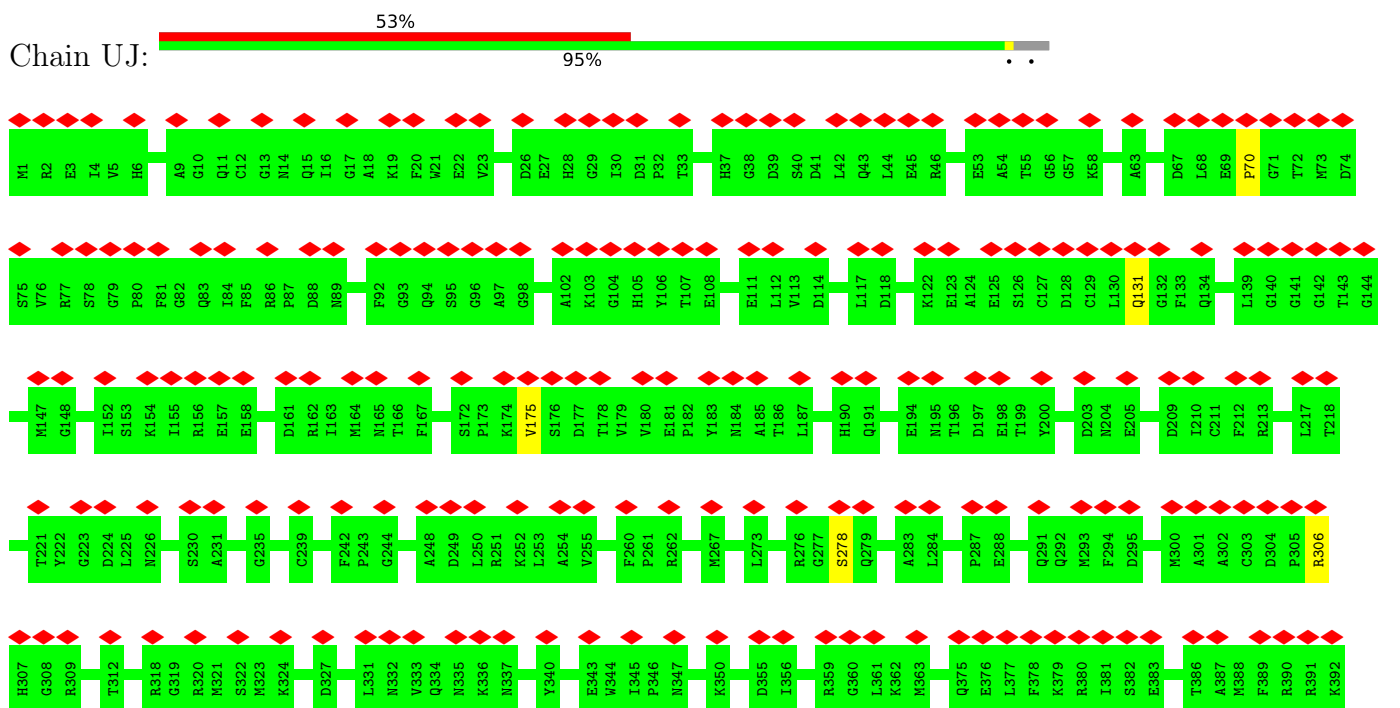
• Molecule 55: Tubulin beta chain



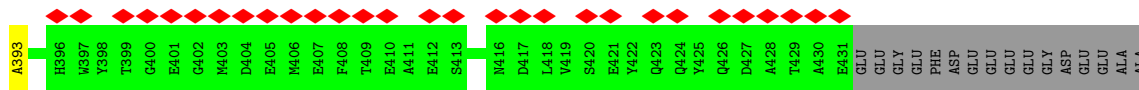
• Molecule 55: Tubulin beta chain



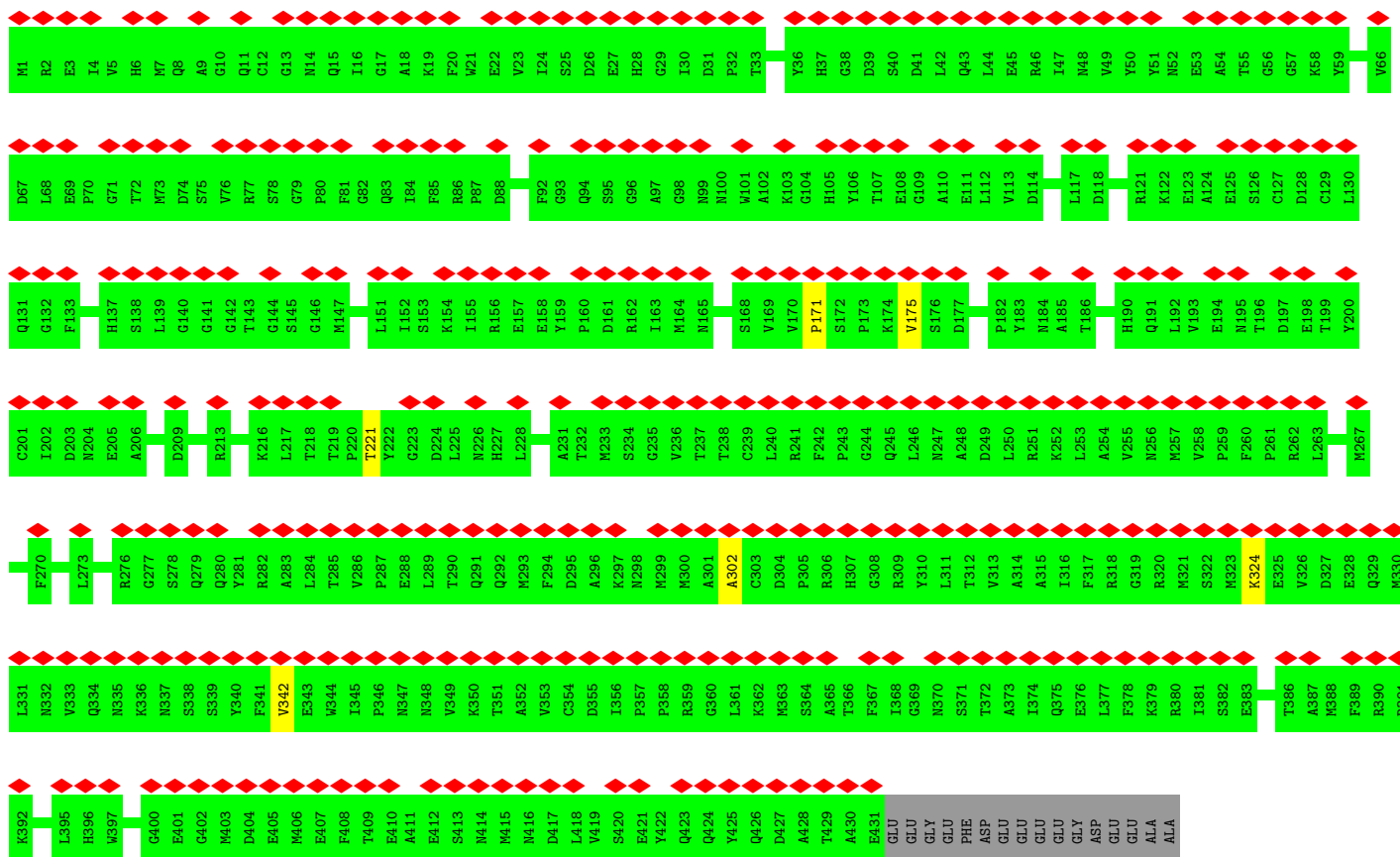
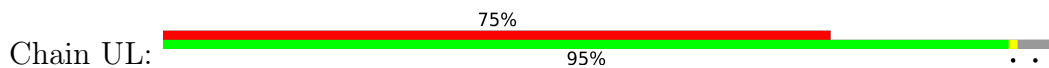
• Molecule 55: Tubulin beta chain



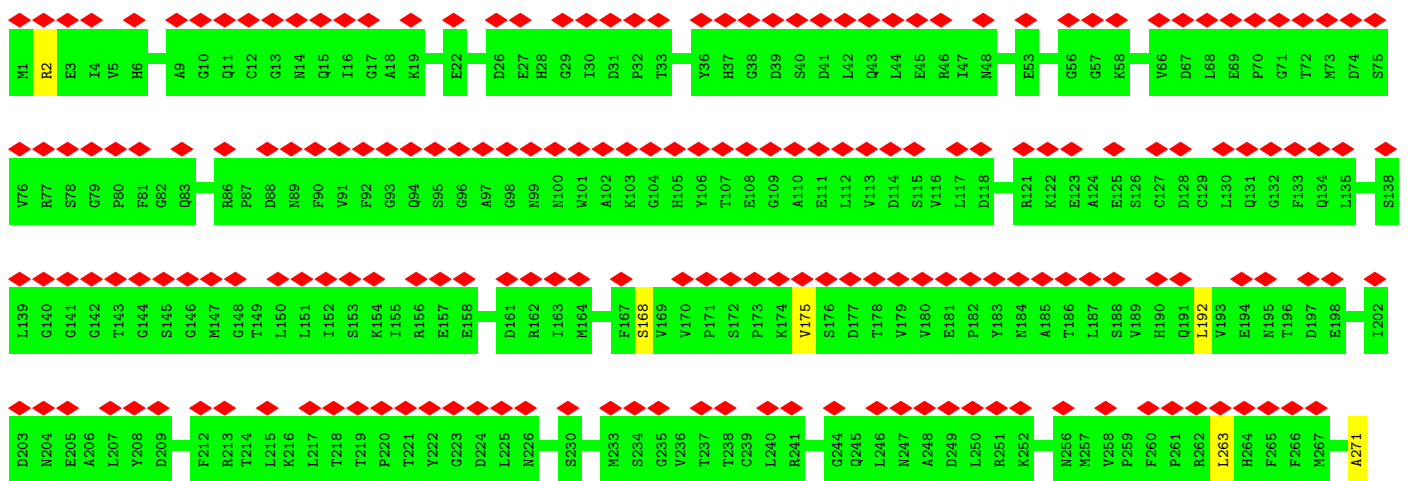


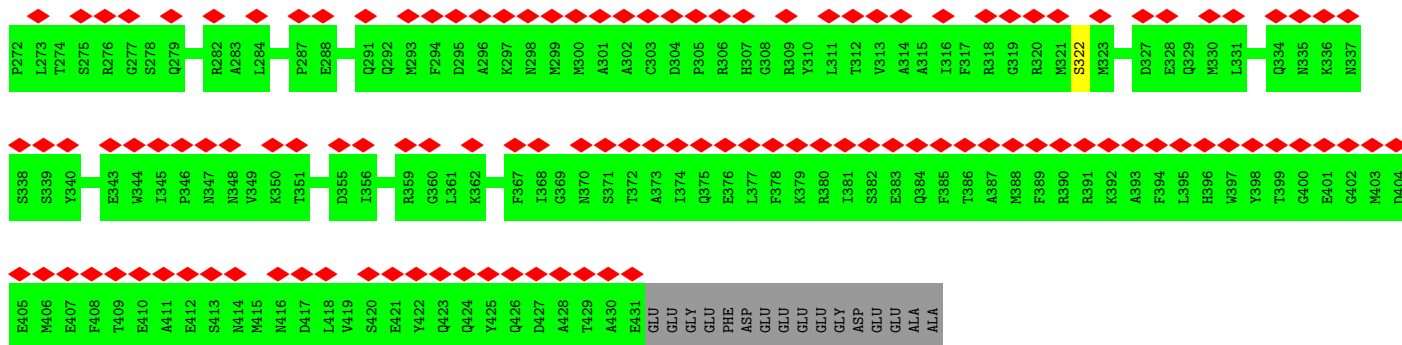


• Molecule 55: Tubulin beta chain

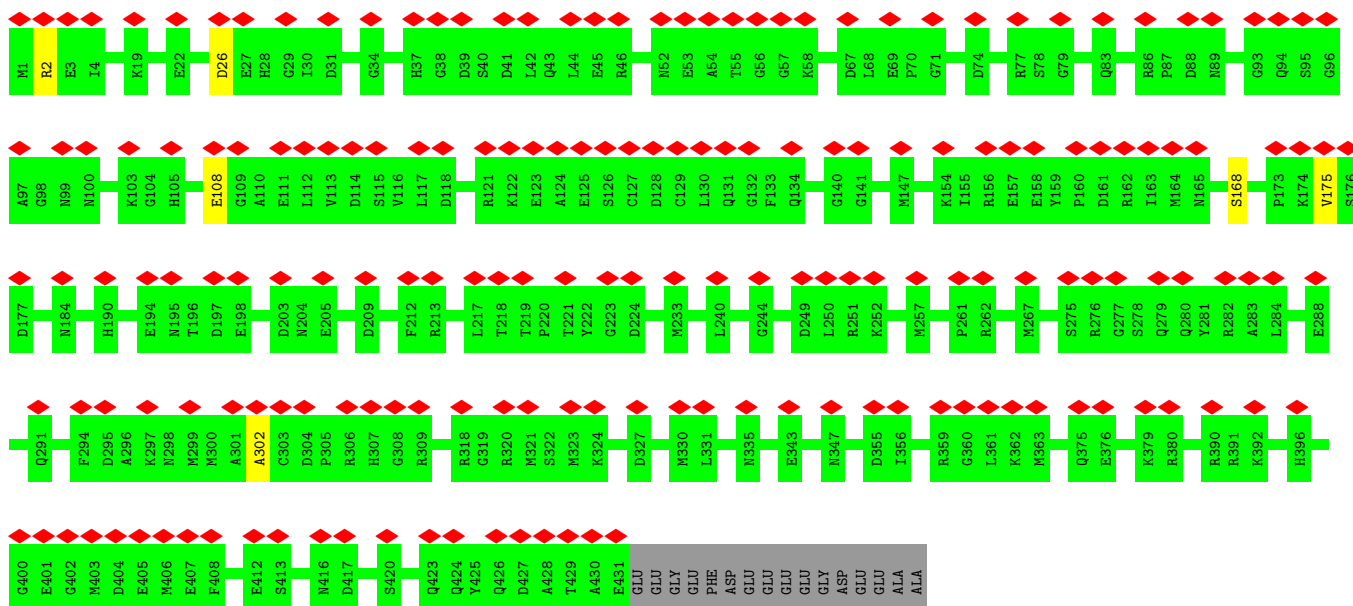
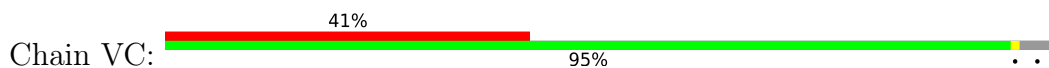


• Molecule 55: Tubulin beta chain

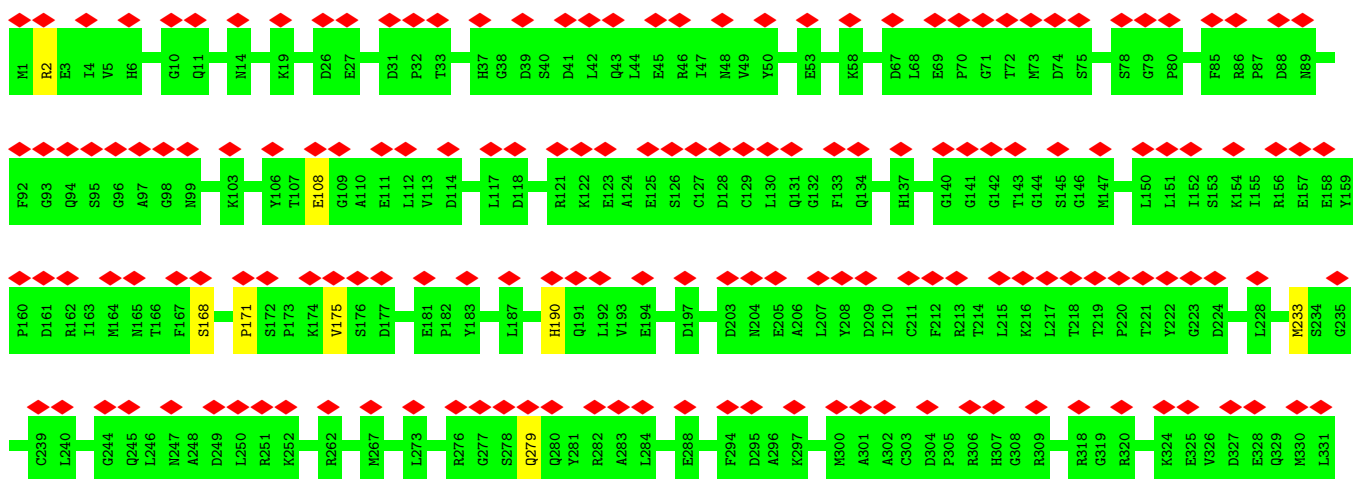


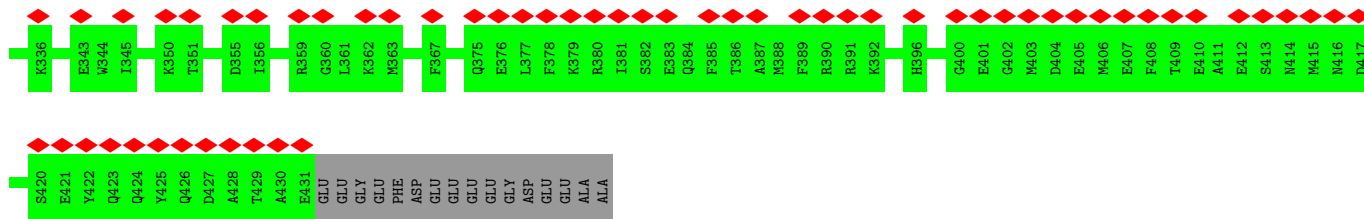


• Molecule 55: Tubulin beta chain

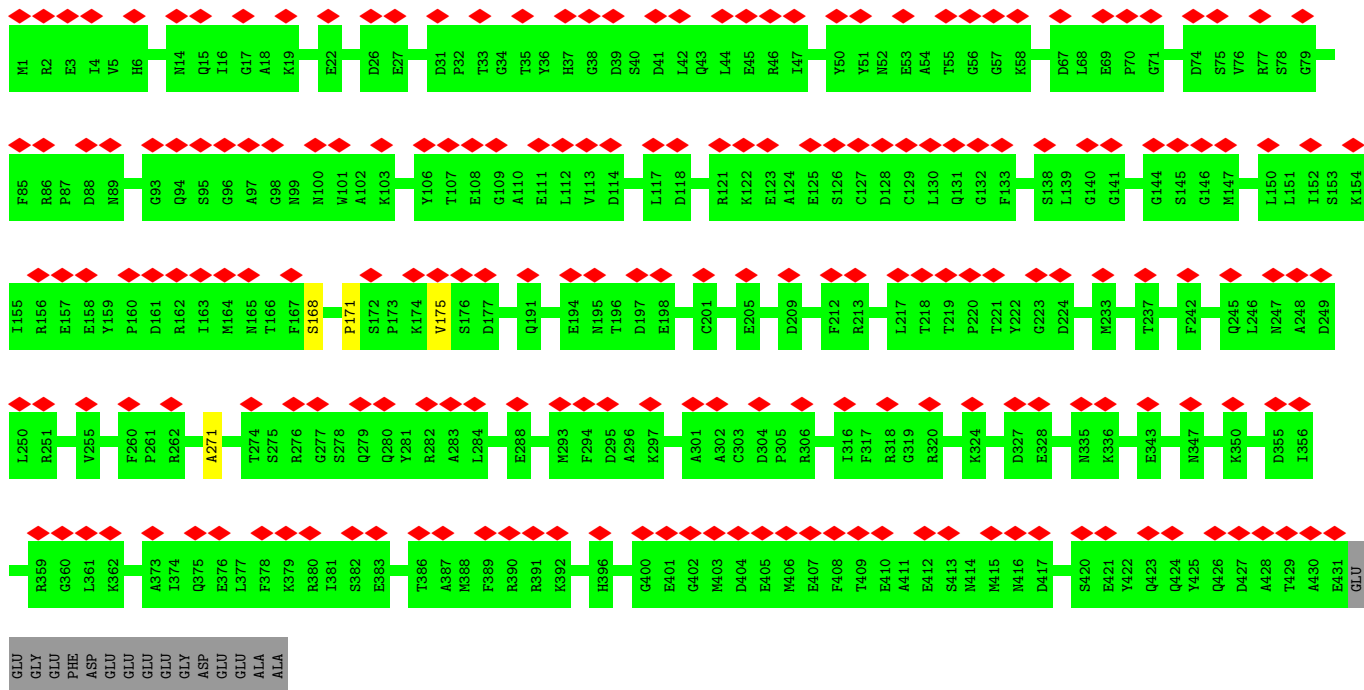


• Molecule 55: Tubulin beta chain

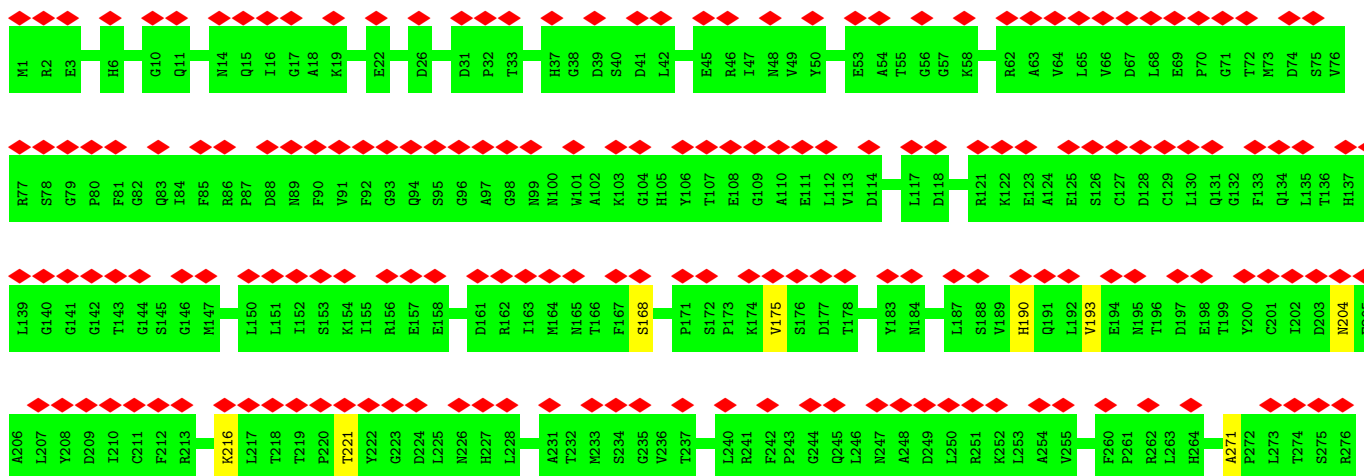


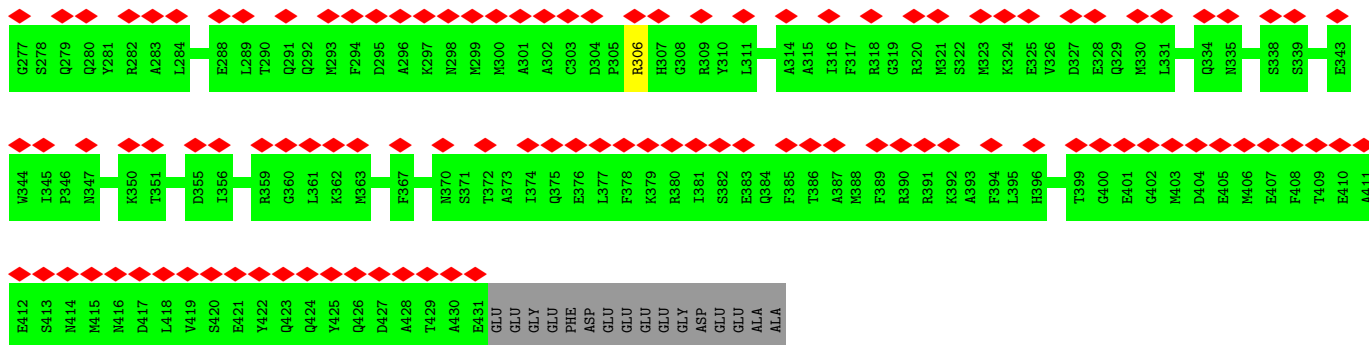


• Molecule 55: Tubulin beta chain

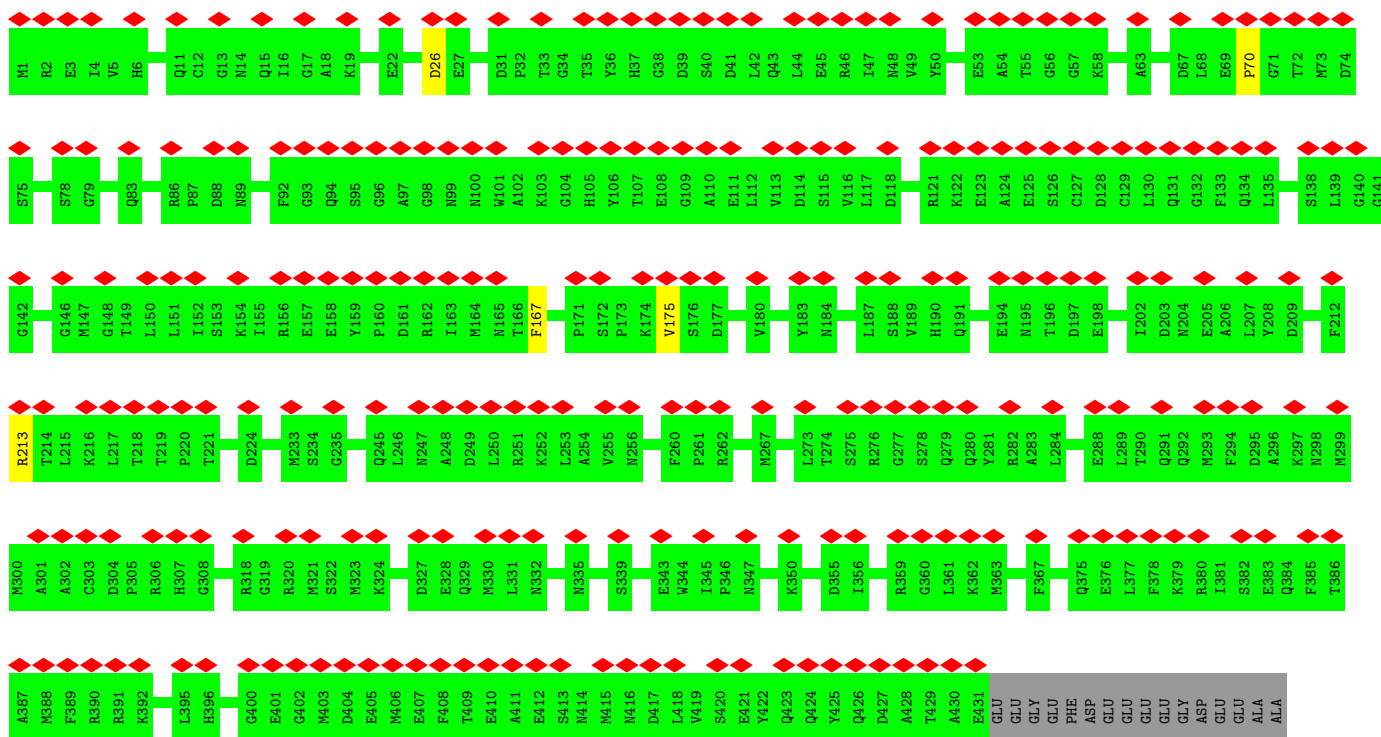


• Molecule 55: Tubulin beta chain

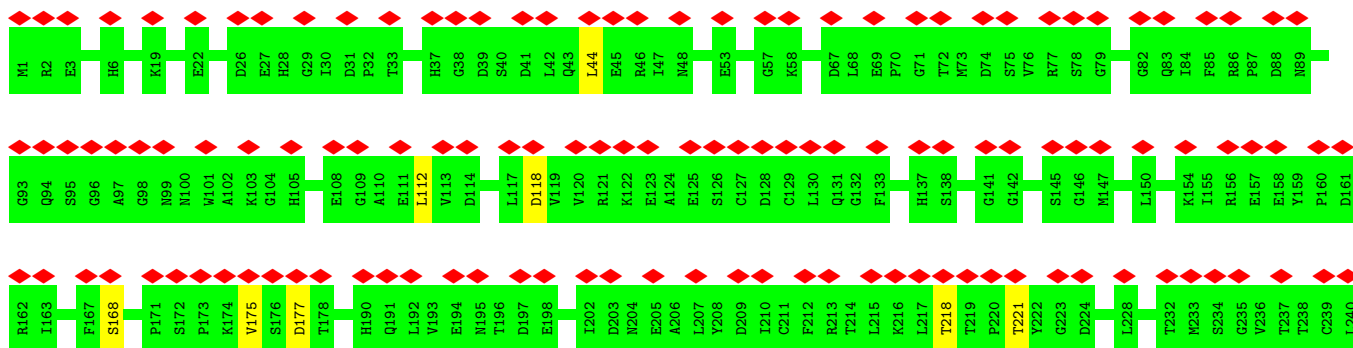


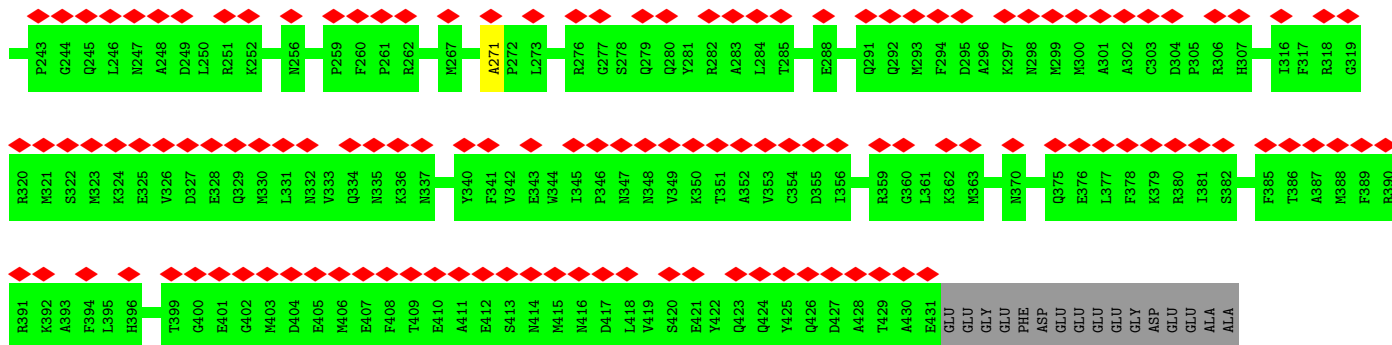


• Molecule 55: Tubulin beta chain

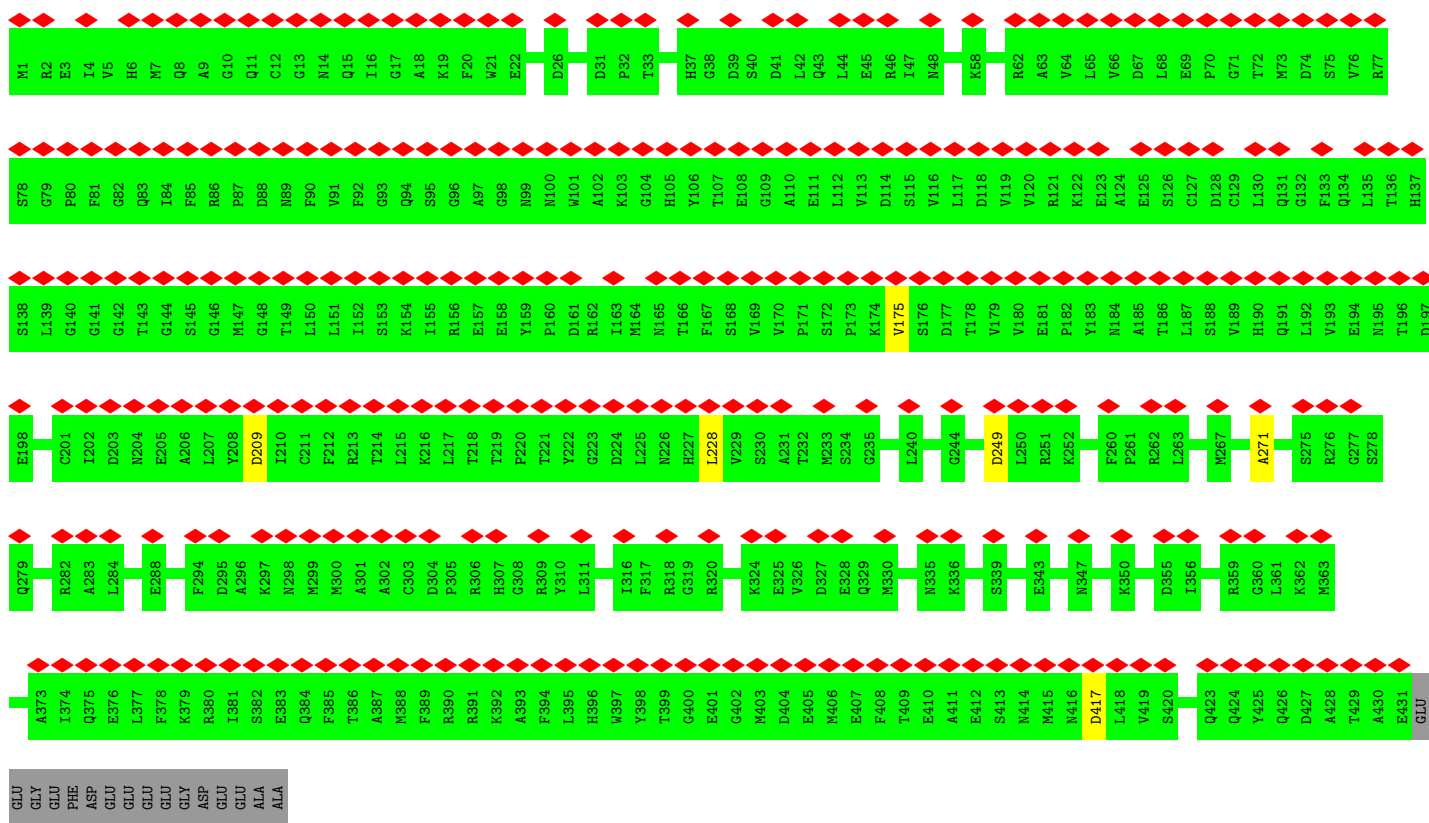
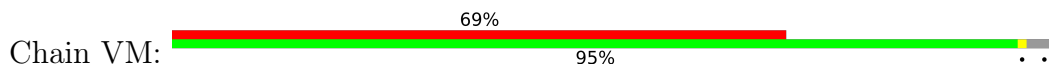


• Molecule 55: Tubulin beta chain

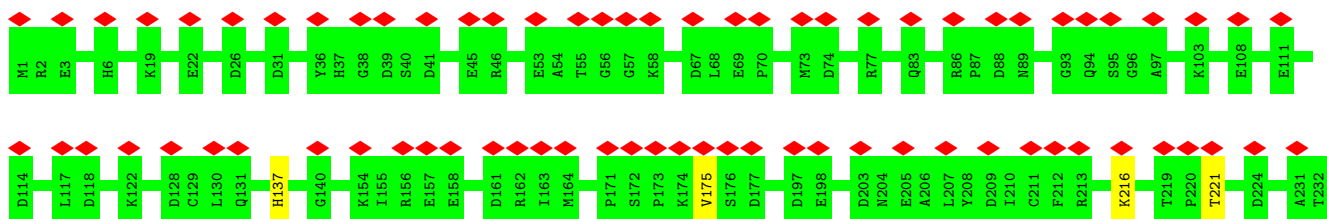


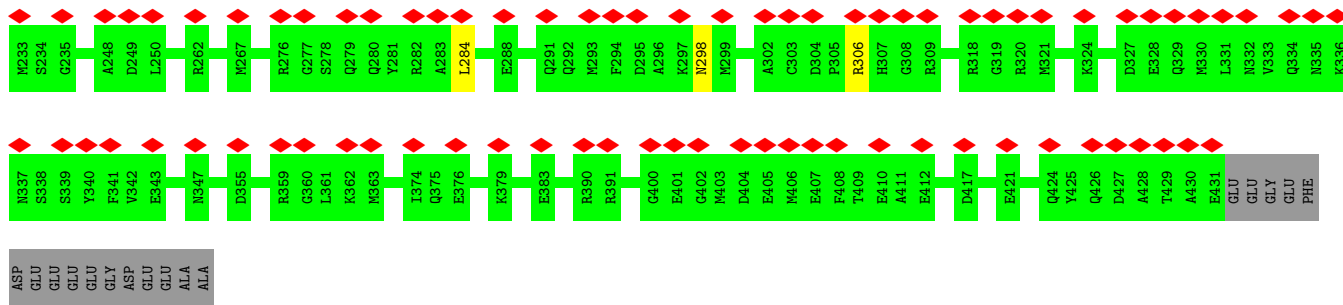


• Molecule 55: Tubulin beta chain

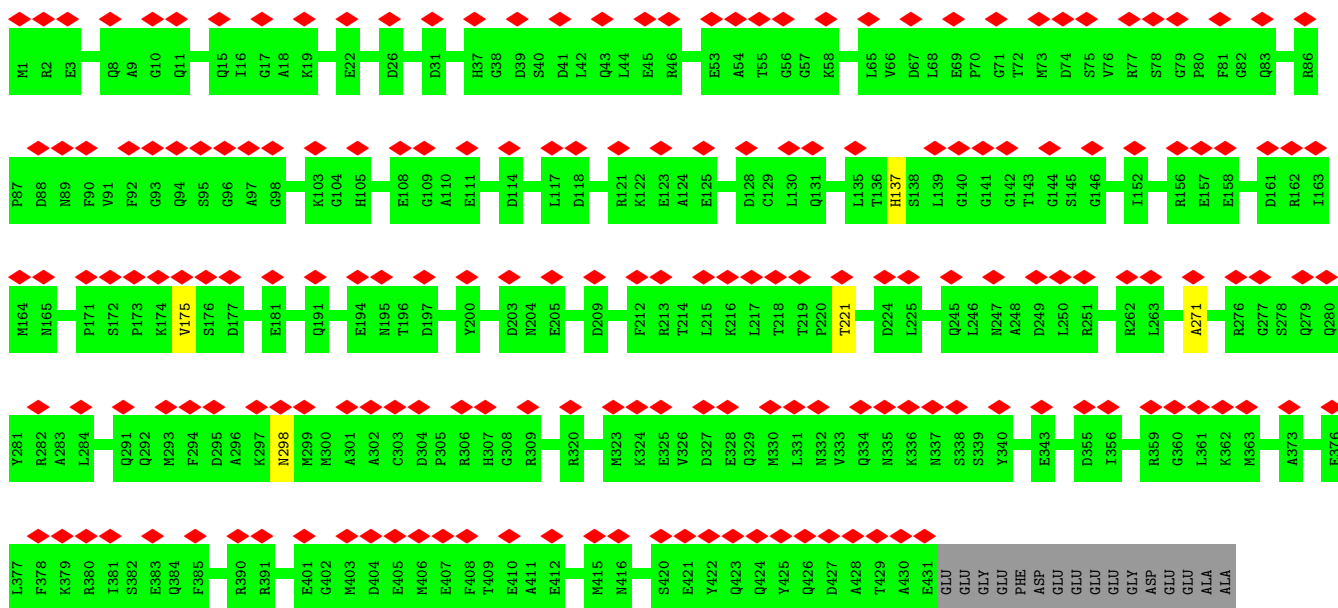
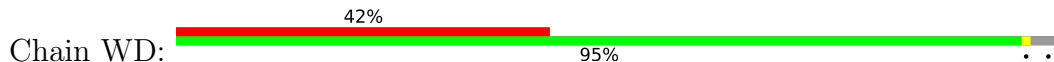


• Molecule 55: Tubulin beta chain

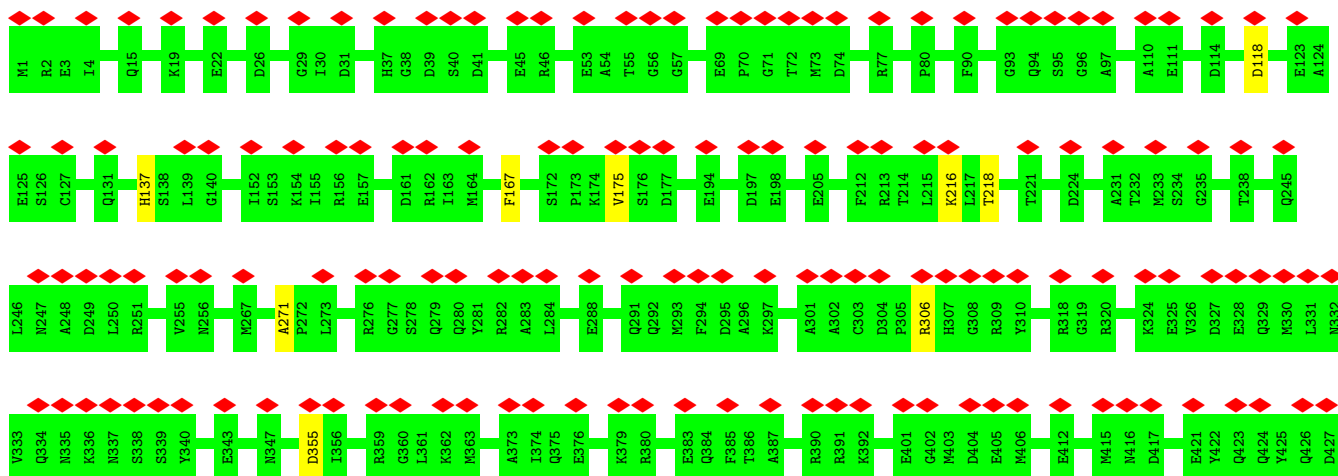


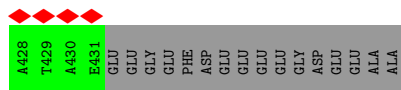


● Molecule 55: Tubulin beta chain

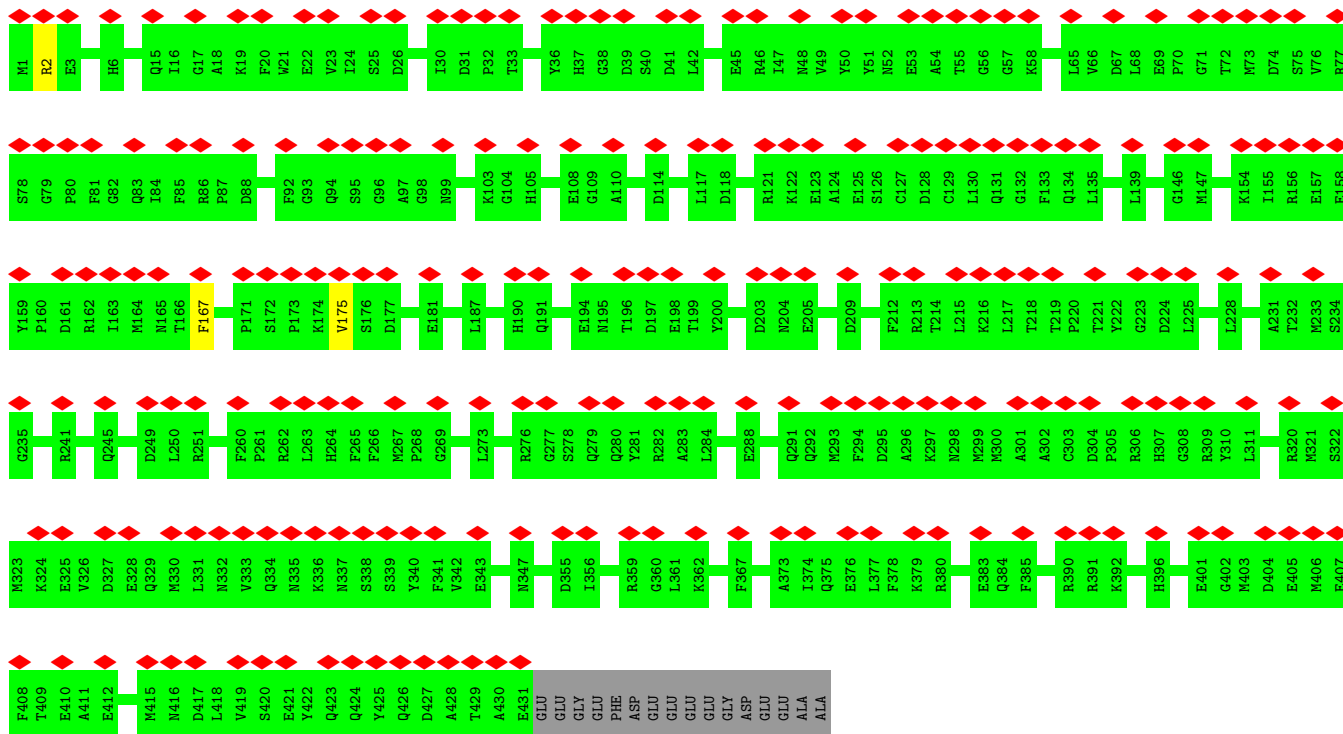


● Molecule 55: Tubulin beta chain

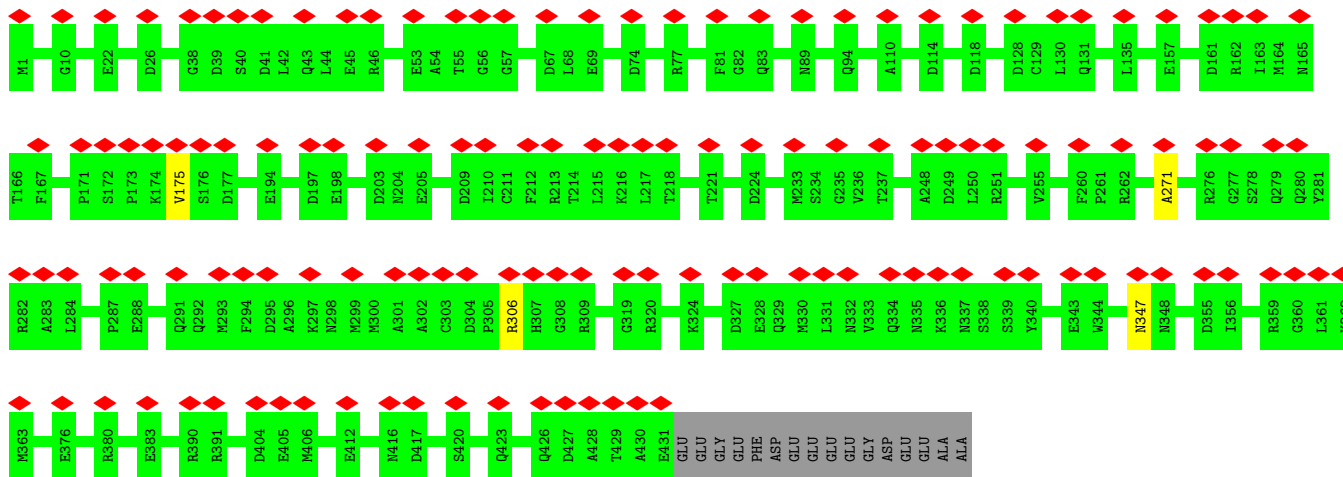




• Molecule 55: Tubulin beta chain



• Molecule 55: Tubulin beta chain



• Molecule 55: Tubulin beta chain



M1	D26	D31	P32	T33	H57	G38	D39	S40	D41	L42	Q43	L44	E45	R46	I47	M48	E53	A54	T55	G56	G57	K58	D67	L68	E69	P70	G71	T72	M73	D74	S75	V76	R77	S78	G79	P80	R86	P87	D88	Q94	A97	K103	E108	D114	D118	R121			
C127	D128	Q131	L135	T136	H137	S138	L139	G140	G141	G142	K154	I155	R156	E157	E158	D161	R162	I163	M164	F167	S168	P173	K174	V175	S176	D177	A185	Q191	E194	D197	E198	D203	N204	E205	A206	L207	Y208	D209	F212	R213	K216	L217	T218	D224					
L225	H233	T238	G244	Q245	L246	N247	A248	D249	L250	L273	R276	G277	S278	Q279	R282	A283	L284	P287	E288	Q291	Q292	M293	F294	D295	A296	K297	A301	A302	C303	D304	P305	R306	H307	G308	R320	M321	S322	M323	K324	E325	V326	D327	E328	Q329	M330	L331	N332	V333	Q334
N335	K336	N337	S338	S339	Y340	E343	W344	I345	P346	N347	D355	I356	R359	G360	L361	K362	K363	A373	I374	Q375	E376	K379	R380	I381	S382	E383	R390	R391	K392	T399	G400	E401	G402	M403	D404	E405	M406	E410	A411	E412	M415	M416	D417	Q423	Q424	Y425	Q426	D427	A428
T429	A430	E431	GLU	GLU	GLY	GLU	PHE	ASP	W344	GLU	GLU	GLU	GLU	GLY	ASP	GLU	GLU	ALA	ALA																														



## 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

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	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	0.27	0/4020	0.63	1/5438 (0.0%)
20	3K	0.31	0/559	0.74	1/752 (0.1%)
21	3N	0.40	0/2152	0.78	4/2862 (0.1%)
21	3O	0.32	0/2345	0.65	2/3121 (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	0.34	0/3240	0.72	3/4304 (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	0.29	0/3046	0.63	2/4115 (0.0%)
26	4K	0.29	0/3035	0.65	0/4100
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	2.37	7/3492 (0.2%)	0.63	5/4742 (0.1%)
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	2.37	7/3492 (0.2%)	0.64	5/4742 (0.1%)
54	FB	0.29	0/3492	0.61	2/4742 (0.0%)
54	FE	2.37	7/3492 (0.2%)	0.67	5/4742 (0.1%)
54	FG	0.31	0/3492	0.62	3/4742 (0.1%)
54	FI	2.37	8/3492 (0.2%)	0.70	7/4742 (0.1%)
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	0.38	33/1289671 (0.0%)	0.61	419/1747055 (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	EA	0	1
54	EG	0	2
54	EI	0	1
54	EK	0	1
54	FA	0	1
54	FB	0	2
54	FE	0	2
54	FI	0	3
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

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Mol	Chain	#Chirality outliers	#Planarity outliers
54	QI	0	1
54	QK	0	1
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

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	DC	0	1
55	DD	0	1
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

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	KH	0	1
55	KJ	0	2
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

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	SJ	0	1
55	SM	0	2
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	328

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	FI	358	GLN	CG-CD	80.78	3.36	1.51
54	FA	358	GLN	CG-CD	80.26	3.35	1.51
54	EA	358	GLN	CG-CD	79.66	3.34	1.51
54	FE	358	GLN	CG-CD	79.33	3.33	1.51
54	FE	244	PHE	CD2-CE2	54.52	2.48	1.39
54	EA	244	PHE	CE2-CZ	53.69	2.39	1.37
54	FA	244	PHE	CD1-CE1	53.27	2.45	1.39
54	FE	244	PHE	CD1-CE1	53.13	2.45	1.39
54	FI	244	PHE	CE1-CZ	52.37	2.36	1.37
54	FA	244	PHE	CD2-CE2	52.32	2.43	1.39
54	EA	244	PHE	CE1-CZ	52.07	2.36	1.37
54	FI	244	PHE	CD2-CE2	51.92	2.43	1.39
54	EA	244	PHE	CD2-CE2	51.14	2.41	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	FE	244	PHE	CE1-CZ	50.95	2.34	1.37
54	FA	244	PHE	CE1-CZ	50.58	2.33	1.37
54	FI	244	PHE	CE2-CZ	50.51	2.33	1.37
54	FE	244	PHE	CE2-CZ	50.47	2.33	1.37
54	FA	244	PHE	CE2-CZ	50.07	2.32	1.37
54	FI	244	PHE	CD1-CE1	50.05	2.39	1.39
54	EA	244	PHE	CD1-CE1	50.05	2.39	1.39
54	EA	244	PHE	CG-CD1	34.44	1.90	1.38
54	FA	244	PHE	CG-CD2	33.76	1.89	1.38
54	FI	244	PHE	CG-CD2	33.55	1.89	1.38
54	EA	244	PHE	CG-CD2	33.42	1.88	1.38
54	FI	244	PHE	CG-CD1	33.07	1.88	1.38
54	FE	244	PHE	CG-CD2	32.69	1.87	1.38
54	FA	244	PHE	CG-CD1	32.62	1.87	1.38
54	FE	244	PHE	CG-CD1	32.47	1.87	1.38
55	FH	171	PRO	CG-CD	-7.52	1.25	1.50
3	1v	670	CYS	CB-SG	-6.48	1.71	1.82
54	FI	358	GLN	CB-CG	6.17	1.69	1.52
3	1y	670	CYS	CB-SG	-5.45	1.73	1.81
55	TM	194	GLU	CA-CB	5.39	1.65	1.53

All (419) 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
54	FA	244	PHE	CB-CG-CD1	-8.82	114.62	120.80
55	RD	44	LEU	CA-CB-CG	8.81	135.57	115.30
3	1L	134	LEU	CA-CB-CG	8.25	134.27	115.30
54	FE	160	ASP	CB-CG-OD1	8.22	125.70	118.30
54	FA	358	GLN	CB-CG-CD	8.22	132.96	111.60
55	PC	187	LEU	CA-CB-CG	8.19	134.15	115.30
55	PF	171	PRO	C-N-CA	8.18	142.14	121.70
55	JL	177	ASP	CB-CG-OD1	8.15	125.64	118.30
54	FG	248	LEU	CA-CB-CG	8.14	134.03	115.30
55	FJ	171	PRO	C-N-CA	8.13	142.03	121.70
55	MH	171	PRO	C-N-CA	8.00	141.71	121.70
54	FE	358	GLN	CB-CG-CD	7.97	132.32	111.60
55	ED	305	PRO	CA-N-CD	-7.96	100.35	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	EA	358	GLN	CB-CG-CD	7.95	132.27	111.60
55	QC	284	LEU	CA-CB-CG	7.93	133.53	115.30
54	PG	120	ASP	CB-CG-OD2	7.89	125.40	118.30
55	VM	228	LEU	CA-CB-CG	7.86	133.38	115.30
55	TD	187	LEU	CA-CB-CG	7.86	133.38	115.30
55	SM	171	PRO	C-N-CA	7.79	141.19	121.70
21	3N	414	LEU	CA-CB-CG	7.78	133.19	115.30
55	GC	44	LEU	CA-CB-CG	7.74	133.11	115.30
3	1v	598	ASP	CB-CG-OD1	7.69	125.22	118.30
54	CB	47	ASP	CB-CG-OD2	7.68	125.21	118.30
55	JF	118	ASP	CB-CG-OD1	7.68	125.21	118.30
55	FM	42	LEU	CA-CB-CG	7.64	132.87	115.30
54	FE	244	PHE	CD1-CG-CD2	7.62	128.21	118.30
13	2A	99	LEU	CA-CB-CG	7.55	132.67	115.30
7	5H	210	ARG	C-N-CA	7.55	140.58	121.70
55	FL	217	LEU	CA-CB-CG	7.54	132.64	115.30
54	BA	227	LEU	CB-CG-CD2	7.49	123.73	111.00
54	FI	244	PHE	CB-CG-CD2	-7.46	115.58	120.80
1	1B	61	ASP	CB-CG-OD1	7.46	125.01	118.30
31	6A	93	ASP	CB-CG-OD2	7.43	124.99	118.30
54	FA	244	PHE	CD1-CG-CD2	7.43	127.95	118.30
54	FG	245	ASP	CB-CG-OD1	7.43	124.98	118.30
55	NK	128	ASP	CB-CG-OD1	7.42	124.98	118.30
55	DC	417	ASP	CB-CG-OD2	7.41	124.97	118.30
55	CH	209	ASP	CB-CG-OD1	7.38	124.95	118.30
54	KB	298	PRO	CA-N-CD	-7.37	101.19	111.50
55	OH	161	ASP	CB-CG-OD1	7.32	124.88	118.30
55	BD	203	ASP	CB-CG-OD1	7.29	124.86	118.30
54	FI	273	ALA	C-N-CD	-7.28	104.58	120.60
26	4J	215	ASP	CB-CG-OD2	7.26	124.84	118.30
54	BA	160	ASP	CB-CG-OD1	7.25	124.83	118.30
55	VC	26	ASP	CB-CG-OD2	7.21	124.79	118.30
55	QC	41	ASP	CB-CG-OD2	7.20	124.78	118.30
54	EA	244	PHE	CB-CG-CD2	-7.19	115.77	120.80
55	CJ	41	ASP	CB-CG-OD1	7.17	124.76	118.30
54	RE	116	ASP	CB-CG-OD1	7.17	124.75	118.30
55	CC	197	ASP	CB-CG-OD1	7.16	124.74	118.30
55	ID	171	PRO	C-N-CA	7.16	139.59	121.70
40	7U	105	ASP	CB-CG-OD1	7.15	124.73	118.30
55	WF	118	ASP	CB-CG-OD1	7.15	124.73	118.30
54	FE	244	PHE	CB-CG-CD2	-7.12	115.82	120.80
55	QJ	177	ASP	CB-CG-OD1	7.09	124.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	JH	44	LEU	CA-CB-CG	7.09	131.61	115.30
54	CK	39	ASP	CB-CG-OD1	7.09	124.68	118.30
55	PF	41	ASP	CB-CG-OD1	7.08	124.67	118.30
55	OM	203	ASP	CB-CG-OD1	7.08	124.67	118.30
13	2B	222	ASP	CB-CG-OD1	7.06	124.65	118.30
55	FC	225	LEU	CA-CB-CG	7.04	131.48	115.30
54	VG	46	ASP	CB-CG-OD1	7.01	124.61	118.30
55	LL	26	ASP	CB-CG-OD1	6.99	124.59	118.30
55	RM	203	ASP	CB-CG-OD1	6.96	124.56	118.30
55	AD	171	PRO	C-N-CA	6.93	139.04	121.70
55	DD	177	ASP	CB-CG-OD1	6.93	124.54	118.30
54	FE	244	PHE	CB-CG-CD1	-6.93	115.95	120.80
41	7Y	132	ASP	CB-CG-OD1	6.91	124.52	118.30
55	ED	203	ASP	CB-CG-OD1	6.90	124.51	118.30
54	HG	251	ASP	CB-CG-OD1	6.84	124.45	118.30
54	NG	127	ASP	CB-CG-OD2	6.82	124.44	118.30
54	FI	245	ASP	CB-CG-OD1	6.82	124.43	118.30
54	FI	244	PHE	CB-CG-CD1	-6.77	116.06	120.80
23	3Z	158	ASP	CB-CG-OD1	6.76	124.38	118.30
54	JE	273	ALA	C-N-CD	-6.75	105.76	120.60
55	FH	171	PRO	CA-N-CD	-6.71	102.10	111.50
54	MB	205	ASP	CB-CG-OD1	6.70	124.33	118.30
54	EE	431	ASP	CB-CG-OD2	6.70	124.33	118.30
55	UL	171	PRO	C-N-CA	6.70	138.44	121.70
55	UC	217	LEU	CA-CB-CG	6.68	130.67	115.30
55	CL	304	ASP	CB-CG-OD2	6.68	124.31	118.30
55	JD	187	LEU	CA-CB-CG	6.67	130.65	115.30
54	TK	364	PRO	CA-N-CD	-6.66	102.17	111.50
54	VK	252	LEU	CA-CB-CG	6.66	130.62	115.30
54	LG	205	ASP	CB-CG-OD1	6.65	124.28	118.30
24	4A	350	ASP	CB-CG-OD2	6.65	124.28	118.30
22	3R	166	ASP	CB-CG-OD2	6.64	124.28	118.30
2	1H	222	MET	CA-CB-CG	6.63	124.57	113.30
55	RJ	215	LEU	CA-CB-CG	6.61	130.51	115.30
54	JA	367	ASP	CB-CG-OD1	6.60	124.24	118.30
7	5F	171	ASP	CB-CG-OD2	6.60	124.24	118.30
54	WA	33	ASP	CB-CG-OD2	6.59	124.23	118.30
55	QJ	41	ASP	CB-CG-OD2	6.58	124.22	118.30
45	8R	243	ASP	CB-CG-OD2	6.57	124.21	118.30
55	NH	118	ASP	CB-CG-OD1	6.55	124.19	118.30
54	GI	397	LEU	CA-CB-CG	6.54	130.35	115.30
55	NH	177	ASP	CB-CG-OD1	6.54	124.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	SK	205	ASP	CB-CG-OD2	6.53	124.18	118.30
1	1B	257	LEU	CA-CB-CG	6.51	130.28	115.30
55	CL	44	LEU	CA-CB-CG	6.51	130.28	115.30
54	EA	244	PHE	CD1-CG-CD2	6.51	126.76	118.30
54	JA	245	ASP	CB-CG-OD1	6.50	124.16	118.30
54	HA	119	LEU	CA-CB-CG	6.44	130.12	115.30
55	CL	139	LEU	CA-CB-CG	6.43	130.09	115.30
22	3T	166	ASP	CB-CG-OD1	6.42	124.08	118.30
54	IA	205	ASP	CB-CG-OD1	6.42	124.07	118.30
54	PK	211	ASP	CB-CG-OD1	6.39	124.05	118.30
55	VM	417	ASP	CB-CG-OD2	6.38	124.05	118.30
22	3T	10	ASP	CB-CG-OD2	6.38	124.04	118.30
54	TE	322	ASP	CB-CG-OD2	6.37	124.03	118.30
5	1T	215	ASP	CB-CG-OD1	6.37	124.03	118.30
47	9A	128	LEU	CA-CB-CG	6.37	129.94	115.30
42	8A	180	LEU	CA-CB-CG	6.36	129.94	115.30
54	GA	397	LEU	CA-CB-CG	6.36	129.93	115.30
55	FL	112	LEU	CA-CB-CG	6.36	129.93	115.30
54	FI	244	PHE	CD1-CG-CD2	6.33	126.53	118.30
54	FI	358	GLN	CB-CG-CD	6.33	128.05	111.60
55	KH	417	ASP	CB-CG-OD1	6.32	123.99	118.30
55	NC	328	GLU	N-CA-CB	6.30	121.94	110.60
55	QJ	217	LEU	CA-CB-CG	6.27	129.73	115.30
28	4U	89	ASP	CB-CG-OD1	6.26	123.94	118.30
55	AJ	203	ASP	CB-CG-OD1	6.26	123.94	118.30
54	TE	218	ASP	CB-CG-OD1	6.25	123.92	118.30
54	HG	326	LYS	CB-CG-CD	-6.24	95.38	111.60
54	OE	1	MET	CB-CG-SD	-6.24	93.69	112.40
37	7H	475	PRO	CA-N-CD	-6.23	102.78	111.50
55	HL	108	GLU	CA-CB-CG	6.22	127.08	113.40
55	EH	177	ASP	CB-CG-OD1	6.21	123.89	118.30
55	JF	65	LEU	CB-CG-CD2	-6.21	100.44	111.00
3	1w	368	CYS	CA-CB-SG	-6.21	102.83	114.00
55	VD	233	MET	CA-CB-CG	6.19	123.83	113.30
23	3W	93	GLY	N-CA-C	6.18	128.56	113.10
36	7D	107	LEU	CA-CB-CG	6.18	129.52	115.30
47	9A	129	PRO	N-CD-CG	-6.18	93.93	103.20
55	AC	114	ASP	CB-CG-OD1	6.16	123.84	118.30
55	LF	112	LEU	CA-CB-CG	6.14	129.43	115.30
54	FI	358	GLN	CA-CB-CG	6.14	126.91	113.40
54	FK	205	ASP	CB-CG-OD2	6.14	123.83	118.30
54	UB	98	ASP	CB-CG-OD1	6.12	123.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	VG	424	ASP	CB-CG-OD2	6.11	123.80	118.30
54	DM	397	LEU	CA-CB-CG	6.10	129.33	115.30
55	SF	44	LEU	CA-CB-CG	6.10	129.32	115.30
54	AE	251	ASP	CB-CG-OD1	6.09	123.78	118.30
19	3C	138	ASP	CB-CG-OD2	6.09	123.78	118.30
55	CD	324	LYS	CD-CE-NZ	6.08	125.69	111.70
54	VA	396	ASP	CB-CG-OD2	6.08	123.77	118.30
5	1V	237	LEU	CA-CB-CG	6.07	129.26	115.30
45	8S	131	ASP	CB-CG-OD1	6.07	123.77	118.30
54	SA	86	LEU	CA-CB-CG	6.07	129.26	115.30
35	6U	272	ASP	CB-CG-OD2	6.07	123.76	118.30
54	RA	127	ASP	CB-CG-OD1	6.07	123.76	118.30
54	UB	265	ILE	CG1-CB-CG2	-6.07	98.05	111.40
54	EI	205	ASP	CB-CG-OD1	6.07	123.76	118.30
54	TI	245	ASP	CB-CG-OD1	6.06	123.76	118.30
55	QF	217	LEU	CA-CB-CG	6.06	129.24	115.30
55	AF	88	ASP	CB-CG-OD1	6.06	123.75	118.30
55	QF	118	ASP	CB-CG-OD2	6.06	123.75	118.30
54	UI	245	ASP	CB-CG-OD1	6.05	123.75	118.30
55	SM	404	ASP	CB-CG-OD2	6.05	123.75	118.30
55	BJ	31	ASP	CB-CG-OD1	6.04	123.74	118.30
55	GJ	203	ASP	CB-CG-OD2	6.02	123.72	118.30
55	CD	249	ASP	CB-CG-OD1	6.02	123.72	118.30
54	MK	205	ASP	CB-CG-OD1	6.02	123.72	118.30
43	8G	373	ASP	CB-CG-OD2	6.01	123.71	118.30
54	VK	98	ASP	CB-CG-OD1	6.01	123.71	118.30
55	FF	324	LYS	CD-CE-NZ	-6.01	97.89	111.70
54	SA	33	ASP	CB-CG-OD1	6.00	123.70	118.30
54	SA	413	MET	CA-CB-CG	6.00	123.51	113.30
55	SC	44	LEU	CA-CB-CG	6.00	129.09	115.30
36	7D	239	ASP	CB-CG-OD2	5.98	123.69	118.30
55	VL	44	LEU	CA-CB-CG	5.97	129.04	115.30
54	LE	205	ASP	CB-CG-OD1	5.96	123.66	118.30
54	OE	273	ALA	C-N-CD	-5.96	107.49	120.60
47	9A	114	ASP	CB-CG-OD2	5.96	123.66	118.30
55	FJ	88	ASP	CB-CG-OD1	5.95	123.66	118.30
55	NJ	295	ASP	CB-CG-OD1	5.94	123.65	118.30
39	7Q	105	ASP	CB-CG-OD2	5.94	123.64	118.30
26	4J	214	VAL	C-N-CA	5.93	136.52	121.70
55	UM	263	LEU	CA-CB-CG	5.93	128.93	115.30
19	3A	138	ASP	CB-CG-OD1	5.91	123.62	118.30
55	EL	88	ASP	CB-CG-OD2	5.91	123.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	7H	247	ASP	CB-CG-OD1	5.89	123.60	118.30
37	7I	13	ASP	CB-CG-OD2	5.89	123.60	118.30
45	8S	69	ASP	CB-CG-OD2	5.89	123.60	118.30
54	AG	218	ASP	CB-CG-OD1	5.88	123.59	118.30
55	CD	177	ASP	CB-CG-OD1	5.88	123.60	118.30
54	FA	116	ASP	CB-CG-OD1	5.88	123.59	118.30
54	EA	428	LEU	CA-CB-CG	5.88	128.81	115.30
55	SL	112	LEU	CA-CB-CG	5.87	128.81	115.30
54	PB	132	LEU	CA-CB-CG	5.87	128.79	115.30
54	DI	322	ASP	CB-CG-OD1	5.86	123.58	118.30
21	3N	414	LEU	CB-CG-CD1	5.86	120.96	111.00
55	OH	42	LEU	CA-CB-CG	5.85	128.75	115.30
54	RE	39	ASP	CB-CG-OD1	5.85	123.56	118.30
30	9Y	169	LEU	CA-CB-CG	5.84	128.74	115.30
54	DG	428	LEU	CA-CB-CG	5.84	128.74	115.30
55	DF	65	LEU	CB-CG-CD2	5.84	120.92	111.00
55	CL	404	ASP	CB-CG-OD1	5.84	123.55	118.30
55	LC	417	ASP	CB-CG-OD2	5.79	123.51	118.30
43	8D	196	ASP	CB-CG-OD1	5.79	123.51	118.30
54	CK	245	ASP	CB-CG-OD2	5.78	123.50	118.30
54	WI	397	LEU	CA-CB-CG	5.78	128.59	115.30
55	NC	177	ASP	CB-CG-OD1	5.77	123.49	118.30
55	GL	151	LEU	CA-CB-CG	5.74	128.51	115.30
54	HB	397	LEU	CA-CB-CG	5.74	128.51	115.30
54	RE	47	ASP	CB-CG-OD2	5.74	123.47	118.30
55	RD	404	ASP	CB-CG-OD1	5.74	123.46	118.30
55	TC	417	ASP	CB-CG-OD1	5.73	123.46	118.30
55	CJ	42	LEU	CA-CB-CG	5.73	128.47	115.30
55	JL	263	LEU	CA-CB-CG	5.73	128.47	115.30
55	LM	128	ASP	CB-CG-OD2	5.73	123.45	118.30
55	HM	44	LEU	CA-CB-CG	5.71	128.44	115.30
19	3D	127	ASP	CB-CG-OD2	5.71	123.44	118.30
54	FB	33	ASP	CB-CG-OD2	5.71	123.44	118.30
54	GK	189	LEU	CA-CB-CG	5.70	128.42	115.30
55	LM	249	ASP	CB-CG-OD2	5.70	123.43	118.30
55	FJ	41	ASP	CB-CG-OD1	5.70	123.43	118.30
36	7A	107	LEU	CA-CB-CG	5.70	128.40	115.30
55	VM	209	ASP	CB-CG-OD1	5.67	123.40	118.30
54	CM	317	MET	CA-CB-CG	5.66	122.92	113.30
54	EI	245	ASP	CB-CG-OD1	5.65	123.39	118.30
54	DG	66	VAL	CA-CB-CG1	5.65	119.38	110.90
55	FF	41	ASP	CB-CG-OD1	5.65	123.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	EB	217	LEU	CA-CB-CG	5.65	128.29	115.30
55	AC	161	ASP	CB-CG-OD1	5.64	123.38	118.30
55	EM	187	LEU	CA-CB-CG	5.63	128.25	115.30
54	IG	424	ASP	CB-CG-OD1	5.62	123.36	118.30
54	FB	120	ASP	CB-CG-OD2	5.62	123.35	118.30
54	FG	33	ASP	CB-CG-OD2	5.61	123.34	118.30
3	1K	45	LEU	CA-CB-CG	5.60	128.18	115.30
55	KM	304	ASP	CB-CG-OD2	5.60	123.34	118.30
54	SI	116	ASP	CB-CG-OD1	5.60	123.34	118.30
24	4A	21	ASP	CB-CG-OD2	5.59	123.33	118.30
23	3W	97	VAL	C-N-CA	5.59	135.67	121.70
55	FD	187	LEU	CA-CB-CG	5.59	128.15	115.30
54	IM	33	ASP	CB-CG-OD2	5.58	123.33	118.30
55	OC	177	ASP	CB-CG-OD2	5.58	123.32	118.30
55	JJ	171	PRO	C-N-CA	5.58	135.65	121.70
55	CH	177	ASP	CB-CG-OD1	5.58	123.32	118.30
55	CJ	377	LEU	CA-CB-CG	5.57	128.12	115.30
55	JJ	44	LEU	CA-CB-CG	5.57	128.10	115.30
55	FH	187	LEU	CA-CB-CG	5.56	128.09	115.30
55	DC	65	LEU	CA-CB-CG	5.56	128.08	115.30
55	TJ	67	ASP	CB-CG-OD2	5.56	123.30	118.30
55	KH	217	LEU	CA-CB-CG	5.56	128.08	115.30
39	7R	124	LEU	CA-CB-CG	5.55	128.07	115.30
55	LM	263	LEU	CA-CB-CG	5.55	128.06	115.30
55	BD	31	ASP	CB-CG-OD1	5.55	123.29	118.30
10	lj	25	LEU	CA-CB-CG	5.54	128.06	115.30
37	7H	57	ASP	CB-CG-OD2	5.54	123.29	118.30
55	VL	118	ASP	CB-CG-OD1	5.54	123.29	118.30
54	BE	327	ASP	CB-CG-OD1	5.54	123.28	118.30
55	EF	395	LEU	CA-CB-CG	5.54	128.04	115.30
54	TI	218	ASP	CB-CG-OD1	5.54	123.28	118.30
55	VM	249	ASP	CB-CG-OD2	5.53	123.28	118.30
22	3S	84	ASP	CB-CG-OD1	5.53	123.27	118.30
54	KG	251	ASP	CB-CG-OD2	5.53	123.27	118.30
55	PJ	112	LEU	CA-CB-CG	5.52	128.00	115.30
54	BI	86	LEU	CA-CB-CG	5.52	127.99	115.30
22	3S	76	ASP	CB-CG-OD1	5.51	123.26	118.30
54	LA	251	ASP	CB-CG-OD2	5.51	123.26	118.30
34	6Q	294	LEU	CA-CB-CG	5.51	127.97	115.30
2	1H	84	ASP	CB-CG-OD1	5.51	123.26	118.30
55	ED	44	LEU	CA-CB-CG	5.51	127.96	115.30
55	UH	151	LEU	CA-CB-CG	5.50	127.96	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	DM	431	ASP	CB-CG-OD2	5.50	123.25	118.30
55	OC	203	ASP	CB-CG-OD2	5.50	123.25	118.30
55	DH	171	PRO	C-N-CA	5.49	135.42	121.70
54	CK	428	LEU	CA-CB-CG	5.48	127.90	115.30
54	RA	341	ILE	CG1-CB-CG2	-5.48	99.35	111.40
55	OD	217	LEU	CA-CB-CG	5.47	127.88	115.30
54	SA	245	ASP	CB-CG-OD2	5.47	123.22	118.30
55	VL	177	ASP	CB-CG-OD2	5.47	123.22	118.30
5	1T	112	PRO	CA-N-CD	-5.46	103.85	111.50
55	PD	299	MET	CB-CG-SD	-5.46	96.02	112.40
24	4B	21	ASP	CB-CG-OD1	5.46	123.21	118.30
55	FJ	187	LEU	CA-CB-CG	5.45	127.83	115.30
36	7A	129	LEU	CA-CB-CG	5.45	127.83	115.30
55	NK	249	ASP	CB-CG-OD2	5.44	123.20	118.30
22	3S	67	ASP	CB-CG-OD2	5.44	123.20	118.30
36	7A	142	ASP	CB-CG-OD2	5.44	123.20	118.30
55	IH	41	ASP	CB-CG-OD1	5.44	123.20	118.30
54	RK	341	ILE	CG1-CB-CG2	-5.44	99.44	111.40
55	KD	217	LEU	CA-CB-CG	5.43	127.78	115.30
55	JM	26	ASP	CB-CG-OD2	5.42	123.18	118.30
54	SB	203	MET	CB-CG-SD	5.42	128.66	112.40
36	7C	297	ILE	CG1-CB-CG2	-5.42	99.49	111.40
54	NG	116	ASP	CB-CG-OD2	5.42	123.17	118.30
55	HD	41	ASP	CB-CG-OD2	5.41	123.17	118.30
55	QH	118	ASP	CB-CG-OD1	5.41	123.17	118.30
54	RE	33	ASP	CB-CG-OD1	5.39	123.15	118.30
54	VI	160	ASP	CB-CG-OD1	5.39	123.15	118.30
54	QL	171	ILE	CG1-CB-CG2	-5.39	99.55	111.40
55	RJ	427	ASP	CB-CG-OD2	5.39	123.15	118.30
55	EF	187	LEU	CA-CB-CG	5.38	127.68	115.30
55	RF	122	LYS	CA-CB-CG	5.38	125.23	113.40
21	3N	413	ARG	CA-CB-CG	5.38	125.23	113.40
55	VF	171	PRO	C-N-CA	5.37	135.13	121.70
54	CE	47	ASP	CB-CG-OD1	5.37	123.13	118.30
2	1G	84	ASP	CB-CG-OD1	5.36	123.12	118.30
55	IJ	171	PRO	C-N-CA	5.36	135.10	121.70
55	RF	217	LEU	CA-CB-CG	5.36	127.63	115.30
37	7I	283	PRO	CA-N-CD	-5.36	104.00	111.50
55	NC	328	GLU	CA-CB-CG	5.35	125.18	113.40
54	WE	47	ASP	CB-CG-OD1	5.35	123.12	118.30
43	8D	132	LEU	CA-CB-CG	5.35	127.61	115.30
55	DH	295	ASP	CB-CG-OD2	5.34	123.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	MD	401	GLU	CA-CB-CG	5.33	125.14	113.40
55	NK	130	LEU	CA-CB-CG	5.33	127.57	115.30
54	BK	345	ASP	CB-CG-OD1	5.33	123.09	118.30
21	3O	269	ASP	CB-CG-OD2	5.32	123.09	118.30
54	RK	70	LEU	CA-CB-CG	5.32	127.55	115.30
55	NJ	253	LEU	CA-CB-CG	5.31	127.52	115.30
54	EG	36	MET	CB-CG-SD	5.31	128.34	112.40
55	JF	284	LEU	CA-CB-CG	5.31	127.51	115.30
54	UI	251	ASP	CB-CG-OD1	5.30	123.07	118.30
22	3R	32	MET	CA-CB-CG	5.29	122.30	113.30
33	6N	427	LEU	CA-CB-CG	5.29	127.47	115.30
54	JI	211	ASP	CB-CG-OD1	5.28	123.05	118.30
9	1f	36	ARG	CA-CB-CG	5.28	125.02	113.40
55	SM	4	ILE	CG1-CB-CG2	-5.28	99.78	111.40
55	VL	112	LEU	CA-CB-CG	5.28	127.44	115.30
54	EA	127	ASP	CB-CG-OD1	5.28	123.05	118.30
55	BC	151	LEU	CA-CB-CG	5.27	127.43	115.30
55	LJ	177	ASP	CB-CG-OD1	5.27	123.05	118.30
55	UD	284	LEU	CA-CB-CG	5.27	127.43	115.30
55	WC	284	LEU	CA-CB-CG	5.27	127.42	115.30
55	EB	187	LEU	CA-CB-CG	5.26	127.40	115.30
54	RE	127	ASP	CB-CG-OD2	5.26	123.03	118.30
46	8Z	72	VAL	CG1-CB-CG2	-5.25	102.50	110.90
55	EH	26	ASP	CB-CG-OD2	5.25	123.02	118.30
55	MJ	44	LEU	CA-CB-CG	5.25	127.37	115.30
19	3B	183	LEU	CA-CB-CG	5.25	127.37	115.30
24	4C	260	MET	CA-CB-CG	5.25	122.22	113.30
18	2V	266	VAL	CG1-CB-CG2	-5.24	102.51	110.90
1	1A	23	ASP	CB-CG-OD2	5.24	123.02	118.30
54	DG	218	ASP	CB-CG-OD1	5.24	123.01	118.30
54	FK	245	ASP	CB-CG-OD1	5.24	123.01	118.30
55	UC	395	LEU	CA-CB-CG	5.23	127.34	115.30
54	UK	218	ASP	CB-CG-OD1	5.23	123.01	118.30
54	CI	209	ILE	CG1-CB-CG2	-5.23	99.89	111.40
54	KB	326	LYS	CD-CE-NZ	-5.22	99.69	111.70
54	NI	120	ASP	CB-CG-OD1	5.22	122.99	118.30
55	FL	304	ASP	CB-CG-OD2	5.21	122.99	118.30
55	JM	249	ASP	CB-CG-OD2	5.21	122.99	118.30
55	QJ	118	ASP	CB-CG-OD1	5.21	122.99	118.30
55	SJ	217	LEU	CA-CB-CG	5.21	127.27	115.30
55	UM	192	LEU	CA-CB-CG	5.20	127.26	115.30
13	2D	131	THR	C-N-CA	5.20	134.70	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	GK	218	ASP	CB-CG-OD1	5.20	122.98	118.30
54	EC	217	LEU	CA-CB-CG	5.19	127.25	115.30
55	LC	177	ASP	CB-CG-OD1	5.19	122.97	118.30
54	JI	430	LYS	CD-CE-NZ	5.19	123.63	111.70
42	8A	22	ASP	CB-CG-OD1	5.18	122.97	118.30
55	CJ	328	GLU	CA-CB-CG	5.18	124.81	113.40
18	2V	108	MET	CA-CB-CG	5.18	122.11	113.30
46	8Z	20	LEU	CA-CB-CG	5.18	127.21	115.30
55	RC	284	LEU	CA-CB-CG	5.18	127.21	115.30
24	4B	459	ILE	C-N-CA	5.16	134.60	121.70
55	MH	118	ASP	CB-CG-OD1	5.15	122.94	118.30
54	RB	76	ASP	CB-CG-OD2	5.15	122.94	118.30
27	4Q	180	LEU	CA-CB-CG	5.15	127.14	115.30
54	UG	218	ASP	CB-CG-OD1	5.15	122.93	118.30
55	MC	249	ASP	CB-CG-OD1	5.14	122.93	118.30
55	QF	209	ASP	CB-CG-OD1	5.14	122.93	118.30
54	RG	7	ILE	CG1-CB-CG2	-5.14	100.08	111.40
55	EM	299	MET	CB-CG-SD	-5.14	96.98	112.40
21	3N	397	GLU	CA-CB-CG	5.14	124.70	113.40
54	WK	46	ASP	CB-CG-OD1	5.14	122.92	118.30
55	BF	380	ARG	CB-CG-CD	5.13	124.95	111.60
54	LE	397	LEU	CA-CB-CG	5.13	127.11	115.30
55	BH	263	LEU	CA-CB-CG	5.13	127.11	115.30
55	GH	331	LEU	CA-CB-CG	5.13	127.11	115.30
55	EF	177	ASP	CB-CG-OD1	5.13	122.92	118.30
54	RB	275	VAL	CG1-CB-CG2	-5.13	102.70	110.90
36	7D	406	LEU	CA-CB-CG	5.12	127.06	115.30
25	4G	179	ASP	CB-CG-OD2	5.11	122.90	118.30
37	7I	142	LEU	CA-CB-CG	5.11	127.06	115.30
55	VJ	26	ASP	CB-CG-OD2	5.11	122.90	118.30
55	ED	377	LEU	CA-CB-CG	5.11	127.05	115.30
55	KM	225	LEU	CA-CB-CG	5.11	127.05	115.30
55	TM	263	LEU	CA-CB-CG	5.11	127.05	115.30
43	8G	359	LYS	CD-CE-NZ	-5.11	99.96	111.70
55	KC	118	ASP	CB-CG-OD1	5.10	122.89	118.30
31	6C	83	ASP	CB-CG-OD2	5.10	122.89	118.30
55	EL	284	LEU	CA-CB-CG	5.10	127.03	115.30
3	1z	413	ASP	CB-CG-OD1	5.08	122.87	118.30
54	OA	248	LEU	CA-CB-CG	5.08	126.98	115.30
54	SE	259	LEU	CA-CB-CG	5.08	126.98	115.30
36	7A	404	MET	CB-CG-SD	5.08	127.63	112.40
54	LB	23	LEU	CA-CB-CG	5.07	126.97	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	TL	225	LEU	CB-CG-CD1	-5.06	102.39	111.00
55	CF	177	ASP	CB-CG-OD1	5.06	122.85	118.30
55	SC	118	ASP	CB-CG-OD1	5.05	122.85	118.30
22	3R	33	PRO	C-N-CA	5.05	134.32	121.70
54	QA	132	LEU	CA-CB-CG	5.05	126.91	115.30
55	SF	284	LEU	CA-CB-CG	5.04	126.89	115.30
54	FA	244	PHE	CB-CG-CD2	-5.04	117.27	120.80
55	DC	197	ASP	CB-CG-OD2	5.04	122.83	118.30
55	QH	177	ASP	CB-CG-OD1	5.04	122.83	118.30
55	DJ	217	LEU	CA-CB-CG	5.03	126.88	115.30
3	1x	400	GLN	C-N-CA	5.03	134.28	121.70
7	1b	42	GLU	C-N-CA	-5.03	109.13	121.70
20	3K	51	GLU	CA-CB-CG	5.03	124.46	113.40
36	7B	578	ASP	CB-CG-OD1	5.02	122.82	118.30
55	RF	130	LEU	CB-CG-CD2	5.02	119.54	111.00
36	7A	534	ALA	C-N-CA	5.02	134.25	121.70
36	7D	407	LEU	CA-CB-CG	5.02	126.84	115.30
55	NF	377	LEU	CA-CB-CG	5.02	126.84	115.30
54	UA	218	ASP	CB-CG-OD1	5.02	122.82	118.30
23	3W	80	LEU	CA-CB-CG	5.01	126.83	115.30
55	ED	305	PRO	N-CD-CG	-5.01	95.69	103.20
21	3O	202	ASP	CB-CG-OD1	5.00	122.80	118.30
7	5G	94	PHE	C-N-CA	5.00	134.21	121.70

There are no chirality outliers.

All (328) 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
7	1b	38	ILE	Peptide
7	1b	43	MET	Peptide
12	1r	3	GLN	Peptide
3	1v	669	GLN	Peptide
3	1w	400	GLN	Peptide
3	1y	669	GLN	Peptide
3	2a	670	CYS	Peptide
19	3B	95	ASP	Peptide
20	3J	304	ALA	Peptide

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Mol	Chain	Res	Type	Group
20	3J	312	TYR	Peptide
22	3S	116	PRO	Peptide
23	3W	97	VAL	Peptide
23	3W	98	LEU	Peptide
25	4G	27	MET	Peptide
26	4J	330	GLY	Peptide
30	5B	182	SER	Peptide
7	5K	71	VAL	Peptide
7	5K	72	THR	Peptide
31	6B	100	HIS	Peptide
31	6B	99	THR	Peptide
36	7A	534	ALA	Peptide
36	7C	406	LEU	Peptide
36	7D	4	PRO	Peptide
37	7G	59	LEU	Peptide
37	7H	344	ASP	Peptide
37	7I	344	ASP	Peptide
38	7M	232	ALA	Peptide
38	7M	246	GLU	Peptide
40	7U	188	LYS	Peptide
41	7Y	201	HIS	Peptide
42	8A	109	LYS	Peptide
43	8D	252	GLU	Peptide
47	9A	105	ILE	Peptide
48	9D	157	ASN	Peptide
10	9O	154	GLU	Peptide
53	9V	80	TRP	Peptide
53	9V	81	ARG	Sidechain
30	9Z	131	GLU	Peptide
30	9Z	60	HIS	Peptide
54	AB	273	ALA	Peptide
55	AC	85	PHE	Peptide
54	AE	254	GLU	Peptide
55	AF	167	PHE	Peptide
55	AF	271	ALA	Peptide
54	AG	273	ALA	Peptide
55	AH	167	PHE	Peptide
55	AH	271	ALA	Peptide
55	AJ	271	ALA	Peptide
55	AL	137	HIS	Peptide
55	AL	271	ALA	Peptide
54	BA	254	GLU	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
55	BC	167	PHE	Peptide
55	BC	324	LYS	Peptide
55	BC	70	PRO	Peptide
54	BI	273	ALA	Peptide
54	BK	273	ALA	Peptide
54	CA	254	GLU	Peptide
54	CB	409	VAL	Peptide
55	CC	137	HIS	Peptide
55	CC	271	ALA	Peptide
55	CD	271	ALA	Peptide
54	CE	215	ARG	Sidechain
54	CE	273	ALA	Peptide
55	CF	167	PHE	Peptide
55	CH	271	ALA	Peptide
54	CI	100	ALA	Peptide
55	CJ	167	PHE	Peptide
55	CJ	271	ALA	Peptide
54	CK	273	ALA	Peptide
55	CL	271	ALA	Peptide
54	CM	273	ALA	Peptide
55	DC	271	ALA	Peptide
55	DD	167	PHE	Peptide
55	DF	137	HIS	Peptide
55	DF	70	PRO	Peptide
55	DH	137	HIS	Peptide
55	DH	167	PHE	Peptide
55	DH	271	ALA	Peptide
55	DJ	271	ALA	Peptide
55	DJ	70	PRO	Peptide
54	DK	141	PHE	Peptide
55	DL	302	ALA	Peptide
54	EA	273	ALA	Peptide
55	EB	271	ALA	Peptide
55	ED	271	ALA	Peptide
55	EF	271	ALA	Peptide
54	EG	273	ALA	Peptide
54	EG	357	TYR	Peptide
55	EH	88	ASP	Peptide
54	EI	273	ALA	Peptide
55	EJ	271	ALA	Peptide
54	EK	273	ALA	Peptide
55	EL	70	PRO	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
55	EM	271	ALA	Peptide
55	EM	70	PRO	Peptide
54	FA	412	GLY	Peptide
54	FB	273	ALA	Peptide
54	FB	357	TYR	Peptide
55	FC	271	ALA	Peptide
55	FD	271	ALA	Peptide
54	FE	273	ALA	Peptide
54	FE	337	THR	Peptide
55	FF	271	ALA	Peptide
54	FI	172	TYR	Peptide
54	FI	273	ALA	Peptide
54	FI	274	PRO	Peptide
55	FJ	271	ALA	Peptide
55	FL	271	ALA	Peptide
55	FM	167	PHE	Peptide
55	FM	70	PRO	Peptide
54	GB	303	VAL	Peptide
55	GF	271	ALA	Peptide
55	GL	271	ALA	Peptide
55	GM	271	ALA	Peptide
54	HA	159	VAL	Peptide
54	HB	273	ALA	Peptide
55	HC	302	ALA	Peptide
55	HD	137	HIS	Peptide
55	HD	236	VAL	Peptide
55	HF	167	PHE	Peptide
55	HF	271	ALA	Peptide
54	HG	273	ALA	Peptide
55	HH	167	PHE	Peptide
55	HM	195	ASN	Peptide
54	IA	243	ARG	Peptide
54	IB	273	ALA	Peptide
55	IC	271	ALA	Peptide
55	IC	70	PRO	Peptide
55	ID	271	ALA	Peptide
55	IF	302	ALA	Peptide
54	IG	160	ASP	Peptide
54	IG	273	ALA	Peptide
54	II	273	ALA	Peptide
55	IJ	167	PHE	Peptide
54	IK	273	ALA	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
54	IK	316	CYS	Peptide
55	IL	271	ALA	Peptide
54	JA	273	ALA	Peptide
54	JB	273	ALA	Peptide
55	JC	167	PHE	Peptide
55	JC	271	ALA	Peptide
55	JD	70	PRO	Peptide
54	JE	273	ALA	Peptide
55	JF	167	PHE	Peptide
55	JF	271	ALA	Peptide
54	JG	273	ALA	Peptide
55	JH	137	HIS	Peptide
55	JH	271	ALA	Peptide
55	JJ	271	ALA	Peptide
55	JL	271	ALA	Peptide
55	JM	271	ALA	Peptide
54	KB	273	ALA	Peptide
55	KC	271	ALA	Peptide
55	KD	167	PHE	Peptide
55	KD	271	ALA	Peptide
54	KE	273	ALA	Peptide
55	KF	271	ALA	Peptide
54	KG	38	SER	Peptide
55	KH	271	ALA	Peptide
54	KI	1	MET	Peptide
55	KJ	167	PHE	Peptide
55	KJ	271	ALA	Peptide
55	KL	271	ALA	Peptide
54	LA	273	ALA	Peptide
55	LD	401	GLU	Peptide
55	LF	108	GLU	Peptide
55	LF	167	PHE	Peptide
55	LF	271	ALA	Peptide
55	LJ	271	ALA	Peptide
55	LL	137	HIS	Peptide
55	LL	271	ALA	Peptide
55	LM	271	ALA	Peptide
54	MA	273	ALA	Peptide
54	MB	339	ARG	Sidechain
55	MC	107	THR	Peptide
55	MC	125	GLU	Peptide
55	MD	271	ALA	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
55	MF	107	THR	Peptide
55	MH	257	MET	Peptide
54	MI	273	ALA	Peptide
55	MJ	167	PHE	Peptide
55	MJ	271	ALA	Peptide
54	MK	273	ALA	Peptide
55	MM	167	PHE	Peptide
55	MM	271	ALA	Peptide
54	NB	273	ALA	Peptide
55	NC	271	ALA	Peptide
55	ND	271	ALA	Peptide
55	ND	70	PRO	Peptide
55	NH	137	HIS	Peptide
55	NH	216	LYS	Peptide
55	NH	271	ALA	Peptide
55	NH	70	PRO	Peptide
55	NJ	167	PHE	Peptide
55	NJ	257	MET	Peptide
55	NK	271	ALA	Peptide
55	NK	302	ALA	Peptide
55	NM	271	ALA	Peptide
55	NM	393	ALA	Peptide
55	NM	70	PRO	Peptide
55	OC	167	PHE	Peptide
55	OC	70	PRO	Peptide
54	OE	110	ILE	Peptide
54	OE	273	ALA	Peptide
55	OF	167	PHE	Peptide
55	OF	271	ALA	Peptide
55	OH	167	PHE	Peptide
55	OH	271	ALA	Peptide
55	OJ	167	PHE	Peptide
55	OJ	70	PRO	Peptide
54	OK	273	ALA	Peptide
55	OM	271	ALA	Peptide
54	PA	160	ASP	Peptide
55	PC	167	PHE	Peptide
55	PC	271	ALA	Peptide
55	PC	302	ALA	Peptide
55	PD	167	PHE	Peptide
55	PF	167	PHE	Peptide
55	PH	167	PHE	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
55	PH	70	PRO	Peptide
54	PI	316	CYS	Peptide
55	PJ	167	PHE	Peptide
54	QB	202	PHE	Peptide
54	QB	273	ALA	Peptide
55	QC	167	PHE	Peptide
55	QC	187	LEU	Peptide
55	QD	167	PHE	Peptide
55	QD	271	ALA	Peptide
54	QE	273	ALA	Peptide
54	QE	403	ALA	Peptide
55	QF	271	ALA	Peptide
55	QF	58	LYS	Peptide
55	QH	167	PHE	Peptide
54	QI	273	ALA	Peptide
55	QJ	167	PHE	Peptide
55	QJ	271	ALA	Peptide
54	QK	216	ASN	Peptide
55	QM	167	PHE	Peptide
55	QM	271	ALA	Peptide
55	QM	401	GLU	Peptide
54	RA	273	ALA	Peptide
54	RB	141	PHE	Peptide
54	RB	273	ALA	Peptide
55	RC	271	ALA	Peptide
54	RE	273	ALA	Peptide
55	RF	167	PHE	Peptide
55	RF	324	LYS	Peptide
55	RF	401	GLU	Peptide
54	RG	273	ALA	Peptide
55	RH	320	ARG	Peptide
54	RI	273	ALA	Peptide
55	RJ	137	HIS	Peptide
55	RJ	271	ALA	Peptide
54	RK	273	ALA	Peptide
54	RL	273	ALA	Peptide
54	RL	72	PRO	Peptide
54	SB	42	ILE	Peptide
55	SD	167	PHE	Peptide
55	SD	255	VAL	Peptide
55	SD	271	ALA	Peptide
55	SD	323	MET	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
54	SE	411	GLU	Peptide
55	SF	167	PHE	Peptide
54	SG	141	PHE	Peptide
54	SG	273	ALA	Peptide
54	SI	273	ALA	Peptide
55	SJ	44	LEU	Peptide
55	SM	167	PHE	Peptide
55	SM	271	ALA	Peptide
54	TA	31	GLN	Peptide
54	TB	273	ALA	Peptide
54	TB	285	GLN	Peptide
55	TD	212	PHE	Peptide
55	TD	302	ALA	Peptide
54	TG	160	ASP	Peptide
55	TH	70	PRO	Peptide
54	TI	273	ALA	Peptide
55	TJ	216	LYS	Peptide
54	TK	273	ALA	Peptide
54	TK	274	PRO	Peptide
54	UB	273	ALA	Peptide
55	UC	167	PHE	Peptide
55	UC	271	ALA	Peptide
55	UD	271	ALA	Peptide
55	UF	271	ALA	Peptide
54	UG	303	VAL	Peptide
55	UH	234	SER	Peptide
55	UH	271	ALA	Peptide
55	UH	70	PRO	Peptide
54	UI	273	ALA	Peptide
55	UJ	278	SER	Peptide
55	UJ	70	PRO	Peptide
54	UK	221	ARG	Sidechain
55	UL	302	ALA	Peptide
55	UM	271	ALA	Peptide
55	UM	322	SER	Peptide
54	VB	254	GLU	Peptide
55	VC	302	ALA	Peptide
54	VE	273	ALA	Peptide
55	VF	271	ALA	Peptide
54	VG	273	ALA	Peptide
55	VH	193	VAL	Peptide
55	VH	204	ASN	Peptide

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Mol	Chain	Res	Type	Group
55	VH	271	ALA	Peptide
55	VJ	167	PHE	Peptide
55	VJ	70	PRO	Peptide
55	VL	271	ALA	Peptide
55	VM	271	ALA	Peptide
54	WA	273	ALA	Peptide
54	WB	273	ALA	Peptide
55	WC	137	HIS	Peptide
55	WD	137	HIS	Peptide
55	WD	271	ALA	Peptide
54	WE	273	ALA	Peptide
55	WF	137	HIS	Peptide
55	WF	167	PHE	Peptide
55	WF	271	ALA	Peptide
55	WF	355	ASP	Peptide
55	WH	167	PHE	Peptide
54	WI	273	ALA	Peptide
55	WJ	271	ALA	Peptide
54	WK	273	ALA	Peptide
55	WL	137	HIS	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%)	<b>2</b> <b>14</b>
1	1B	265/309 (86%)	219 (83%)	42 (16%)	4 (2%)	<b>10</b> <b>38</b>
2	1E	415/448 (93%)	390 (94%)	22 (5%)	3 (1%)	<b>22</b> <b>54</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1F	164/448 (37%)	149 (91%)	14 (8%)	1 (1%)	25	57
2	1G	290/448 (65%)	279 (96%)	10 (3%)	1 (0%)	41	71
2	1H	416/448 (93%)	379 (91%)	33 (8%)	4 (1%)	15	46
3	1K	173/696 (25%)	154 (89%)	16 (9%)	3 (2%)	9	35
3	1L	173/696 (25%)	156 (90%)	15 (9%)	2 (1%)	13	42
3	1M	173/696 (25%)	160 (92%)	12 (7%)	1 (1%)	25	57
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%)	9	36
3	1y	194/696 (28%)	181 (93%)	13 (7%)	0	100	100
3	1z	85/696 (12%)	83 (98%)	2 (2%)	0	100	100
3	2a	52/696 (8%)	45 (86%)	6 (12%)	1 (2%)	8	34
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%)	17	48
5	1U	107/429 (25%)	97 (91%)	10 (9%)	0	100	100
5	1V	221/429 (52%)	190 (86%)	28 (13%)	3 (1%)	11	38
5	1W	103/429 (24%)	91 (88%)	10 (10%)	2 (2%)	8	34
6	1Y	115/139 (83%)	98 (85%)	17 (15%)	0	100	100
7	1a	132/251 (53%)	106 (80%)	23 (17%)	3 (2%)	6	29
7	1b	120/251 (48%)	95 (79%)	22 (18%)	3 (2%)	5	27
7	5E	152/251 (61%)	115 (76%)	35 (23%)	2 (1%)	12	40
7	5F	110/251 (44%)	89 (81%)	19 (17%)	2 (2%)	8	35
7	5G	140/251 (56%)	109 (78%)	29 (21%)	2 (1%)	11	38
7	5H	115/251 (46%)	90 (78%)	21 (18%)	4 (4%)	3	21
7	5I	25/251 (10%)	20 (80%)	4 (16%)	1 (4%)	3	18
7	5J	231/251 (92%)	189 (82%)	37 (16%)	5 (2%)	6	30
7	5K	132/251 (53%)	99 (75%)	30 (23%)	3 (2%)	6	29
7	5L	123/251 (49%)	99 (80%)	21 (17%)	3 (2%)	6	28
7	5M	12/251 (5%)	11 (92%)	0	1 (8%)	1	5
7	5N	242/251 (96%)	194 (80%)	44 (18%)	4 (2%)	9	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	4	23
10	1j	29/188 (15%)	24 (83%)	4 (14%)	1 (3%)	3	22
10	9M	82/188 (44%)	67 (82%)	15 (18%)	0	100	100
10	9N	82/188 (44%)	71 (87%)	10 (12%)	1 (1%)	13	42
10	9O	39/188 (21%)	25 (64%)	11 (28%)	3 (8%)	1	6
11	1l	37/176 (21%)	25 (68%)	12 (32%)	0	100	100
11	1m	37/176 (21%)	26 (70%)	11 (30%)	0	100	100
12	1o	27/142 (19%)	24 (89%)	1 (4%)	2 (7%)	1	7
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%)	13	42
13	2B	249/258 (96%)	212 (85%)	30 (12%)	7 (3%)	5	25
13	2C	249/258 (96%)	209 (84%)	35 (14%)	5 (2%)	7	32
13	2D	77/258 (30%)	67 (87%)	8 (10%)	2 (3%)	5	27
14	2G	225/235 (96%)	187 (83%)	36 (16%)	2 (1%)	17	48
15	2J	105/141 (74%)	91 (87%)	14 (13%)	0	100	100
15	2K	105/141 (74%)	93 (89%)	10 (10%)	2 (2%)	8	34
15	2L	105/141 (74%)	95 (90%)	8 (8%)	2 (2%)	8	34
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%)	41	71
18	2V	282/292 (97%)	239 (85%)	38 (14%)	5 (2%)	8	35
18	2W	282/292 (97%)	243 (86%)	35 (12%)	4 (1%)	11	38
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	3D	170/195 (87%)	151 (89%)	18 (11%)	1 (1%)	25	57
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%)	406 (83%)	72 (15%)	13 (3%)	5	27
20	3K	68/592 (12%)	52 (76%)	14 (21%)	2 (3%)	4	24
21	3N	256/560 (46%)	246 (96%)	8 (3%)	2 (1%)	19	51
21	3O	276/560 (49%)	265 (96%)	9 (3%)	2 (1%)	22	54
22	3R	163/172 (95%)	130 (80%)	31 (19%)	2 (1%)	13	42
22	3S	125/172 (73%)	105 (84%)	19 (15%)	1 (1%)	19	51
22	3T	163/172 (95%)	137 (84%)	24 (15%)	2 (1%)	13	42
23	3W	382/541 (71%)	357 (94%)	22 (6%)	3 (1%)	19	51
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%)	25	57
24	4A	615/635 (97%)	549 (89%)	65 (11%)	1 (0%)	47	77
24	4B	613/635 (96%)	564 (92%)	49 (8%)	0	100	100
24	4C	615/635 (97%)	551 (90%)	63 (10%)	1 (0%)	47	77
25	4F	311/516 (60%)	301 (97%)	10 (3%)	0	100	100
25	4G	204/516 (40%)	188 (92%)	12 (6%)	4 (2%)	7	32
26	4J	376/380 (99%)	323 (86%)	49 (13%)	4 (1%)	14	45
26	4K	374/380 (98%)	314 (84%)	55 (15%)	5 (1%)	12	40
27	4N	147/243 (60%)	130 (88%)	13 (9%)	4 (3%)	5	26
27	4O	104/243 (43%)	93 (89%)	9 (9%)	2 (2%)	8	34
27	4P	146/243 (60%)	131 (90%)	14 (10%)	1 (1%)	22	54
27	4Q	91/243 (37%)	74 (81%)	16 (18%)	1 (1%)	14	45
28	4T	141/231 (61%)	126 (89%)	11 (8%)	4 (3%)	5	25
28	4U	141/231 (61%)	128 (91%)	12 (8%)	1 (1%)	22	54
28	4V	12/231 (5%)	12 (100%)	0	0	100	100
29	4Y	298/302 (99%)	272 (91%)	23 (8%)	3 (1%)	15	46
30	5A	33/277 (12%)	28 (85%)	4 (12%)	1 (3%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	5B	209/277 (76%)	170 (81%)	34 (16%)	5 (2%)	6	28
30	9Y	136/277 (49%)	102 (75%)	28 (21%)	6 (4%)	2	16
30	9Z	97/277 (35%)	65 (67%)	29 (30%)	3 (3%)	4	23
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
33	6M	389/469 (83%)	370 (95%)	18 (5%)	1 (0%)	41	71
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%)	22	54
35	6W	241/379 (64%)	229 (95%)	9 (4%)	3 (1%)	13	42
35	6X	119/379 (31%)	111 (93%)	7 (6%)	1 (1%)	19	51
36	7A	721/744 (97%)	612 (85%)	96 (13%)	13 (2%)	8	35
36	7B	445/744 (60%)	372 (84%)	68 (15%)	5 (1%)	14	45
36	7C	533/744 (72%)	441 (83%)	81 (15%)	11 (2%)	7	31
36	7D	720/744 (97%)	621 (86%)	87 (12%)	12 (2%)	9	35
37	7G	525/645 (81%)	437 (83%)	77 (15%)	11 (2%)	7	31
37	7H	525/645 (81%)	432 (82%)	80 (15%)	13 (2%)	5	27
37	7I	610/645 (95%)	519 (85%)	79 (13%)	12 (2%)	7	32
38	7M	261/322 (81%)	239 (92%)	21 (8%)	1 (0%)	34	66
38	7N	66/322 (20%)	64 (97%)	2 (3%)	0	100	100
39	7Q	141/185 (76%)	118 (84%)	21 (15%)	2 (1%)	11	38
39	7R	138/185 (75%)	122 (88%)	16 (12%)	0	100	100
40	7U	91/200 (46%)	61 (67%)	25 (28%)	5 (6%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	7V	51/200 (26%)	44 (86%)	6 (12%)	1 (2%)	7	32
41	7Y	198/204 (97%)	162 (82%)	31 (16%)	5 (2%)	5	27
41	7Z	62/204 (30%)	40 (64%)	20 (32%)	2 (3%)	4	22
42	8A	241/268 (90%)	203 (84%)	35 (14%)	3 (1%)	13	42
43	8D	395/462 (86%)	383 (97%)	11 (3%)	1 (0%)	41	71
43	8E	174/462 (38%)	170 (98%)	3 (2%)	1 (1%)	25	57
43	8F	261/462 (56%)	252 (97%)	9 (3%)	0	100	100
43	8G	395/462 (86%)	379 (96%)	15 (4%)	1 (0%)	41	71
44	8J	401/430 (93%)	380 (95%)	19 (5%)	2 (0%)	29	61
44	8K	318/430 (74%)	307 (96%)	10 (3%)	1 (0%)	41	71
44	8L	401/430 (93%)	383 (96%)	16 (4%)	2 (0%)	29	61
44	8M	124/430 (29%)	112 (90%)	11 (9%)	1 (1%)	19	51
44	8N	15/430 (4%)	12 (80%)	2 (13%)	1 (7%)	1	8
45	8Q	19/402 (5%)	19 (100%)	0	0	100	100
45	8R	398/402 (99%)	386 (97%)	10 (2%)	2 (0%)	29	61
45	8S	300/402 (75%)	290 (97%)	8 (3%)	2 (1%)	22	54
45	8T	398/402 (99%)	384 (96%)	13 (3%)	1 (0%)	41	71
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%)	7	32
46	8Z	102/119 (86%)	85 (83%)	15 (15%)	2 (2%)	7	32
47	9A	205/220 (93%)	163 (80%)	37 (18%)	5 (2%)	6	28
48	9D	94/171 (55%)	79 (84%)	15 (16%)	0	100	100
49	9G	148/150 (99%)	133 (90%)	12 (8%)	3 (2%)	7	32
50	9J	99/179 (55%)	95 (96%)	3 (3%)	1 (1%)	15	46
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%)	29	61
54	AB	435/451 (96%)	406 (93%)	29 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	AE	435/451 (96%)	402 (92%)	33 (8%)	0	100	100
54	AG	435/451 (96%)	399 (92%)	35 (8%)	1 (0%)	47	77
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%)	47	77
54	BB	435/451 (96%)	409 (94%)	24 (6%)	2 (0%)	29	61
54	BE	435/451 (96%)	406 (93%)	29 (7%)	0	100	100
54	BG	435/451 (96%)	409 (94%)	25 (6%)	1 (0%)	47	77
54	BI	435/451 (96%)	407 (94%)	28 (6%)	0	100	100
54	BK	435/451 (96%)	401 (92%)	33 (8%)	1 (0%)	47	77
54	BM	435/451 (96%)	403 (93%)	31 (7%)	1 (0%)	47	77
54	CA	435/451 (96%)	402 (92%)	32 (7%)	1 (0%)	47	77
54	CB	435/451 (96%)	397 (91%)	37 (8%)	1 (0%)	47	77
54	CE	435/451 (96%)	401 (92%)	32 (7%)	2 (0%)	29	61
54	CG	435/451 (96%)	409 (94%)	25 (6%)	1 (0%)	47	77
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%)	29	61
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%)	47	77
54	DG	435/451 (96%)	385 (88%)	48 (11%)	2 (0%)	29	61
54	DI	435/451 (96%)	395 (91%)	39 (9%)	1 (0%)	47	77
54	DK	435/451 (96%)	395 (91%)	39 (9%)	1 (0%)	47	77
54	DM	435/451 (96%)	398 (92%)	36 (8%)	1 (0%)	47	77
54	EA	435/451 (96%)	406 (93%)	29 (7%)	0	100	100
54	EC	435/451 (96%)	411 (94%)	23 (5%)	1 (0%)	47	77
54	EE	435/451 (96%)	402 (92%)	32 (7%)	1 (0%)	47	77
54	EG	435/451 (96%)	408 (94%)	27 (6%)	0	100	100
54	EI	435/451 (96%)	398 (92%)	35 (8%)	2 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	EK	435/451 (96%)	404 (93%)	31 (7%)	0	100	100
54	FA	435/451 (96%)	404 (93%)	30 (7%)	1 (0%)	47	77
54	FB	435/451 (96%)	409 (94%)	25 (6%)	1 (0%)	47	77
54	FE	435/451 (96%)	387 (89%)	46 (11%)	2 (0%)	29	61
54	FG	435/451 (96%)	397 (91%)	37 (8%)	1 (0%)	47	77
54	FI	435/451 (96%)	394 (91%)	39 (9%)	2 (0%)	29	61
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%)	47	77
54	GE	435/451 (96%)	411 (94%)	23 (5%)	1 (0%)	47	77
54	GG	435/451 (96%)	408 (94%)	26 (6%)	1 (0%)	47	77
54	GI	435/451 (96%)	396 (91%)	39 (9%)	0	100	100
54	GK	435/451 (96%)	388 (89%)	45 (10%)	2 (0%)	29	61
54	HA	435/451 (96%)	402 (92%)	31 (7%)	2 (0%)	29	61
54	HB	435/451 (96%)	399 (92%)	36 (8%)	0	100	100
54	HE	428/451 (95%)	395 (92%)	31 (7%)	2 (0%)	29	61
54	HG	431/451 (96%)	400 (93%)	29 (7%)	2 (0%)	29	61
54	HI	435/451 (96%)	401 (92%)	33 (8%)	1 (0%)	47	77
54	HK	431/451 (96%)	404 (94%)	26 (6%)	1 (0%)	47	77
54	IA	435/451 (96%)	399 (92%)	35 (8%)	1 (0%)	47	77
54	IB	430/451 (95%)	400 (93%)	28 (6%)	2 (0%)	29	61
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%)	29	61
54	IM	435/451 (96%)	392 (90%)	43 (10%)	0	100	100
54	JA	428/451 (95%)	397 (93%)	30 (7%)	1 (0%)	47	77
54	JB	435/451 (96%)	406 (93%)	28 (6%)	1 (0%)	47	77
54	JE	435/451 (96%)	410 (94%)	24 (6%)	1 (0%)	47	77
54	JG	435/451 (96%)	404 (93%)	31 (7%)	0	100	100
54	JI	435/451 (96%)	401 (92%)	33 (8%)	1 (0%)	47	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	JK	435/451 (96%)	409 (94%)	25 (6%)	1 (0%)	47	77
54	KA	435/451 (96%)	416 (96%)	18 (4%)	1 (0%)	47	77
54	KB	430/451 (95%)	401 (93%)	29 (7%)	0	100	100
54	KE	435/451 (96%)	405 (93%)	29 (7%)	1 (0%)	47	77
54	KG	435/451 (96%)	404 (93%)	29 (7%)	2 (0%)	29	61
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%)	47	77
54	LE	435/451 (96%)	414 (95%)	20 (5%)	1 (0%)	47	77
54	LG	435/451 (96%)	408 (94%)	25 (6%)	2 (0%)	29	61
54	LI	435/451 (96%)	414 (95%)	21 (5%)	0	100	100
54	LK	435/451 (96%)	416 (96%)	18 (4%)	1 (0%)	47	77
54	MA	435/451 (96%)	403 (93%)	30 (7%)	2 (0%)	29	61
54	MB	435/451 (96%)	412 (95%)	22 (5%)	1 (0%)	47	77
54	ME	435/451 (96%)	409 (94%)	25 (6%)	1 (0%)	47	77
54	MG	435/451 (96%)	412 (95%)	23 (5%)	0	100	100
54	MI	435/451 (96%)	401 (92%)	32 (7%)	2 (0%)	29	61
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%)	29	61
54	NB	435/451 (96%)	387 (89%)	44 (10%)	4 (1%)	17	48
54	NE	435/451 (96%)	402 (92%)	32 (7%)	1 (0%)	47	77
54	NG	435/451 (96%)	401 (92%)	32 (7%)	2 (0%)	29	61
54	NI	430/451 (95%)	395 (92%)	34 (8%)	1 (0%)	47	77
54	NL	429/451 (95%)	389 (91%)	39 (9%)	1 (0%)	47	77
54	OA	435/451 (96%)	396 (91%)	38 (9%)	1 (0%)	47	77
54	OB	430/451 (95%)	405 (94%)	23 (5%)	2 (0%)	29	61
54	OE	435/451 (96%)	401 (92%)	32 (7%)	2 (0%)	29	61
54	OG	435/451 (96%)	404 (93%)	31 (7%)	0	100	100
54	OI	435/451 (96%)	405 (93%)	28 (6%)	2 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	OK	435/451 (96%)	402 (92%)	32 (7%)	1 (0%)	47	77
54	OL	435/451 (96%)	393 (90%)	42 (10%)	0	100	100
54	PA	435/451 (96%)	403 (93%)	31 (7%)	1 (0%)	47	77
54	PB	435/451 (96%)	399 (92%)	35 (8%)	1 (0%)	47	77
54	PE	435/451 (96%)	400 (92%)	33 (8%)	2 (0%)	29	61
54	PG	435/451 (96%)	402 (92%)	33 (8%)	0	100	100
54	PI	435/451 (96%)	398 (92%)	36 (8%)	1 (0%)	47	77
54	PK	435/451 (96%)	392 (90%)	40 (9%)	3 (1%)	22	54
54	PL	435/451 (96%)	403 (93%)	32 (7%)	0	100	100
54	QA	435/451 (96%)	407 (94%)	25 (6%)	3 (1%)	22	54
54	QB	435/451 (96%)	392 (90%)	43 (10%)	0	100	100
54	QE	435/451 (96%)	390 (90%)	44 (10%)	1 (0%)	47	77
54	QG	435/451 (96%)	388 (89%)	45 (10%)	2 (0%)	29	61
54	QI	435/451 (96%)	398 (92%)	35 (8%)	2 (0%)	29	61
54	QK	429/451 (95%)	404 (94%)	24 (6%)	1 (0%)	47	77
54	QL	432/451 (96%)	389 (90%)	42 (10%)	1 (0%)	47	77
54	RA	435/451 (96%)	414 (95%)	18 (4%)	3 (1%)	22	54
54	RB	435/451 (96%)	391 (90%)	42 (10%)	2 (0%)	29	61
54	RE	435/451 (96%)	392 (90%)	41 (9%)	2 (0%)	29	61
54	RG	435/451 (96%)	395 (91%)	38 (9%)	2 (0%)	29	61
54	RI	435/451 (96%)	400 (92%)	35 (8%)	0	100	100
54	RK	435/451 (96%)	404 (93%)	30 (7%)	1 (0%)	47	77
54	RL	435/451 (96%)	399 (92%)	35 (8%)	1 (0%)	47	77
54	SA	435/451 (96%)	398 (92%)	37 (8%)	0	100	100
54	SB	435/451 (96%)	411 (94%)	23 (5%)	1 (0%)	47	77
54	SE	435/451 (96%)	402 (92%)	33 (8%)	0	100	100
54	SG	435/451 (96%)	409 (94%)	23 (5%)	3 (1%)	22	54
54	SI	435/451 (96%)	408 (94%)	26 (6%)	1 (0%)	47	77
54	SK	435/451 (96%)	399 (92%)	35 (8%)	1 (0%)	47	77
54	TA	432/451 (96%)	404 (94%)	28 (6%)	0	100	100
54	TB	432/451 (96%)	410 (95%)	21 (5%)	1 (0%)	47	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	TE	435/451 (96%)	406 (93%)	29 (7%)	0	100	100
54	TG	435/451 (96%)	402 (92%)	31 (7%)	2 (0%)	29	61
54	TI	435/451 (96%)	404 (93%)	31 (7%)	0	100	100
54	TK	435/451 (96%)	399 (92%)	34 (8%)	2 (0%)	29	61
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%)	47	77
54	UK	435/451 (96%)	394 (91%)	41 (9%)	0	100	100
54	VA	435/451 (96%)	399 (92%)	33 (8%)	3 (1%)	22	54
54	VB	435/451 (96%)	401 (92%)	34 (8%)	0	100	100
54	VE	435/451 (96%)	407 (94%)	26 (6%)	2 (0%)	29	61
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%)	47	77
54	WA	435/451 (96%)	408 (94%)	26 (6%)	1 (0%)	47	77
54	WB	432/451 (96%)	397 (92%)	33 (8%)	2 (0%)	29	61
54	WE	435/451 (96%)	394 (91%)	40 (9%)	1 (0%)	47	77
54	WG	435/451 (96%)	400 (92%)	33 (8%)	2 (0%)	29	61
54	WI	435/451 (96%)	389 (89%)	45 (10%)	1 (0%)	47	77
54	WK	435/451 (96%)	392 (90%)	39 (9%)	4 (1%)	17	48
55	AC	429/447 (96%)	396 (92%)	30 (7%)	3 (1%)	22	54
55	AD	429/447 (96%)	398 (93%)	29 (7%)	2 (0%)	29	61
55	AF	429/447 (96%)	396 (92%)	30 (7%)	3 (1%)	22	54
55	AH	429/447 (96%)	391 (91%)	32 (8%)	6 (1%)	11	38
55	AJ	429/447 (96%)	395 (92%)	31 (7%)	3 (1%)	22	54
55	AL	429/447 (96%)	398 (93%)	30 (7%)	1 (0%)	47	77
55	BC	429/447 (96%)	394 (92%)	32 (8%)	3 (1%)	22	54
55	BD	429/447 (96%)	385 (90%)	42 (10%)	2 (0%)	29	61
55	BF	429/447 (96%)	388 (90%)	38 (9%)	3 (1%)	22	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	BH	429/447 (96%)	393 (92%)	34 (8%)	2 (0%)	29	61
55	BJ	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	29	61
55	BL	429/447 (96%)	392 (91%)	33 (8%)	4 (1%)	17	48
55	CC	429/447 (96%)	371 (86%)	54 (13%)	4 (1%)	17	48
55	CD	429/447 (96%)	385 (90%)	40 (9%)	4 (1%)	17	48
55	CF	429/447 (96%)	390 (91%)	38 (9%)	1 (0%)	47	77
55	CH	429/447 (96%)	390 (91%)	37 (9%)	2 (0%)	29	61
55	CJ	429/447 (96%)	382 (89%)	45 (10%)	2 (0%)	29	61
55	CL	429/447 (96%)	386 (90%)	41 (10%)	2 (0%)	29	61
55	DC	429/447 (96%)	391 (91%)	35 (8%)	3 (1%)	22	54
55	DD	429/447 (96%)	386 (90%)	40 (9%)	3 (1%)	22	54
55	DF	429/447 (96%)	380 (89%)	44 (10%)	5 (1%)	13	42
55	DH	429/447 (96%)	393 (92%)	35 (8%)	1 (0%)	47	77
55	DJ	429/447 (96%)	389 (91%)	36 (8%)	4 (1%)	17	48
55	DL	429/447 (96%)	389 (91%)	36 (8%)	4 (1%)	17	48
55	EB	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	29	61
55	ED	429/447 (96%)	383 (89%)	42 (10%)	4 (1%)	17	48
55	EF	429/447 (96%)	394 (92%)	34 (8%)	1 (0%)	47	77
55	EH	429/447 (96%)	387 (90%)	36 (8%)	6 (1%)	11	38
55	EJ	429/447 (96%)	389 (91%)	39 (9%)	1 (0%)	47	77
55	EL	429/447 (96%)	389 (91%)	38 (9%)	2 (0%)	29	61
55	EM	429/447 (96%)	385 (90%)	40 (9%)	4 (1%)	17	48
55	FC	429/447 (96%)	386 (90%)	42 (10%)	1 (0%)	47	77
55	FD	429/447 (96%)	394 (92%)	32 (8%)	3 (1%)	22	54
55	FF	429/447 (96%)	403 (94%)	26 (6%)	0	100	100
55	FH	429/447 (96%)	384 (90%)	44 (10%)	1 (0%)	47	77
55	FJ	429/447 (96%)	390 (91%)	35 (8%)	4 (1%)	17	48
55	FL	429/447 (96%)	384 (90%)	40 (9%)	5 (1%)	13	42
55	FM	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	29	61
55	GC	429/447 (96%)	382 (89%)	44 (10%)	3 (1%)	22	54
55	GD	429/447 (96%)	376 (88%)	50 (12%)	3 (1%)	22	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	GF	429/447 (96%)	386 (90%)	39 (9%)	4 (1%)	17	48
55	GH	429/447 (96%)	391 (91%)	34 (8%)	4 (1%)	17	48
55	GJ	429/447 (96%)	393 (92%)	33 (8%)	3 (1%)	22	54
55	GL	429/447 (96%)	390 (91%)	37 (9%)	2 (0%)	29	61
55	GM	429/447 (96%)	399 (93%)	29 (7%)	1 (0%)	47	77
55	HC	429/447 (96%)	398 (93%)	28 (6%)	3 (1%)	22	54
55	HD	429/447 (96%)	382 (89%)	45 (10%)	2 (0%)	29	61
55	HF	429/447 (96%)	395 (92%)	32 (8%)	2 (0%)	29	61
55	HH	429/447 (96%)	393 (92%)	32 (8%)	4 (1%)	17	48
55	HJ	429/447 (96%)	398 (93%)	27 (6%)	4 (1%)	17	48
55	HL	429/447 (96%)	384 (90%)	40 (9%)	5 (1%)	13	42
55	HM	429/447 (96%)	393 (92%)	33 (8%)	3 (1%)	22	54
55	IC	429/447 (96%)	385 (90%)	42 (10%)	2 (0%)	29	61
55	ID	429/447 (96%)	390 (91%)	36 (8%)	3 (1%)	22	54
55	IF	429/447 (96%)	393 (92%)	34 (8%)	2 (0%)	29	61
55	IH	429/447 (96%)	396 (92%)	30 (7%)	3 (1%)	22	54
55	IJ	429/447 (96%)	386 (90%)	40 (9%)	3 (1%)	22	54
55	IL	429/447 (96%)	385 (90%)	39 (9%)	5 (1%)	13	42
55	JC	429/447 (96%)	407 (95%)	20 (5%)	2 (0%)	29	61
55	JD	429/447 (96%)	391 (91%)	36 (8%)	2 (0%)	29	61
55	JF	429/447 (96%)	385 (90%)	40 (9%)	4 (1%)	17	48
55	JH	429/447 (96%)	379 (88%)	45 (10%)	5 (1%)	13	42
55	JJ	429/447 (96%)	393 (92%)	32 (8%)	4 (1%)	17	48
55	JL	429/447 (96%)	382 (89%)	45 (10%)	2 (0%)	29	61
55	JM	429/447 (96%)	400 (93%)	27 (6%)	2 (0%)	29	61
55	KC	429/447 (96%)	389 (91%)	36 (8%)	4 (1%)	17	48
55	KD	429/447 (96%)	388 (90%)	38 (9%)	3 (1%)	22	54
55	KF	429/447 (96%)	399 (93%)	27 (6%)	3 (1%)	22	54
55	KH	429/447 (96%)	398 (93%)	28 (6%)	3 (1%)	22	54
55	KJ	429/447 (96%)	390 (91%)	37 (9%)	2 (0%)	29	61
55	KL	429/447 (96%)	386 (90%)	42 (10%)	1 (0%)	47	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	KM	429/447 (96%)	409 (95%)	19 (4%)	1 (0%)	47	77
55	LC	429/447 (96%)	396 (92%)	30 (7%)	3 (1%)	22	54
55	LD	429/447 (96%)	397 (92%)	30 (7%)	2 (0%)	29	61
55	LF	429/447 (96%)	395 (92%)	32 (8%)	2 (0%)	29	61
55	LH	429/447 (96%)	388 (90%)	37 (9%)	4 (1%)	17	48
55	LJ	429/447 (96%)	397 (92%)	30 (7%)	2 (0%)	29	61
55	LL	429/447 (96%)	392 (91%)	34 (8%)	3 (1%)	22	54
55	LM	429/447 (96%)	397 (92%)	31 (7%)	1 (0%)	47	77
55	MC	429/447 (96%)	392 (91%)	35 (8%)	2 (0%)	29	61
55	MD	429/447 (96%)	402 (94%)	23 (5%)	4 (1%)	17	48
55	MF	429/447 (96%)	407 (95%)	21 (5%)	1 (0%)	47	77
55	MH	429/447 (96%)	385 (90%)	40 (9%)	4 (1%)	17	48
55	MJ	429/447 (96%)	395 (92%)	30 (7%)	4 (1%)	17	48
55	MM	429/447 (96%)	389 (91%)	38 (9%)	2 (0%)	29	61
55	NC	429/447 (96%)	383 (89%)	44 (10%)	2 (0%)	29	61
55	ND	429/447 (96%)	391 (91%)	33 (8%)	5 (1%)	13	42
55	NF	429/447 (96%)	388 (90%)	36 (8%)	5 (1%)	13	42
55	NH	429/447 (96%)	386 (90%)	42 (10%)	1 (0%)	47	77
55	NJ	429/447 (96%)	381 (89%)	44 (10%)	4 (1%)	17	48
55	NK	429/447 (96%)	388 (90%)	40 (9%)	1 (0%)	47	77
55	NM	429/447 (96%)	381 (89%)	45 (10%)	3 (1%)	22	54
55	OC	429/447 (96%)	391 (91%)	36 (8%)	2 (0%)	29	61
55	OD	429/447 (96%)	386 (90%)	41 (10%)	2 (0%)	29	61
55	OF	429/447 (96%)	395 (92%)	32 (8%)	2 (0%)	29	61
55	OH	429/447 (96%)	391 (91%)	38 (9%)	0	100	100
55	OJ	429/447 (96%)	392 (91%)	34 (8%)	3 (1%)	22	54
55	OM	429/447 (96%)	393 (92%)	33 (8%)	3 (1%)	22	54
55	PC	429/447 (96%)	389 (91%)	36 (8%)	4 (1%)	17	48
55	PD	429/447 (96%)	396 (92%)	31 (7%)	2 (0%)	29	61
55	PF	429/447 (96%)	389 (91%)	38 (9%)	2 (0%)	29	61
55	PH	429/447 (96%)	391 (91%)	36 (8%)	2 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	PJ	429/447 (96%)	377 (88%)	49 (11%)	3 (1%)	22	54
55	PM	429/447 (96%)	387 (90%)	38 (9%)	4 (1%)	17	48
55	QC	429/447 (96%)	386 (90%)	39 (9%)	4 (1%)	17	48
55	QD	429/447 (96%)	391 (91%)	37 (9%)	1 (0%)	47	77
55	QF	429/447 (96%)	383 (89%)	43 (10%)	3 (1%)	22	54
55	QH	429/447 (96%)	388 (90%)	38 (9%)	3 (1%)	22	54
55	QJ	429/447 (96%)	379 (88%)	49 (11%)	1 (0%)	47	77
55	QM	429/447 (96%)	393 (92%)	35 (8%)	1 (0%)	47	77
55	RC	429/447 (96%)	383 (89%)	44 (10%)	2 (0%)	29	61
55	RD	429/447 (96%)	395 (92%)	30 (7%)	4 (1%)	17	48
55	RF	429/447 (96%)	391 (91%)	36 (8%)	2 (0%)	29	61
55	RH	429/447 (96%)	388 (90%)	38 (9%)	3 (1%)	22	54
55	RJ	429/447 (96%)	381 (89%)	46 (11%)	2 (0%)	29	61
55	RM	429/447 (96%)	396 (92%)	29 (7%)	4 (1%)	17	48
55	SC	429/447 (96%)	396 (92%)	31 (7%)	2 (0%)	29	61
55	SD	429/447 (96%)	380 (89%)	48 (11%)	1 (0%)	47	77
55	SF	429/447 (96%)	405 (94%)	21 (5%)	3 (1%)	22	54
55	SH	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	29	61
55	SJ	429/447 (96%)	389 (91%)	38 (9%)	2 (0%)	29	61
55	SL	429/447 (96%)	384 (90%)	42 (10%)	3 (1%)	22	54
55	SM	429/447 (96%)	390 (91%)	36 (8%)	3 (1%)	22	54
55	TC	429/447 (96%)	386 (90%)	40 (9%)	3 (1%)	22	54
55	TD	429/447 (96%)	384 (90%)	42 (10%)	3 (1%)	22	54
55	TF	429/447 (96%)	395 (92%)	32 (8%)	2 (0%)	29	61
55	TH	429/447 (96%)	385 (90%)	41 (10%)	3 (1%)	22	54
55	TJ	429/447 (96%)	386 (90%)	39 (9%)	4 (1%)	17	48
55	TL	429/447 (96%)	381 (89%)	47 (11%)	1 (0%)	47	77
55	TM	429/447 (96%)	384 (90%)	42 (10%)	3 (1%)	22	54
55	UC	429/447 (96%)	380 (89%)	46 (11%)	3 (1%)	22	54
55	UD	429/447 (96%)	392 (91%)	33 (8%)	4 (1%)	17	48
55	UF	429/447 (96%)	379 (88%)	46 (11%)	4 (1%)	17	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	UH	429/447 (96%)	380 (89%)	45 (10%)	4 (1%)	17	48
55	UJ	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	29	61
55	UL	429/447 (96%)	381 (89%)	45 (10%)	3 (1%)	22	54
55	UM	429/447 (96%)	387 (90%)	40 (9%)	2 (0%)	29	61
55	VC	429/447 (96%)	378 (88%)	48 (11%)	3 (1%)	22	54
55	VD	429/447 (96%)	386 (90%)	39 (9%)	4 (1%)	17	48
55	VF	429/447 (96%)	388 (90%)	39 (9%)	2 (0%)	29	61
55	VH	429/447 (96%)	372 (87%)	53 (12%)	4 (1%)	17	48
55	VJ	429/447 (96%)	384 (90%)	44 (10%)	1 (0%)	47	77
55	VL	429/447 (96%)	377 (88%)	48 (11%)	4 (1%)	17	48
55	VM	429/447 (96%)	397 (92%)	31 (7%)	1 (0%)	47	77
55	WC	429/447 (96%)	396 (92%)	30 (7%)	3 (1%)	22	54
55	WD	429/447 (96%)	392 (91%)	35 (8%)	2 (0%)	29	61
55	WF	429/447 (96%)	390 (91%)	36 (8%)	3 (1%)	22	54
55	WH	429/447 (96%)	394 (92%)	34 (8%)	1 (0%)	47	77
55	WJ	429/447 (96%)	405 (94%)	23 (5%)	1 (0%)	47	77
55	WL	429/447 (96%)	390 (91%)	36 (8%)	3 (1%)	22	54
All	All	159050/186788 (85%)	144892 (91%)	13287 (8%)	871 (0%)	32	61

All (871) 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
3	1M	16	LYS
7	1a	156	VAL
7	1a	247	ILE
7	1b	16	ALA
10	1i	5	PHE
10	1j	30	LYS
3	1x	445	ARG
13	2B	142	SER
13	2B	253	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	2C	132	VAL
13	2D	132	VAL
13	2D	156	GLU
17	2S	269	GLU
18	2V	70	VAL
18	2V	227	CYS
3	2a	669	GLN
20	3J	160	THR
20	3J	224	ASP
20	3J	313	PRO
20	3J	516	ILE
21	3O	47	VAL
22	3R	34	TYR
23	3W	81	ILE
25	4G	30	LYS
26	4J	172	ILE
26	4J	290	LYS
26	4K	63	LEU
28	4T	94	TYR
28	4U	26	ASP
30	5B	94	HIS
30	5B	146	MET
7	5E	137	ASN
7	5F	247	ILE
7	5G	95	LYS
7	5H	160	ARG
7	5K	73	ARG
7	5L	247	ILE
7	5N	247	ILE
36	7A	108	GLU
36	7A	130	ILE
36	7A	316	ILE
36	7A	504	LEU
36	7B	445	VAL
36	7C	108	GLU
36	7C	316	ILE
36	7C	445	VAL
36	7D	108	GLU
36	7D	316	ILE
37	7G	41	ILE
37	7G	131	HIS
37	7G	363	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
37	7H	7	PRO
37	7H	363	ILE
38	7M	231	ARG
40	7U	110	GLU
40	7U	189	VAL
41	7Y	36	ALA
41	7Y	59	ILE
41	7Y	147	VAL
41	7Y	202	PRO
41	7Z	10	LEU
42	8A	48	PRO
43	8E	265	VAL
45	8R	207	ILE
45	8S	204	VAL
45	8T	208	GLU
47	9A	134	GLU
47	9A	202	THR
10	9O	161	ASP
53	9V	88	PRO
30	9Y	140	HIS
30	9Y	273	VAL
30	9Z	123	PRO
30	9Z	131	GLU
54	AA	219	ILE
54	AA	281	ALA
55	AH	175	VAL
55	AH	355	ASP
55	AJ	175	VAL
55	AL	175	VAL
55	BC	175	VAL
55	BD	175	VAL
55	BF	175	VAL
55	BF	221	THR
55	BH	175	VAL
55	BJ	175	VAL
55	BL	175	VAL
54	CA	109	THR
54	CB	74	VAL
55	CD	175	VAL
55	CD	218	THR
55	CF	323	MET
54	CG	278	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	CJ	175	VAL
54	CM	161	TYR
55	DC	221	THR
55	DD	175	VAL
54	DE	74	VAL
55	DF	176	SER
54	DG	74	VAL
55	DH	175	VAL
55	DJ	175	VAL
55	DJ	355	ASP
55	DL	176	SER
54	EC	42	ILE
55	ED	175	VAL
55	ED	177	ASP
54	EE	74	VAL
55	EF	221	THR
55	EH	89	ASN
55	EH	221	THR
54	EI	74	VAL
55	EJ	175	VAL
55	EL	175	VAL
55	EM	175	VAL
55	EM	218	THR
55	EM	221	THR
54	FA	74	VAL
55	FD	175	VAL
54	FE	74	VAL
55	FH	221	THR
55	FJ	175	VAL
55	FJ	221	THR
55	FL	221	THR
55	FM	175	VAL
55	FM	221	THR
55	GD	176	SER
55	GF	218	THR
55	GF	221	THR
55	GH	221	THR
55	HD	175	VAL
54	HE	219	ILE
54	HG	48	SER
55	HH	218	THR
55	HJ	175	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	HK	82	THR
55	HL	175	VAL
55	ID	175	VAL
55	IJ	175	VAL
55	IL	175	VAL
55	IL	221	THR
54	JA	281	ALA
54	JB	42	ILE
55	JC	221	THR
55	JD	175	VAL
55	JD	218	THR
55	JH	176	SER
54	JI	278	ALA
55	JJ	175	VAL
55	JL	175	VAL
55	KC	218	THR
54	KE	339	ARG
55	KF	175	VAL
55	KJ	175	VAL
55	KM	175	VAL
54	LE	82	THR
55	LF	175	VAL
55	LH	175	VAL
55	LH	218	THR
55	LH	221	THR
55	LJ	221	THR
54	LK	74	VAL
55	LL	218	THR
54	MA	74	VAL
54	MB	39	ASP
55	MH	175	VAL
54	MI	252	LEU
55	MJ	108	GLU
55	MJ	221	THR
55	MM	175	VAL
54	NB	281	ALA
55	ND	175	VAL
55	ND	221	THR
55	NF	175	VAL
54	NG	161	TYR
54	NI	281	ALA
55	NJ	175	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	NK	175	VAL
55	NM	175	VAL
55	NM	221	THR
55	OD	175	VAL
55	OJ	175	VAL
54	OK	240	ALA
55	OM	175	VAL
54	PA	40	LYS
54	PB	278	ALA
55	PC	176	SER
55	PD	176	SER
55	PD	221	THR
55	PF	175	VAL
55	PF	221	THR
54	PI	161	TYR
55	PJ	175	VAL
54	PK	74	VAL
54	PK	82	THR
55	PM	175	VAL
55	PM	221	THR
55	QC	221	THR
55	QD	175	VAL
54	QE	39	ASP
55	QF	175	VAL
54	QG	48	SER
54	QG	73	THR
55	QH	176	SER
54	QI	73	THR
55	QJ	175	VAL
54	QK	219	ILE
54	QL	82	THR
55	QM	175	VAL
54	RB	74	VAL
55	RC	175	VAL
55	RD	175	VAL
54	RE	40	LYS
55	RF	175	VAL
54	RG	74	VAL
55	RJ	175	VAL
55	RM	175	VAL
55	SC	175	VAL
55	SD	175	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	SF	218	THR
54	SG	340	THR
55	SJ	175	VAL
55	SL	342	VAL
55	SM	175	VAL
55	TC	262	ARG
55	TD	175	VAL
55	TF	221	THR
55	TH	175	VAL
55	TJ	175	VAL
55	TL	175	VAL
55	TM	175	VAL
55	UC	175	VAL
55	UC	221	THR
55	UD	175	VAL
55	UF	175	VAL
55	UF	339	SER
55	UF	342	VAL
55	UH	175	VAL
55	UH	279	GLN
55	UJ	175	VAL
55	UL	175	VAL
55	UL	342	VAL
55	VC	175	VAL
55	VD	175	VAL
55	VD	279	GLN
55	VF	175	VAL
55	VH	175	VAL
55	VJ	175	VAL
55	VL	175	VAL
54	WA	82	THR
55	WD	175	VAL
54	WE	275	VAL
55	WF	218	THR
55	WH	175	VAL
54	WI	74	VAL
1	1A	23	ASP
1	1B	114	LEU
1	1B	155	THR
2	1E	247	ASN
2	1G	132	ARG
5	1V	238	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	1o	27	MET
12	1o	28	THR
3	1x	401	PHE
13	2A	93	LYS
13	2B	20	VAL
13	2B	98	PRO
13	2C	20	VAL
15	2K	42	ILE
18	2W	70	VAL
20	3J	83	VAL
20	3J	206	PHE
20	3J	212	VAL
20	3K	51	GLU
20	3K	83	VAL
22	3R	138	LYS
22	3S	138	LYS
23	3W	112	THR
23	3W	151	GLN
26	4J	44	LYS
27	4N	170	ASN
27	4O	173	ILE
29	4Y	36	ALA
30	5A	42	ARG
30	5B	98	THR
7	5H	247	ILE
7	5J	101	SER
35	6V	124	PRO
35	6V	262	SER
35	6W	40	VAL
35	6X	40	VAL
36	7A	473	ILE
36	7B	473	ILE
36	7B	632	ASN
36	7C	130	ILE
36	7D	130	ILE
36	7D	473	ILE
36	7D	709	VAL
37	7G	269	VAL
37	7H	269	VAL
37	7I	41	ILE
37	7I	143	ILE
37	7I	269	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	7Q	99	VAL
40	7U	141	GLU
40	7V	35	VAL
49	9G	33	SER
50	9J	172	THR
10	9N	112	SER
10	9O	160	ASN
55	AF	216	LYS
55	AF	218	THR
55	AH	108	GLU
55	AH	218	THR
55	AH	221	THR
55	AH	302	ALA
54	BB	42	ILE
55	BC	108	GLU
55	BC	218	THR
55	BD	221	THR
55	BJ	218	THR
55	BL	218	THR
55	BL	221	THR
54	BM	46	ASP
55	CC	176	SER
55	CD	168	SER
54	CE	72	PRO
55	CJ	347	ASN
54	CM	264	ARG
55	DD	221	THR
55	DF	108	GLU
55	DF	336	LYS
54	DI	42	ILE
55	EB	175	VAL
55	ED	221	THR
55	EH	108	GLU
55	EH	176	SER
54	FE	145	THR
54	FG	82	THR
55	FJ	99	ASN
55	FL	95	SER
55	GC	108	GLU
55	GC	214	THR
55	GH	216	LYS
55	GJ	175	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	GJ	216	LYS
55	GJ	218	THR
54	HE	82	THR
55	HF	216	LYS
55	HH	216	LYS
54	HI	82	THR
55	HJ	108	GLU
55	HJ	217	LEU
55	HL	95	SER
55	HL	143	THR
55	HM	175	VAL
55	HM	177	ASP
54	IA	161	TYR
54	IB	40	LYS
55	ID	218	THR
55	IH	168	SER
55	IH	221	THR
54	IK	41	THR
55	IL	218	THR
54	JE	109	THR
55	JF	176	SER
55	JF	201	CYS
55	JM	175	VAL
55	KD	108	GLU
55	KD	221	THR
55	KF	218	THR
54	KG	37	PRO
55	KH	218	THR
54	LB	82	THR
55	LC	216	LYS
55	LD	175	VAL
55	LJ	95	SER
55	LL	175	VAL
55	LL	216	LYS
54	MA	82	THR
55	MC	108	GLU
55	MC	216	LYS
55	MD	218	THR
55	MF	108	GLU
55	MH	108	GLU
55	MH	168	SER
55	MH	216	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	MI	38	SER
55	MJ	218	THR
54	NA	41	THR
55	ND	218	THR
54	NE	110	ILE
55	NF	107	THR
55	NF	216	LYS
55	NF	218	THR
55	NJ	221	THR
54	NL	110	ILE
54	OA	110	ILE
54	OB	110	ILE
55	OD	221	THR
55	OF	95	SER
55	OJ	77	ARG
55	OJ	216	LYS
55	OM	221	THR
55	PC	218	THR
55	PC	221	THR
55	PH	218	THR
54	QA	72	PRO
54	QA	73	THR
55	QF	221	THR
54	RA	82	THR
54	RB	48	SER
55	RD	218	THR
54	RG	42	ILE
55	RH	176	SER
55	RM	221	THR
55	SF	221	THR
55	SL	175	VAL
55	SM	218	THR
55	TC	175	VAL
55	TF	355	ASP
55	TJ	108	GLU
55	TJ	195	ASN
55	TM	108	GLU
55	UD	108	GLU
55	UD	221	THR
55	UF	218	THR
55	UH	216	LYS
54	UI	41	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	VA	82	THR
55	VD	108	GLU
54	VE	220	GLU
55	VL	221	THR
55	WC	175	VAL
55	WC	221	THR
54	WG	41	THR
54	WG	82	THR
54	WK	42	ILE
55	WL	175	VAL
55	WL	218	THR
2	1H	360	THR
5	1T	147	LYS
5	1V	147	LYS
5	1V	272	GLU
5	1W	147	LYS
5	1W	177	LYS
7	1a	172	LEU
7	1b	73	ARG
7	1b	77	ASP
3	1x	449	PHE
13	2B	156	GLU
13	2C	156	GLU
14	2G	101	LYS
15	2L	8	ASN
18	2W	284	LYS
25	4G	8	ARG
26	4J	232	ARG
26	4K	44	LYS
26	4K	83	ASP
26	4K	356	ASN
27	4N	102	ASP
27	4O	170	ASN
7	5F	184	VAL
7	5H	157	TYR
7	5I	6	TYR
7	5K	9	THR
36	7A	383	ASN
37	7G	143	ILE
37	7G	355	TYR
37	7G	458	ILE
37	7H	143	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
37	7H	402	LYS
37	7H	458	ILE
37	7I	35	ALA
37	7I	402	LYS
40	7U	162	ILE
41	7Y	8	ARG
44	8J	3	ILE
44	8L	3	ILE
45	8R	204	VAL
47	9A	164	PHE
49	9G	7	THR
53	9V	92	ARG
30	9Y	153	ARG
30	9Y	200	LYS
55	AC	168	SER
55	AD	218	THR
55	AJ	176	SER
54	BB	48	SER
55	BF	218	THR
55	CH	216	LYS
55	DF	168	SER
55	DJ	108	GLU
55	DJ	282	ARG
54	DK	38	SER
55	DL	168	SER
55	ED	216	LYS
55	EL	168	SER
54	FB	274	PRO
55	FJ	216	LYS
54	GB	38	SER
55	GD	168	SER
54	GE	42	ILE
54	GG	41	THR
54	GK	109	THR
55	GL	175	VAL
54	HA	82	THR
55	HD	168	SER
55	IC	168	SER
55	ID	216	LYS
55	IL	168	SER
55	JC	176	SER
55	JH	175	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	JJ	216	LYS
55	JL	221	THR
55	KC	168	SER
54	KG	41	THR
55	KH	168	SER
55	KJ	221	THR
55	KL	175	VAL
55	LC	168	SER
54	LG	40	LYS
55	LH	216	LYS
55	MD	175	VAL
55	MD	216	LYS
55	MJ	216	LYS
55	MM	221	THR
54	NB	145	THR
55	NC	176	SER
55	NF	168	SER
55	NJ	218	THR
55	NM	168	SER
55	OC	216	LYS
54	OI	82	THR
55	OM	216	LYS
54	PE	39	ASP
54	PE	41	THR
55	PJ	216	LYS
54	QA	278	ALA
55	QC	177	ASP
55	QH	143	THR
54	QI	40	LYS
54	RA	274	PRO
55	RD	216	LYS
55	RH	216	LYS
55	RJ	221	THR
54	RL	38	SER
55	SC	216	LYS
55	SH	216	LYS
54	SK	39	ASP
55	SM	216	LYS
54	TB	274	PRO
55	TD	216	LYS
55	TD	221	THR
55	TH	147	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	TH	355	ASP
54	TK	274	PRO
55	UH	221	THR
55	UM	168	SER
55	UM	175	VAL
55	VC	168	SER
55	VH	221	THR
55	VL	168	SER
55	VL	218	THR
54	WB	274	PRO
55	WC	216	LYS
55	WF	175	VAL
55	WF	216	LYS
55	WL	168	SER
1	1B	139	ILE
2	1H	261	THR
3	1K	3	GLU
3	1L	6	SER
5	1T	419	ARG
13	2C	217	LEU
14	2G	227	ARG
21	3N	491	VAL
23	3Z	81	ILE
27	4N	169	MET
28	4T	88	VAL
28	4T	129	TYR
30	5B	210	ILE
7	5J	157	TYR
7	5J	180	SER
7	5J	184	VAL
7	5L	184	VAL
7	5M	247	ILE
7	5N	157	TYR
7	5N	184	VAL
33	6M	170	ALA
35	6W	124	PRO
36	7A	542	ILE
36	7C	473	ILE
36	7C	505	TYR
36	7D	380	ALA
37	7G	430	LYS
37	7I	430	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
37	7I	448	PHE
39	7Q	160	VAL
41	7Z	59	ILE
44	8M	3	ILE
45	8S	6	LYS
10	9O	166	PHE
30	9Y	210	ILE
55	AC	175	VAL
55	AD	168	SER
55	BH	216	LYS
54	BK	109	THR
55	CC	101	TRP
55	CC	175	VAL
55	CC	221	THR
55	CH	217	LEU
55	CL	168	SER
55	DC	176	SER
55	DF	175	VAL
55	DL	175	VAL
55	EH	175	VAL
54	EI	274	PRO
55	FC	168	SER
55	FD	259	PRO
55	FL	218	THR
55	GD	175	VAL
55	GF	168	SER
55	GM	175	VAL
55	HC	216	LYS
54	HG	274	PRO
55	HJ	168	SER
55	HL	216	LYS
55	IJ	216	LYS
55	JF	175	VAL
55	JH	168	SER
55	JM	221	THR
55	LM	175	VAL
55	MD	221	THR
54	NB	274	PRO
55	ND	168	SER
55	PC	175	VAL
54	PK	219	ILE
55	PM	168	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	QC	178	THR
55	QF	168	SER
55	QH	175	VAL
54	RA	161	TYR
55	RC	168	SER
55	RF	221	THR
55	RH	168	SER
55	RM	168	SER
55	SF	175	VAL
55	SJ	168	SER
55	TJ	217	LEU
55	TM	168	SER
55	VD	168	SER
55	VF	168	SER
55	VM	175	VAL
55	WJ	175	VAL
54	WK	403	ALA
2	1H	51	ASP
3	1K	19	THR
13	2A	253	ILE
18	2V	190	VAL
18	2V	284	LYS
18	2W	190	VAL
20	3J	196	ARG
20	3J	562	VAL
21	3N	528	VAL
25	4G	35	HIS
26	4K	331	PRO
27	4N	168	ASN
27	4Q	168	ASN
28	4T	98	SER
29	4Y	10	VAL
7	5G	101	SER
7	5H	184	VAL
7	5J	247	ILE
35	6W	127	VAL
36	7A	184	ILE
36	7C	184	ILE
36	7D	184	ILE
36	7D	504	LEU
37	7G	197	ALA
37	7G	457	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
37	7H	35	ALA
37	7H	430	LYS
37	7I	197	ALA
42	8A	29	GLN
43	8G	265	VAL
44	8L	328	PRO
46	8Y	110	LYS
46	8Z	73	GLU
47	9A	152	TYR
49	9G	2	SER
53	9V	89	PRO
55	AC	218	THR
55	AJ	216	LYS
55	BL	108	GLU
54	CE	73	THR
55	CL	175	VAL
55	DC	216	LYS
54	DM	40	LYS
55	EB	168	SER
55	EH	88	ASP
55	FL	175	VAL
55	GF	175	VAL
55	HH	393	ALA
54	IB	163	LYS
55	IJ	217	LEU
54	IK	274	PRO
55	JF	101	TRP
55	JJ	176	SER
54	JK	42	ILE
55	KD	218	THR
55	KF	216	LYS
55	LC	108	GLU
55	LD	216	LYS
54	ME	46	ASP
55	NC	216	LYS
55	ND	247	ASN
54	NG	58	ALA
55	NH	176	SER
55	NJ	216	LYS
54	OE	220	GLU
54	OE	274	PRO
55	OF	175	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	PJ	218	THR
54	RE	160	ASP
54	RK	109	THR
55	RM	218	THR
55	SH	176	SER
54	SI	274	PRO
55	SL	97	ALA
55	TC	108	GLU
55	UJ	393	ALA
55	VH	168	SER
54	WB	261	PRO
55	WD	221	THR
54	WK	404	PHE
1	1A	35	GLU
3	1K	15	HIS
3	1x	450	ASN
13	2C	188	MET
15	2K	38	PHE
18	2W	146	THR
20	3J	97	ALA
20	3J	109	SER
20	3J	111	LYS
29	4Y	191	GLN
30	5B	255	TYR
7	5E	9	THR
7	5L	157	TYR
7	5N	20	THR
36	7A	505	TYR
36	7A	513	HIS
36	7B	437	LEU
36	7B	505	TYR
36	7D	505	TYR
37	7I	367	THR
43	8D	265	VAL
44	8J	328	PRO
44	8K	328	PRO
46	8Z	110	LYS
47	9A	181	THR
55	AF	108	GLU
54	AG	65	ALA
54	BA	46	ASP
55	CD	216	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	DD	218	THR
55	DL	177	ASP
55	EM	216	LYS
55	FD	108	GLU
55	GC	175	VAL
55	GH	168	SER
54	GK	37	PRO
55	GL	221	THR
55	HC	221	THR
55	HH	394	PHE
55	HL	168	SER
55	HM	241	ARG
55	IF	97	ALA
55	IH	175	VAL
55	JH	216	LYS
55	JJ	108	GLU
55	KC	216	LYS
55	KC	221	THR
55	KH	216	LYS
55	LF	216	LYS
54	OB	40	LYS
55	OC	221	THR
54	OI	41	THR
55	PH	216	LYS
55	PM	218	THR
55	QC	316	ILE
54	SB	278	ALA
54	TG	243	ARG
55	UC	218	THR
55	UD	216	LYS
55	UL	221	THR
54	VA	42	ILE
54	VA	74	VAL
55	VC	108	GLU
55	VH	216	LYS
20	3J	208	VAL
24	4A	121	VAL
36	7A	54	GLN
44	8N	328	PRO
55	FL	272	PRO
55	GH	175	VAL
55	HC	175	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	IF	175	VAL
54	NB	110	ILE
54	SG	42	ILE
13	2A	20	VAL
13	2B	132	VAL
15	2L	42	ILE
37	7I	458	ILE
30	9Y	134	HIS
54	TK	110	ILE
54	WK	274	PRO
13	2B	92	PRO
18	2V	236	VAL
19	3D	178	PRO
22	3T	121	GLU
25	4G	28	PRO
37	7H	377	LEU
40	7U	134	ILE
54	DG	66	VAL
54	FI	110	ILE
55	HF	175	VAL
55	IC	175	VAL
55	IL	70	PRO
54	LG	110	ILE
55	RD	70	PRO
54	TG	110	ILE
54	VE	274	PRO
21	3O	108	ILE
22	3T	33	PRO
7	5K	108	GLY
36	7A	186	ALA
36	7A	389	PRO
36	7C	6	LEU
36	7C	54	GLN
36	7C	186	ALA
36	7C	389	PRO
36	7D	54	GLN
37	7G	377	LEU
37	7H	197	ALA
37	7H	457	ILE
37	7H	478	PRO
37	7I	457	ILE
42	8A	55	GLY

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Mol	Chain	Res	Type
30	9Z	52	PRO
54	BG	261	PRO
54	HA	110	ILE
55	JH	316	ILE
54	KA	110	ILE
54	VK	110	ILE
1	1B	97	PRO
24	4C	121	VAL
27	4P	89	VAL
36	7D	186	ALA
36	7D	389	PRO
37	7H	470	MET
37	7I	470	MET
46	8Y	73	GLU
54	FI	274	PRO
54	NA	110	ILE
54	SG	274	PRO

### 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%)	92	96
2	1F	140/374 (37%)	139 (99%)	1 (1%)	84	90
2	1G	248/374 (66%)	247 (100%)	1 (0%)	91	95
2	1H	352/374 (94%)	350 (99%)	2 (1%)	86	91
3	1K	159/612 (26%)	159 (100%)	0	100	100
3	1L	159/612 (26%)	158 (99%)	1 (1%)	86	91
3	1M	155/612 (25%)	155 (100%)	0	100	100
3	1v	187/612 (31%)	187 (100%)	0	100	100
3	1w	81/612 (13%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1x	226/612 (37%)	225 (100%)	1 (0%)	91	95
3	1y	178/612 (29%)	178 (100%)	0	100	100
3	1z	81/612 (13%)	80 (99%)	1 (1%)	71	83
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%)	81	89
5	1T	199/383 (52%)	198 (100%)	1 (0%)	88	93
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%)	27	58
7	5J	197/213 (92%)	197 (100%)	0	100	100
7	5K	109/213 (51%)	108 (99%)	1 (1%)	78	87
7	5L	110/213 (52%)	109 (99%)	1 (1%)	78	87
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%)	52	74
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
10	9N	76/164 (46%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	41	68
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%)	49	73
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%)	78	87
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%)	92	96
18	2V	252/259 (97%)	251 (100%)	1 (0%)	91	95
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%)	86	91
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%)	86	91
20	3J	428/509 (84%)	426 (100%)	2 (0%)	88	93
20	3K	61/509 (12%)	60 (98%)	1 (2%)	62	79
21	3N	221/478 (46%)	218 (99%)	3 (1%)	67	82
21	3O	239/478 (50%)	239 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	3R	147/154 (96%)	146 (99%)	1 (1%)	84	90
22	3S	112/154 (73%)	112 (100%)	0	100	100
22	3T	147/154 (96%)	147 (100%)	0	100	100
23	3W	341/480 (71%)	340 (100%)	1 (0%)	92	96
23	3X	278/480 (58%)	276 (99%)	2 (1%)	84	90
23	3Y	89/480 (18%)	89 (100%)	0	100	100
23	3Z	153/480 (32%)	152 (99%)	1 (1%)	84	90
24	4A	532/546 (97%)	532 (100%)	0	100	100
24	4B	530/546 (97%)	528 (100%)	2 (0%)	91	95
24	4C	532/546 (97%)	531 (100%)	1 (0%)	93	97
25	4F	266/454 (59%)	266 (100%)	0	100	100
25	4G	191/454 (42%)	191 (100%)	0	100	100
26	4J	323/327 (99%)	322 (100%)	1 (0%)	92	96
26	4K	322/327 (98%)	322 (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%)	69	82
28	4T	133/209 (64%)	133 (100%)	0	100	100
28	4U	133/209 (64%)	132 (99%)	1 (1%)	81	89
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%)	73	85
30	9Y	122/237 (52%)	120 (98%)	2 (2%)	62	79
30	9Z	82/237 (35%)	82 (100%)	0	100	100
31	6A	195/204 (96%)	194 (100%)	1 (0%)	88	93
31	6B	188/204 (92%)	187 (100%)	1 (0%)	88	93
31	6C	192/204 (94%)	192 (100%)	0	100	100
31	6D	194/204 (95%)	194 (100%)	0	100	100
31	6E	194/204 (95%)	193 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	6F	194/204 (95%)	194 (100%)	0	100	100
32	6I	70/106 (66%)	69 (99%)	1 (1%)	67	82
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%)	81	89
35	6V	240/338 (71%)	238 (99%)	2 (1%)	81	89
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%)	92	96
36	7B	410/660 (62%)	408 (100%)	2 (0%)	88	93
36	7C	480/660 (73%)	478 (100%)	2 (0%)	91	95
36	7D	643/660 (97%)	643 (100%)	0	100	100
37	7G	477/577 (83%)	476 (100%)	1 (0%)	93	97
37	7H	477/577 (83%)	474 (99%)	3 (1%)	86	91
37	7I	553/577 (96%)	550 (100%)	3 (0%)	88	93
38	7M	230/283 (81%)	229 (100%)	1 (0%)	91	95
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%)	73	85
40	7V	49/183 (27%)	48 (98%)	1 (2%)	55	76
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%)	88	93
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%)	91	95
43	8G	364/412 (88%)	364 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	86	91
45	8S	278/365 (76%)	277 (100%)	1 (0%)	91	95
45	8T	363/365 (100%)	362 (100%)	1 (0%)	92	96
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%)	76	86
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%)	84	90
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%)	92	96
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%)	88	93
54	AM	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	BA	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	BB	365/376 (97%)	365 (100%)	0	100	100
54	BE	365/376 (97%)	363 (100%)	2 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	BG	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	BI	365/376 (97%)	365 (100%)	0	100	100
54	BK	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	BM	365/376 (97%)	363 (100%)	2 (0%)	88	93
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%)	88	93
54	CG	365/376 (97%)	363 (100%)	2 (0%)	88	93
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%)	92	96
54	DA	365/376 (97%)	365 (100%)	0	100	100
54	DB	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	DE	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	DG	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	DI	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	DK	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	DM	365/376 (97%)	365 (100%)	0	100	100
54	EA	365/376 (97%)	365 (100%)	0	100	100
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%)	88	93
54	FA	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	FB	365/376 (97%)	365 (100%)	0	100	100
54	FE	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	FG	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	FI	365/376 (97%)	365 (100%)	0	100	100
54	FK	365/376 (97%)	365 (100%)	0	100	100
54	GA	365/376 (97%)	364 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	GB	365/376 (97%)	365 (100%)	0	100	100
54	GE	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	GG	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	GI	365/376 (97%)	364 (100%)	1 (0%)	92	96
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%)	92	96
54	HG	365/376 (97%)	362 (99%)	3 (1%)	81	89
54	HI	365/376 (97%)	365 (100%)	0	100	100
54	HK	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	IA	365/376 (97%)	364 (100%)	1 (0%)	92	96
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%)	92	96
54	IM	365/376 (97%)	362 (99%)	3 (1%)	81	89
54	JA	363/376 (96%)	363 (100%)	0	100	100
54	JB	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	JE	365/376 (97%)	365 (100%)	0	100	100
54	JG	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	JI	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	JK	365/376 (97%)	365 (100%)	0	100	100
54	KA	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	KB	364/376 (97%)	362 (100%)	2 (0%)	88	93
54	KE	365/376 (97%)	365 (100%)	0	100	100
54	KG	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	KI	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	KK	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	LA	365/376 (97%)	363 (100%)	2 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	LB	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	LE	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	LG	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	LI	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	LK	365/376 (97%)	365 (100%)	0	100	100
54	MA	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	MB	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	ME	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	MG	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	MI	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	MK	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	ML	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	NA	365/376 (97%)	365 (100%)	0	100	100
54	NB	365/376 (97%)	364 (100%)	1 (0%)	92	96
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%)	92	96
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%)	88	93
54	OE	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	OG	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	OI	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	OK	365/376 (97%)	365 (100%)	0	100	100
54	OL	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	PA	365/376 (97%)	364 (100%)	1 (0%)	92	96
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%)	92	96
54	PI	365/376 (97%)	365 (100%)	0	100	100
54	PK	365/376 (97%)	364 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	PL	365/376 (97%)	365 (100%)	0	100	100
54	QA	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	QB	365/376 (97%)	365 (100%)	0	100	100
54	QE	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	QG	365/376 (97%)	361 (99%)	4 (1%)	73	85
54	QI	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	QK	363/376 (96%)	362 (100%)	1 (0%)	92	96
54	QL	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	RA	365/376 (97%)	365 (100%)	0	100	100
54	RB	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	RE	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	RG	365/376 (97%)	365 (100%)	0	100	100
54	RI	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	RK	365/376 (97%)	364 (100%)	1 (0%)	92	96
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%)	92	96
54	SK	365/376 (97%)	365 (100%)	0	100	100
54	TA	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	TB	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	TE	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	TG	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	TI	365/376 (97%)	365 (100%)	0	100	100
54	TK	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	UA	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	UB	363/376 (96%)	362 (100%)	1 (0%)	92	96
54	UE	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	UG	365/376 (97%)	365 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	92	96
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%)	88	93
54	VK	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	WA	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	WB	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	WE	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	WG	365/376 (97%)	363 (100%)	2 (0%)	88	93
54	WI	365/376 (97%)	364 (100%)	1 (0%)	92	96
54	WK	365/376 (97%)	364 (100%)	1 (0%)	92	96
55	AC	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	AD	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	AF	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	AH	369/381 (97%)	369 (100%)	0	100	100
55	AJ	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	AL	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	BC	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	BD	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	BF	369/381 (97%)	366 (99%)	3 (1%)	81	89
55	BH	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	BJ	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	BL	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	CC	369/381 (97%)	369 (100%)	0	100	100
55	CD	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	CF	369/381 (97%)	369 (100%)	0	100	100
55	CH	369/381 (97%)	369 (100%)	0	100	100
55	CJ	369/381 (97%)	369 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	CL	369/381 (97%)	368 (100%)	1 (0%)	92	96
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%)	92	96
55	DL	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	EB	369/381 (97%)	369 (100%)	0	100	100
55	ED	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	EF	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	EH	369/381 (97%)	369 (100%)	0	100	100
55	EJ	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	EL	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	EM	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	FC	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	FD	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	FF	369/381 (97%)	368 (100%)	1 (0%)	92	96
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%)	92	96
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%)	92	96
55	GH	369/381 (97%)	368 (100%)	1 (0%)	92	96
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%)	88	93
55	HC	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	HD	369/381 (97%)	366 (99%)	3 (1%)	81	89
55	HF	369/381 (97%)	368 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	HH	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	HJ	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	HL	369/381 (97%)	367 (100%)	2 (0%)	88	93
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%)	92	96
55	IF	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	IH	369/381 (97%)	369 (100%)	0	100	100
55	IJ	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	IL	369/381 (97%)	369 (100%)	0	100	100
55	JC	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	JD	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	JF	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	JH	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	JJ	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	JL	369/381 (97%)	368 (100%)	1 (0%)	92	96
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%)	92	96
55	KJ	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	KL	369/381 (97%)	369 (100%)	0	100	100
55	KM	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	LC	369/381 (97%)	369 (100%)	0	100	100
55	LD	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	LF	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	LH	369/381 (97%)	369 (100%)	0	100	100
55	LJ	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	LL	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	LM	369/381 (97%)	369 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	MC	369/381 (97%)	369 (100%)	0	100	100
55	MD	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	MF	369/381 (97%)	368 (100%)	1 (0%)	92	96
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%)	92	96
55	NC	369/381 (97%)	366 (99%)	3 (1%)	81	89
55	ND	369/381 (97%)	369 (100%)	0	100	100
55	NF	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	NH	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	NJ	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	NK	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	NM	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	OC	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	OD	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	OF	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	OH	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	OJ	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	OM	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	PC	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	PD	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	PF	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	PH	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	PJ	369/381 (97%)	369 (100%)	0	100	100
55	PM	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	QC	369/381 (97%)	366 (99%)	3 (1%)	81	89
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%)	92	96
55	QJ	369/381 (97%)	369 (100%)	0	100	100
55	QM	369/381 (97%)	368 (100%)	1 (0%)	92	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	RC	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	RD	369/381 (97%)	367 (100%)	2 (0%)	88	93
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%)	92	96
55	RM	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	SC	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	SD	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	SF	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	SH	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	SJ	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	SL	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	SM	369/381 (97%)	369 (100%)	0	100	100
55	TC	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	TD	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	TF	369/381 (97%)	369 (100%)	0	100	100
55	TH	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	TJ	369/381 (97%)	369 (100%)	0	100	100
55	TL	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	TM	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	UC	369/381 (97%)	366 (99%)	3 (1%)	81	89
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%)	88	93
55	UJ	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	UL	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	UM	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	VC	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	VD	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	VF	369/381 (97%)	369 (100%)	0	100	100
55	VH	369/381 (97%)	367 (100%)	2 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	VJ	369/381 (97%)	368 (100%)	1 (0%)	92	96
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%)	88	93
55	WD	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	WF	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	WH	369/381 (97%)	368 (100%)	1 (0%)	92	96
55	WJ	369/381 (97%)	367 (100%)	2 (0%)	88	93
55	WL	369/381 (97%)	368 (100%)	1 (0%)	92	96
All	All	136631/159445 (86%)	136293 (100%)	338 (0%)	93	97

All (338) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1E	301	ARG
2	1F	73	ARG
2	1G	147	HIS
2	1H	388	ARG
2	1H	442	ARG
3	1L	136	ARG
4	1Q	197	ARG
5	1T	405	ARG
8	1d	311	LYS
8	1d	324	ARG
11	1m	155	ASN
12	1q	118	GLN
3	1x	607	ARG
3	1z	443	LYS
13	2B	94	ARG
13	2B	249	LYS
17	2S	357	GLN
18	2V	136	GLN
19	3B	170	ARG
19	3G	124	ARG
20	3J	151	ARG
20	3J	514	LYS
20	3K	38	ASN
21	3N	383	ARG
21	3N	400	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
21	3N	413	ARG
22	3R	51	ASN
23	3W	365	ARG
23	3X	374	LYS
23	3X	534	ARG
23	3Z	178	GLN
24	4B	26	MET
24	4B	462	ARG
24	4C	349	ASN
26	4J	146	LYS
27	4Q	159	LYS
28	4U	63	ARG
30	5B	115	LYS
30	5B	224	MET
7	5I	2	ASN
7	5K	73	ARG
7	5L	202	ASN
31	6A	13	ARG
31	6B	27	LYS
31	6E	194	GLN
32	6I	67	LYS
35	6U	232	ARG
35	6V	233	ARG
35	6V	293	ARG
36	7A	532	LYS
36	7A	611	LYS
36	7B	210	ARG
36	7B	385	ARG
36	7C	9	ASN
36	7C	279	ARG
37	7G	375	MET
37	7H	17	ARG
37	7H	72	LYS
37	7H	375	MET
37	7I	211	LYS
37	7I	576	ASN
37	7I	640	LYS
38	7M	131	ARG
40	7U	109	ARG
40	7V	65	ARG
42	8A	26	ARG
43	8F	436	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	8R	189	ARG
45	8R	398	ASN
45	8S	189	ARG
45	8T	277	LYS
46	8Z	101	LYS
49	9G	96	ASN
30	9Y	155	ARG
30	9Y	224	MET
55	AC	2	ARG
55	AC	347	ASN
55	AD	2	ARG
54	AE	84	ARG
55	AF	298	ASN
55	AJ	262	ARG
55	AJ	306	ARG
54	AK	2	ARG
54	AK	308	ARG
55	AL	298	ASN
55	AL	306	ARG
54	AM	308	ARG
54	BA	2	ARG
54	BA	339	ARG
55	BC	306	ARG
55	BD	2	ARG
55	BD	347	ASN
54	BE	2	ARG
54	BE	373	ARG
55	BF	1	MET
55	BF	2	ARG
55	BF	174	LYS
54	BG	2	ARG
54	BG	243	ARG
55	BH	306	ARG
55	BJ	2	ARG
54	BK	243	ARG
55	BL	247	ASN
54	BM	2	ARG
54	BM	258	ASN
55	CD	2	ARG
54	CE	215	ARG
54	CE	339	ARG
54	CG	300	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	CG	309	HIS
55	CL	195	ASN
54	CM	2	ARG
54	DB	101	ASN
54	DB	373	ARG
54	DE	101	ASN
54	DE	128	GLN
54	DG	233	GLN
54	DG	300	ASN
54	DI	40	LYS
55	DJ	298	ASN
54	DK	339	ARG
55	DL	190	HIS
55	ED	334	GLN
55	EF	336	LYS
55	EJ	306	ARG
54	EK	2	ARG
54	EK	35	GLN
55	EL	324	LYS
55	EM	247	ASN
55	EM	306	ARG
54	FA	128	GLN
55	FC	195	ASN
55	FC	247	ASN
55	FD	1	MET
55	FD	2	ARG
54	FE	2	ARG
54	FE	112	LYS
55	FF	2	ARG
54	FG	326	LYS
55	FL	406	MET
54	GA	18	ASN
54	GE	2	ARG
55	GF	122	LYS
54	GG	2	ARG
55	GH	204	ASN
54	GI	2	ARG
55	GM	2	ARG
55	GM	347	ASN
55	HC	2	ARG
55	HC	306	ARG
55	HD	2	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	HD	100	ASN
55	HD	204	ASN
54	HE	133	GLN
55	HF	306	ARG
54	HG	2	ARG
54	HG	50	ASN
54	HG	221	ARG
55	HH	2	ARG
55	HJ	306	ARG
54	HK	308	ARG
55	HL	2	ARG
55	HL	190	HIS
54	IA	2	ARG
55	ID	2	ARG
55	IF	121	ARG
55	IJ	121	ARG
54	IK	133	GLN
54	IM	18	ASN
54	IM	243	ARG
54	IM	308	ARG
54	JB	2	ARG
55	JC	2	ARG
55	JC	347	ASN
55	JD	162	ARG
55	JD	204	ASN
55	JF	121	ARG
54	JG	308	ARG
55	JH	347	ASN
54	JI	50	ASN
55	JJ	347	ASN
55	JL	324	LYS
54	KA	2	ARG
54	KB	2	ARG
54	KB	221	ARG
54	KG	2	ARG
54	KG	373	ARG
55	KH	2	ARG
54	KI	2	ARG
55	KJ	2	ARG
54	KK	308	ARG
55	KM	347	ASN
54	LA	2	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	LA	79	ARG
54	LB	308	ARG
55	LD	306	ARG
54	LE	308	ARG
54	LE	373	ARG
55	LF	347	ASN
54	LG	308	ARG
54	LI	326	LYS
54	LI	422	ARG
55	LJ	291	GLN
55	LL	298	ASN
55	LL	306	ARG
54	MA	326	LYS
54	MB	112	LYS
55	MD	347	ASN
54	ME	2	ARG
54	ME	308	ARG
55	MF	336	LYS
54	MG	2	ARG
54	MI	2	ARG
54	MK	243	ARG
54	MK	373	ARG
54	ML	221	ARG
55	MM	321	MET
54	NB	356	ASN
55	NC	83	GLN
55	NC	307	HIS
55	NC	347	ASN
55	NF	2	ARG
55	NH	306	ARG
54	NI	40	LYS
55	NJ	282	ARG
55	NJ	321	MET
55	NK	195	ASN
55	NK	347	ASN
55	NM	282	ARG
54	OB	308	ARG
54	OB	370	LYS
55	OC	329	GLN
55	OD	347	ASN
54	OE	2	ARG
55	OF	190	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	OG	18	ASN
54	OG	221	ARG
55	OH	204	ASN
55	OH	347	ASN
54	OI	372	GLN
55	OJ	2	ARG
54	OL	2	ARG
55	OM	2	ARG
54	PA	326	LYS
55	PC	347	ASN
55	PD	347	ASN
55	PF	195	ASN
54	PG	2	ARG
55	PH	2	ARG
54	PK	285	GLN
55	PM	2	ARG
54	QA	2	ARG
55	QC	2	ARG
55	QC	337	ASN
55	QC	347	ASN
54	QE	102	ASN
54	QG	2	ARG
54	QG	40	LYS
54	QG	339	ARG
54	QG	373	ARG
55	QH	195	ASN
54	QI	2	ARG
54	QI	84	ARG
54	QK	258	ASN
54	QL	2	ARG
55	QM	2	ARG
54	RB	79	ARG
55	RC	337	ASN
55	RD	121	ARG
55	RD	390	ARG
54	RE	40	LYS
54	RE	308	ARG
54	RI	339	ARG
55	RJ	2	ARG
54	RK	2	ARG
55	RM	337	ASN
55	SC	2	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	SD	279	GLN
55	SD	347	ASN
55	SF	282	ARG
55	SH	347	ASN
54	SI	112	LYS
55	SJ	2	ARG
55	SL	362	LYS
54	TA	358	GLN
54	TB	2	ARG
54	TB	326	LYS
55	TC	2	ARG
55	TD	2	ARG
55	TD	227	HIS
54	TE	2	ARG
54	TG	2	ARG
55	TH	2	ARG
55	TH	324	LYS
54	TK	163	LYS
55	TL	121	ARG
55	TL	362	LYS
55	TM	103	LYS
54	UA	401	LYS
54	UB	308	ARG
55	UC	2	ARG
55	UC	174	LYS
55	UC	347	ASN
54	UE	18	ASN
54	UE	215	ARG
55	UH	2	ARG
55	UH	318	ARG
55	UJ	131	GLN
55	UJ	306	ARG
55	UL	324	LYS
55	UM	2	ARG
54	VA	373	ARG
55	VC	2	ARG
55	VD	2	ARG
55	VD	190	HIS
55	VH	190	HIS
55	VH	306	ARG
54	VI	221	ARG
54	VI	373	ARG

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Mol	Chain	Res	Type
55	VJ	213	ARG
54	VK	206	ASN
54	VK	300	ASN
54	WA	308	ARG
54	WB	308	ARG
55	WC	298	ASN
55	WC	306	ARG
55	WD	298	ASN
54	WE	163	LYS
54	WE	308	ARG
55	WF	306	ARG
54	WG	2	ARG
54	WG	308	ARG
55	WH	2	ARG
54	WI	308	ARG
55	WJ	306	ARG
55	WJ	347	ASN
54	WK	308	ARG
55	WL	306	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (385) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	14	GLN
1	1B	180	GLN
2	1E	296	GLN
3	1M	139	GLN
5	1T	398	HIS
5	1T	416	ASN
5	1T	422	ASN
5	1V	230	GLN
11	1m	155	ASN
12	1r	3	GLN
3	1y	478	GLN
13	2A	72	GLN
13	2A	250	HIS
14	2G	28	ASN
15	2K	9	GLN
15	2K	12	GLN
15	2L	9	GLN
18	2V	206	GLN
19	3A	131	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
19	3B	159	ASN
19	3C	109	GLN
19	3F	131	GLN
21	3N	322	GLN
21	3O	143	GLN
23	3W	388	ASN
23	3W	448	GLN
23	3X	432	GLN
23	3Z	178	GLN
24	4C	349	ASN
25	4F	454	GLN
26	4K	355	HIS
27	4N	168	ASN
27	4O	80	ASN
7	5E	39	ASN
7	5F	248	GLN
7	5H	240	GLN
7	5K	45	GLN
7	5N	136	ASN
31	6C	194	GLN
31	6E	171	GLN
34	6Q	51	GLN
36	7B	555	GLN
36	7B	556	HIS
36	7D	171	GLN
36	7D	555	GLN
36	7D	556	HIS
37	7G	261	GLN
37	7G	353	GLN
37	7I	261	GLN
39	7Q	148	GLN
43	8F	400	GLN
43	8F	436	ASN
43	8G	178	GLN
44	8M	207	ASN
45	8R	398	ASN
45	8S	389	GLN
47	9A	201	ASN
54	AA	11	GLN
55	AC	8	GLN
55	AC	134	GLN
55	AD	37	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	AD	347	ASN
54	AE	101	ASN
54	AE	206	ASN
55	AF	256	ASN
55	AF	298	ASN
55	AF	334	GLN
54	AG	11	GLN
55	AH	6	HIS
55	AH	134	GLN
55	AH	190	HIS
55	AH	347	ASN
55	AL	334	GLN
54	AM	35	GLN
55	BC	131	GLN
54	BG	91	GLN
54	BG	285	GLN
54	BI	8	HIS
55	BJ	6	HIS
55	BJ	134	GLN
54	BM	329	ASN
54	CB	85	GLN
54	CB	128	GLN
55	CC	165	ASN
55	CD	347	ASN
55	CF	134	GLN
54	CG	285	GLN
55	CH	204	ASN
55	CJ	8	GLN
55	CL	14	ASN
55	CL	134	GLN
55	DC	14	ASN
55	DC	165	ASN
55	DD	134	GLN
55	DD	256	ASN
54	DE	128	GLN
54	DI	11	GLN
55	DJ	11	GLN
55	DJ	14	ASN
55	DL	14	ASN
55	DL	204	ASN
54	DM	101	ASN
54	EA	358	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	EA	372	GLN
55	EB	99	ASN
54	EE	256	GLN
55	EF	6	HIS
55	EF	134	GLN
55	EF	195	ASN
54	EG	91	GLN
54	EG	101	ASN
55	EJ	8	GLN
55	EJ	14	ASN
54	FB	258	ASN
55	FF	375	GLN
55	FF	426	GLN
54	FG	293	ASN
54	FI	11	GLN
54	FI	206	ASN
54	FI	216	ASN
55	FJ	94	GLN
55	FJ	334	GLN
55	FJ	347	ASN
55	FJ	348	ASN
55	FL	8	GLN
55	FL	99	ASN
55	FL	137	HIS
55	FL	375	GLN
55	FL	423	GLN
55	FL	426	GLN
55	FM	6	HIS
55	FM	134	GLN
54	GA	8	HIS
54	GA	18	ASN
54	GA	258	ASN
55	GC	48	ASN
55	GC	256	ASN
55	GD	334	GLN
55	GF	14	ASN
55	GF	99	ASN
55	GF	256	ASN
55	GH	99	ASN
55	GJ	204	ASN
54	GK	101	ASN
55	GL	134	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	GM	15	GLN
55	GM	204	ASN
55	GM	348	ASN
54	HB	11	GLN
55	HD	100	ASN
54	HE	128	GLN
54	HE	283	HIS
55	HF	298	ASN
54	HI	101	ASN
55	HL	375	GLN
55	HL	423	GLN
55	HL	426	GLN
55	HM	292	GLN
55	HM	298	ASN
54	IA	258	ASN
54	IA	329	ASN
54	IB	11	GLN
54	IB	285	GLN
55	IC	99	ASN
55	IC	337	ASN
55	ID	298	ASN
55	IJ	100	ASN
54	IK	133	GLN
55	IL	165	ASN
55	IL	329	GLN
54	IM	88	HIS
54	IM	356	ASN
54	JA	101	ASN
54	JA	128	GLN
54	JA	206	ASN
54	JA	329	ASN
54	JB	11	GLN
54	JB	101	ASN
54	JB	206	ASN
54	JB	356	ASN
55	JD	334	GLN
54	JE	11	GLN
54	JE	15	GLN
55	JF	14	ASN
55	JF	247	ASN
54	JG	11	GLN
55	JH	99	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	JH	298	ASN
55	JL	137	HIS
55	JL	226	ASN
55	JM	6	HIS
55	JM	134	GLN
55	JM	204	ASN
55	JM	256	ASN
54	KA	50	ASN
54	KA	285	GLN
54	KB	101	ASN
55	KD	334	GLN
54	KG	206	ASN
55	KJ	100	ASN
55	KL	131	GLN
55	KM	184	ASN
54	LB	101	ASN
55	LC	134	GLN
55	LD	334	GLN
54	LG	35	GLN
55	LH	347	ASN
54	LI	35	GLN
54	LI	226	ASN
55	LJ	8	GLN
55	LJ	134	GLN
55	LJ	414	ASN
54	LK	197	HIS
54	MA	91	GLN
54	MB	206	ASN
55	MC	204	ASN
55	MF	190	HIS
55	MF	334	GLN
55	MJ	8	GLN
55	MJ	134	GLN
55	MJ	256	ASN
55	MJ	347	ASN
54	MK	101	ASN
54	MK	329	ASN
55	MM	337	ASN
54	NA	258	ASN
54	NB	128	GLN
55	NC	6	HIS
55	NC	347	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	ND	94	GLN
55	ND	256	ASN
54	NE	101	ASN
54	NE	176	GLN
55	NF	334	GLN
55	NH	6	HIS
55	NH	134	GLN
55	NH	298	ASN
55	NH	334	GLN
54	NI	356	ASN
55	NJ	165	ASN
55	NK	334	GLN
54	NL	101	ASN
54	OA	11	GLN
55	OC	329	GLN
55	OD	337	ASN
55	OD	347	ASN
54	OE	258	ASN
55	OF	99	ASN
55	OF	256	ASN
54	OG	206	ASN
55	OH	8	GLN
55	OH	204	ASN
55	OH	256	ASN
55	OJ	99	ASN
55	OJ	347	ASN
54	OK	356	ASN
55	OM	375	GLN
55	OM	426	GLN
55	PC	347	ASN
55	PD	89	ASN
55	PD	131	GLN
55	PD	256	ASN
54	PE	101	ASN
54	PE	197	HIS
55	PH	99	ASN
54	PK	101	ASN
54	PK	300	ASN
55	PM	14	ASN
55	PM	131	GLN
55	PM	134	GLN
55	PM	334	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	QA	128	GLN
55	QD	11	GLN
54	QE	11	GLN
54	QE	102	ASN
54	QE	258	ASN
55	QF	100	ASN
55	QF	347	ASN
54	QG	372	GLN
55	QH	337	ASN
54	QI	133	GLN
55	QJ	191	GLN
55	QJ	298	ASN
55	QJ	334	GLN
55	QJ	347	ASN
54	QK	128	GLN
54	QK	133	GLN
55	QM	11	GLN
54	RA	11	GLN
54	RA	139	HIS
55	RC	256	ASN
55	RC	334	GLN
55	RC	426	GLN
55	RD	131	GLN
55	RD	396	HIS
54	RE	15	GLN
54	RE	356	ASN
55	RF	94	GLN
55	RF	334	GLN
55	RH	37	HIS
55	RH	256	ASN
54	RI	101	ASN
55	RJ	100	ASN
55	RJ	227	HIS
55	RJ	334	GLN
54	RL	28	HIS
55	RM	99	ASN
55	RM	247	ASN
54	SA	35	GLN
54	SB	11	GLN
55	SC	426	GLN
55	SD	184	ASN
55	SD	256	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
54	SE	101	ASN
54	SE	102	ASN
55	SF	256	ASN
55	SF	291	GLN
54	SG	11	GLN
54	SG	256	GLN
54	SG	293	ASN
55	SH	347	ASN
54	SI	11	GLN
55	SJ	298	ASN
55	SJ	334	GLN
54	SK	258	ASN
55	SL	8	GLN
55	SL	204	ASN
55	SL	292	GLN
55	SL	298	ASN
54	TA	139	HIS
54	TA	226	ASN
54	TA	293	ASN
54	TB	226	ASN
54	TB	258	ASN
55	TC	292	GLN
55	TC	334	GLN
55	TD	334	GLN
54	TE	206	ASN
55	TH	8	GLN
55	TH	256	ASN
55	TH	334	GLN
54	TI	35	GLN
55	TJ	99	ASN
54	TK	8	HIS
54	TK	139	HIS
54	TK	293	ASN
55	TL	396	HIS
55	TM	256	ASN
55	TM	416	ASN
54	UA	8	HIS
54	UA	372	GLN
55	UC	334	GLN
55	UD	416	ASN
54	UE	8	HIS
54	UE	128	GLN

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Mol	Chain	Res	Type
54	UG	293	ASN
55	UH	14	ASN
54	UI	372	GLN
55	UJ	279	GLN
55	UJ	416	ASN
55	UM	329	GLN
54	VA	256	GLN
55	VC	134	GLN
55	VD	337	ASN
54	VE	101	ASN
54	VG	28	HIS
54	VG	101	ASN
55	VH	347	ASN
54	VK	101	ASN
55	VL	134	GLN
55	VL	226	ASN
55	VM	279	GLN
54	WA	285	GLN
55	WD	8	GLN
55	WD	165	ASN
54	WG	15	GLN
55	WH	94	GLN
55	WH	334	GLN
55	WH	426	GLN
54	WI	102	ASN
55	WJ	256	ASN
54	WK	206	ASN
54	WK	285	GLN
55	WL	8	GLN
55	WL	14	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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	II	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.60	7 (21%)
56	GTP	LI	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.64	7 (21%)
58	GDP	TF	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
58	GDP	EL	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.33	4 (13%)
56	GTP	FG	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.58	7 (21%)
56	GTP	GE	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.67	7 (21%)
58	GDP	QJ	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	5 (16%)
56	GTP	DE	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.62	7 (21%)
58	GDP	WH	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.31	4 (13%)
58	GDP	QC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
58	GDP	CH	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.38	4 (13%)
58	GDP	VM	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
56	GTP	QB	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.66	7 (21%)
56	GTP	VB	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.63	7 (21%)
56	GTP	IG	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.58	7 (21%)
58	GDP	TD	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.39	5 (16%)
56	GTP	UA	501	57	26,34,34	1.13	2 (7%)	32,54,54	1.67	7 (21%)
56	GTP	RA	501	57	26,34,34	1.17	2 (7%)	32,54,54	1.64	7 (21%)
56	GTP	NB	501	57	26,34,34	1.13	2 (7%)	32,54,54	1.58	7 (21%)
58	GDP	FJ	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
56	GTP	AA	501	57	26,34,34	1.13	2 (7%)	32,54,54	1.59	7 (21%)
56	GTP	TG	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.61	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	GTP	QA	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.62	7 (21%)
58	GDP	IF	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
58	GDP	JM	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
56	GTP	AI	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.70	7 (21%)
56	GTP	CK	501	-	26,34,34	1.13	2 (7%)	32,54,54	1.56	8 (25%)
58	GDP	DJ	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.34	4 (13%)
58	GDP	KH	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
58	GDP	KF	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
56	GTP	RE	501	57	26,34,34	1.19	2 (7%)	32,54,54	1.65	7 (21%)
58	GDP	VJ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
56	GTP	BI	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.61	7 (21%)
56	GTP	EI	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.63	7 (21%)
56	GTP	IE	501	57	26,34,34	1.13	2 (7%)	32,54,54	1.60	7 (21%)
56	GTP	UE	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.77	7 (21%)
58	GDP	MD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
56	GTP	BA	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.62	7 (21%)
58	GDP	EM	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	4 (13%)
56	GTP	EK	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.63	7 (21%)
58	GDP	AL	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
58	GDP	OH	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.37	4 (13%)
56	GTP	ML	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.65	7 (21%)
58	GDP	FM	502	-	24,30,30	0.96	1 (4%)	30,47,47	1.36	5 (16%)
58	GDP	ND	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
58	GDP	NH	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
56	GTP	NG	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.62	7 (21%)
56	GTP	NL	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.61	7 (21%)
58	GDP	BH	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.35	4 (13%)
58	GDP	JD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
56	GTP	VE	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.59	7 (21%)
58	GDP	PC	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.36	4 (13%)
56	GTP	FI	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.66	7 (21%)
56	GTP	HA	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.64	7 (21%)
56	GTP	PG	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.59	7 (21%)
58	GDP	EJ	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
58	GDP	UJ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	GDP	KD	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
58	GDP	SJ	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.35	4 (13%)
58	GDP	MM	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.27	4 (13%)
58	GDP	OM	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.36	5 (16%)
56	GTP	ME	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.56	7 (21%)
56	GTP	KB	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.65	7 (21%)
58	GDP	TM	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
56	GTP	KG	501	57	26,34,34	1.17	2 (7%)	32,54,54	1.68	7 (21%)
58	GDP	IC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.37	4 (13%)
56	GTP	AE	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.61	7 (21%)
56	GTP	LE	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.61	6 (18%)
56	GTP	BG	501	57	26,34,34	1.13	2 (7%)	32,54,54	1.53	8 (25%)
56	GTP	QI	501	57,54	26,34,34	1.17	2 (7%)	32,54,54	1.60	7 (21%)
58	GDP	DF	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.16	3 (10%)
58	GDP	LC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
58	GDP	LM	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	4 (13%)
56	GTP	TB	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.61	7 (21%)
56	GTP	HB	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.60	7 (21%)
58	GDP	JC	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.35	5 (16%)
56	GTP	RI	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.54	7 (21%)
58	GDP	ED	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.37	4 (13%)
58	GDP	IH	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
56	GTP	QK	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.69	7 (21%)
56	GTP	GK	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.69	7 (21%)
58	GDP	LF	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.29	4 (13%)
58	GDP	RJ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
58	GDP	VL	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.21	3 (10%)
56	GTP	JE	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.63	7 (21%)
56	GTP	LK	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.60	7 (21%)
56	GTP	NI	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.60	7 (21%)
56	GTP	OK	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.62	7 (21%)
58	GDP	RF	501	-	24,30,30	0.92	1 (4%)	30,47,47	1.21	3 (10%)
58	GDP	TH	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.33	4 (13%)
56	GTP	KE	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.66	7 (21%)
56	GTP	UK	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.65	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	GDP	VD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.41	6 (20%)
56	GTP	WG	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.64	7 (21%)
58	GDP	QD	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.30	4 (13%)
56	GTP	VI	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.62	7 (21%)
58	GDP	HD	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
56	GTP	LG	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.64	7 (21%)
56	GTP	KI	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.64	7 (21%)
56	GTP	HK	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.62	7 (21%)
56	GTP	QE	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.61	7 (21%)
58	GDP	GF	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
58	GDP	QM	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	4 (13%)
56	GTP	VK	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.62	7 (21%)
58	GDP	AF	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
58	GDP	AJ	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
56	GTP	DG	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.56	7 (21%)
56	GTP	OE	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.61	7 (21%)
58	GDP	UD	501	-	24,30,30	0.91	1 (4%)	30,47,47	1.36	4 (13%)
58	GDP	WJ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
58	GDP	QF	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.32	3 (10%)
58	GDP	WC	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
56	GTP	TE	501	57	26,34,34	1.17	2 (7%)	32,54,54	1.75	7 (21%)
56	GTP	GA	501	57	26,34,34	1.12	2 (7%)	32,54,54	1.57	6 (18%)
56	GTP	GG	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.70	6 (18%)
56	GTP	SI	501	57	26,34,34	1.17	2 (7%)	32,54,54	1.61	7 (21%)
56	GTP	OA	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.68	7 (21%)
56	GTP	QG	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.54	7 (21%)
58	GDP	SM	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
58	GDP	OD	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.33	4 (13%)
58	GDP	LL	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
58	GDP	KM	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.29	4 (13%)
56	GTP	AB	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.67	7 (21%)
56	GTP	VA	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.65	7 (21%)
56	GTP	BK	501	57	26,34,34	1.11	2 (7%)	32,54,54	1.58	8 (25%)
56	GTP	JI	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.65	7 (21%)
58	GDP	HJ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	GTP	FK	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.61	7 (21%)
56	GTP	CM	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.60	7 (21%)
56	GTP	OB	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.67	7 (21%)
56	GTP	PI	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.61	7 (21%)
58	GDP	BF	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
58	GDP	CJ	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.33	4 (13%)
58	GDP	TJ	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
58	GDP	NF	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.34	4 (13%)
56	GTP	RG	501	57	26,34,34	1.17	2 (7%)	32,54,54	1.64	7 (21%)
56	GTP	UI	501	57	26,34,34	1.13	2 (7%)	32,54,54	1.62	7 (21%)
56	GTP	NE	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.65	7 (21%)
56	GTP	SK	501	57	26,34,34	1.17	2 (7%)	32,54,54	1.61	7 (21%)
56	GTP	QL	501	57,54	26,34,34	1.12	2 (7%)	32,54,54	1.57	7 (21%)
56	GTP	OG	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.65	7 (21%)
58	GDP	QH	501	55	24,30,30	0.99	1 (4%)	30,47,47	1.29	4 (13%)
58	GDP	UC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
58	GDP	LJ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
56	GTP	KK	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.58	7 (21%)
56	GTP	WB	501	57	26,34,34	1.13	2 (7%)	32,54,54	1.60	7 (21%)
58	GDP	BD	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.30	5 (16%)
58	GDP	FH	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
58	GDP	IJ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.34	4 (13%)
58	GDP	RH	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.38	4 (13%)
56	GTP	MG	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.57	7 (21%)
56	GTP	JA	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.64	7 (21%)
58	GDP	SH	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
58	GDP	CF	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.35	4 (13%)
58	GDP	IL	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
58	GDP	MH	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.34	4 (13%)
56	GTP	LA	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.61	7 (21%)
56	GTP	MB	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.57	7 (21%)
56	GTP	IK	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.60	7 (21%)
56	GTP	WE	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.62	7 (21%)
58	GDP	CD	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	4 (13%)
58	GDP	GH	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.37	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	GTP	JK	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.59	7 (21%)
58	GDP	NK	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
56	GTP	DK	501	57	26,34,34	1.11	2 (7%)	32,54,54	1.54	7 (21%)
56	GTP	TI	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.61	7 (21%)
58	GDP	GJ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
58	GDP	EF	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.38	4 (13%)
56	GTP	BE	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.74	7 (21%)
56	GTP	KA	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.66	7 (21%)
58	GDP	JL	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.15	2 (6%)
58	GDP	KC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.37	4 (13%)
58	GDP	GM	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
58	GDP	KJ	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
56	GTP	BB	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.65	7 (21%)
56	GTP	NA	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.67	7 (21%)
58	GDP	BJ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
58	GDP	DC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
58	GDP	HM	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
58	GDP	MF	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
56	GTP	FB	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.68	7 (21%)
58	GDP	SL	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.33	4 (13%)
58	GDP	EB	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.30	4 (13%)
58	GDP	BC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
58	GDP	PM	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
56	GTP	WA	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.67	7 (21%)
56	GTP	JG	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.63	7 (21%)
56	GTP	UG	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.60	7 (21%)
56	GTP	CB	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.63	7 (21%)
56	GTP	RL	501	57,54	26,34,34	1.12	2 (7%)	32,54,54	1.60	7 (21%)
56	GTP	PB	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.70	7 (21%)
58	GDP	UH	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.33	4 (13%)
56	GTP	MA	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.66	7 (21%)
56	GTP	GB	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.68	7 (21%)
56	GTP	PE	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.64	7 (21%)
58	GDP	FF	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.39	4 (13%)
58	GDP	DH	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.33	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	GDP	OC	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
56	GTP	HE	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.63	7 (21%)
58	GDP	BL	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.38	4 (13%)
56	GTP	EG	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.65	7 (21%)
56	GTP	CG	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.58	7 (21%)
58	GDP	KL	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
58	GDP	NJ	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.32	4 (13%)
56	GTP	IB	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.67	7 (21%)
56	GTP	TA	501	57	26,34,34	1.17	2 (7%)	32,54,54	1.58	7 (21%)
56	GTP	RK	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.64	7 (21%)
58	GDP	SF	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
58	GDP	HC	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.26	3 (10%)
56	GTP	IA	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.64	7 (21%)
56	GTP	CE	501	57	26,34,34	1.13	2 (7%)	32,54,54	1.67	6 (18%)
56	GTP	AK	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.56	7 (21%)
58	GDP	TC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
58	GDP	TL	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
58	GDP	MC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
56	GTP	DI	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.63	7 (21%)
56	GTP	MI	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.61	7 (21%)
56	GTP	MK	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.57	6 (18%)
58	GDP	NM	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
58	GDP	JF	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.35	5 (16%)
56	GTP	PL	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.63	7 (21%)
58	GDP	LD	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.31	4 (13%)
58	GDP	FD	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	4 (13%)
58	GDP	FL	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.35	4 (13%)
58	GDP	HF	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
58	GDP	WL	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	5 (16%)
56	GTP	OL	501	57	26,34,34	1.13	2 (7%)	32,54,54	1.59	7 (21%)
58	GDP	RM	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.46	5 (16%)
58	GDP	AC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
56	GTP	RB	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.54	7 (21%)
58	GDP	HH	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
56	GTP	WI	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.58	7 (21%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	GTP	PK	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.64	7 (21%)
58	GDP	PD	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.28	4 (13%)
56	GTP	UB	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.65	7 (21%)
58	GDP	JJ	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
56	GTP	TK	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.67	7 (21%)
56	GTP	SE	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.61	7 (21%)
58	GDP	RD	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.31	4 (13%)
56	GTP	BM	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.57	8 (25%)
56	GTP	DB	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.61	7 (21%)
58	GDP	SD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.31	4 (13%)
58	GDP	DL	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.23	3 (10%)
58	GDP	GD	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)
56	GTP	FM	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.69	7 (21%)
58	GDP	UL	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.21	5 (16%)
58	GDP	HL	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.32	4 (13%)
56	GTP	DM	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.62	7 (21%)
56	GTP	CI	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.63	7 (21%)
56	GTP	CA	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.67	6 (18%)
58	GDP	MJ	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.37	4 (13%)
56	GTP	HI	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.60	7 (21%)
56	GTP	OI	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.63	7 (21%)
58	GDP	RC	501	-	24,30,30	0.97	1 (4%)	30,47,47	1.32	4 (13%)
56	GTP	LB	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.62	7 (21%)
56	GTP	AG	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.65	7 (21%)
56	GTP	AM	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.59	7 (21%)
56	GTP	IM	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.58	7 (21%)
56	GTP	DA	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.63	7 (21%)
56	GTP	EC	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.62	7 (21%)
58	GDP	DD	501	-	24,30,30	0.98	1 (4%)	30,47,47	1.33	4 (13%)
58	GDP	FC	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.38	4 (13%)
56	GTP	EA	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.65	7 (21%)
56	GTP	JB	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.66	7 (21%)
58	GDP	PF	501	55	24,30,30	0.85	0	30,47,47	1.67	7 (23%)
58	GDP	SC	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.36	4 (13%)
58	GDP	LH	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.35	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
56	GTP	PA	501	57	26,34,34	1.23	2 (7%)	32,54,54	1.60	7 (21%)
56	GTP	HG	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.63	7 (21%)
56	GTP	WK	501	57	26,34,34	1.14	2 (7%)	32,54,54	1.63	7 (21%)
58	GDP	AD	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.30	4 (13%)
58	GDP	AH	501	-	24,30,30	0.93	1 (4%)	30,47,47	1.34	4 (13%)
58	GDP	UF	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.38	4 (13%)
58	GDP	VC	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
58	GDP	OJ	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
58	GDP	PJ	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.35	4 (13%)
58	GDP	GC	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
58	GDP	WF	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.36	4 (13%)
58	GDP	GL	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.30	4 (13%)
56	GTP	FE	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.64	7 (21%)
58	GDP	EH	501	-	24,30,30	0.96	1 (4%)	30,47,47	1.37	5 (16%)
58	GDP	UM	501	55	24,30,30	0.93	1 (4%)	30,47,47	1.35	4 (13%)
58	GDP	PH	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.33	4 (13%)
56	GTP	SA	502	57	26,34,34	1.15	2 (7%)	32,54,54	1.58	7 (21%)
58	GDP	JH	501	-	24,30,30	0.95	1 (4%)	30,47,47	1.30	4 (13%)
58	GDP	NC	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.30	4 (13%)
58	GDP	VF	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
58	GDP	WD	501	-	24,30,30	0.99	1 (4%)	30,47,47	1.34	4 (13%)
56	GTP	SB	501	57	26,34,34	1.17	2 (7%)	32,54,54	1.66	7 (21%)
58	GDP	VH	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.39	4 (13%)
56	GTP	SG	501	57	26,34,34	1.16	2 (7%)	32,54,54	1.60	7 (21%)
56	GTP	VG	501	57	26,34,34	1.15	2 (7%)	32,54,54	1.65	7 (21%)
58	GDP	CL	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
56	GTP	EE	501	57	26,34,34	1.18	2 (7%)	32,54,54	1.69	7 (21%)
58	GDP	OF	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.32	4 (13%)
58	GDP	CC	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.36	4 (13%)
58	GDP	ID	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.34	4 (13%)
56	GTP	GI	501	57	26,34,34	1.13	2 (7%)	32,54,54	1.58	7 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	II	501	57	-	8/18/38/38	0/3/3/3
56	GTP	LI	501	57	-	2/18/38/38	0/3/3/3
58	GDP	TF	501	-	-	1/12/32/32	0/3/3/3
58	GDP	EL	501	-	-	1/12/32/32	0/3/3/3
56	GTP	FG	501	57	-	5/18/38/38	0/3/3/3
56	GTP	GE	501	57	-	2/18/38/38	0/3/3/3
58	GDP	QJ	501	-	-	1/12/32/32	0/3/3/3
56	GTP	DE	501	57	-	3/18/38/38	0/3/3/3
58	GDP	WH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	QC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	CH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	VM	501	-	-	3/12/32/32	0/3/3/3
56	GTP	QB	501	57	-	2/18/38/38	0/3/3/3
56	GTP	VB	501	57	-	6/18/38/38	0/3/3/3
56	GTP	IG	501	57	-	6/18/38/38	0/3/3/3
58	GDP	TD	501	-	-	3/12/32/32	0/3/3/3
56	GTP	UA	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	NB	501	57	-	10/18/38/38	0/3/3/3
58	GDP	FJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	AA	501	57	-	7/18/38/38	0/3/3/3
56	GTP	TG	501	57	-	6/18/38/38	0/3/3/3
56	GTP	QA	501	57	-	6/18/38/38	0/3/3/3
58	GDP	IF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	JM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	AI	501	57	-	3/18/38/38	0/3/3/3
56	GTP	CK	501	-	-	7/18/38/38	0/3/3/3
58	GDP	DJ	501	-	-	4/12/32/32	0/3/3/3
58	GDP	KH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	KF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	RE	501	57	-	3/18/38/38	0/3/3/3
58	GDP	VJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	BI	501	57	-	7/18/38/38	0/3/3/3
56	GTP	EI	501	57	-	2/18/38/38	0/3/3/3
56	GTP	IE	501	57	-	6/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	UE	501	57	-	4/18/38/38	0/3/3/3
58	GDP	MD	501	-	-	1/12/32/32	0/3/3/3
56	GTP	BA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	EM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	EK	501	57	-	2/18/38/38	0/3/3/3
58	GDP	AL	501	-	-	2/12/32/32	0/3/3/3
58	GDP	OH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	ML	501	57	-	3/18/38/38	0/3/3/3
58	GDP	FM	502	-	-	1/12/32/32	0/3/3/3
58	GDP	ND	501	-	-	2/12/32/32	0/3/3/3
58	GDP	NH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	NG	501	57	-	6/18/38/38	0/3/3/3
56	GTP	NL	501	57	-	4/18/38/38	0/3/3/3
58	GDP	BH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	JD	501	-	-	2/12/32/32	0/3/3/3
56	GTP	VE	501	57	-	4/18/38/38	0/3/3/3
58	GDP	PC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	FI	501	57	-	3/18/38/38	0/3/3/3
56	GTP	HA	501	57	-	4/18/38/38	0/3/3/3
56	GTP	PG	501	57	-	7/18/38/38	0/3/3/3
58	GDP	EJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	UJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	KD	501	-	-	2/12/32/32	0/3/3/3
58	GDP	SJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	MM	501	-	-	2/12/32/32	0/3/3/3
58	GDP	OM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	ME	501	57	-	6/18/38/38	0/3/3/3
56	GTP	KB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	TM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	KG	501	57	-	3/18/38/38	0/3/3/3
58	GDP	IC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	AE	501	57	-	6/18/38/38	0/3/3/3
56	GTP	LE	501	57	-	3/18/38/38	0/3/3/3
56	GTP	BG	501	57	-	8/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	QI	501	57,54	-	3/18/38/38	0/3/3/3
58	GDP	DF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	LC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	LM	501	-	-	1/12/32/32	0/3/3/3
56	GTP	TB	501	57	-	8/18/38/38	0/3/3/3
56	GTP	HB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	JC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	RI	501	57	-	4/18/38/38	0/3/3/3
58	GDP	ED	501	-	-	2/12/32/32	0/3/3/3
58	GDP	IH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	QK	501	57	-	3/18/38/38	0/3/3/3
56	GTP	GK	501	57	-	4/18/38/38	0/3/3/3
58	GDP	LF	501	-	-	3/12/32/32	0/3/3/3
58	GDP	RJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	VL	501	-	-	5/12/32/32	0/3/3/3
56	GTP	JE	501	57	-	3/18/38/38	0/3/3/3
56	GTP	LK	501	57	-	6/18/38/38	0/3/3/3
56	GTP	NI	501	57	-	6/18/38/38	0/3/3/3
56	GTP	OK	501	57	-	6/18/38/38	0/3/3/3
58	GDP	RF	501	-	-	5/12/32/32	0/3/3/3
58	GDP	TH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	KE	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	VD	501	-	-	2/12/32/32	0/3/3/3
56	GTP	WG	501	57	-	3/18/38/38	0/3/3/3
58	GDP	QD	501	-	-	2/12/32/32	0/3/3/3
56	GTP	VI	501	57	-	3/18/38/38	0/3/3/3
58	GDP	HD	501	-	-	2/12/32/32	0/3/3/3
56	GTP	LG	501	57	-	3/18/38/38	0/3/3/3
56	GTP	KI	501	57	-	2/18/38/38	0/3/3/3
56	GTP	HK	501	57	-	10/18/38/38	0/3/3/3
56	GTP	QE	501	57	-	3/18/38/38	0/3/3/3
58	GDP	GF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	QM	501	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	VK	501	57	-	7/18/38/38	0/3/3/3
58	GDP	AF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	AJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	DG	501	57	-	5/18/38/38	0/3/3/3
56	GTP	OE	501	57	-	7/18/38/38	0/3/3/3
58	GDP	UD	501	-	-	3/12/32/32	0/3/3/3
58	GDP	WJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	QF	501	-	-	3/12/32/32	0/3/3/3
58	GDP	WC	501	-	-	1/12/32/32	0/3/3/3
56	GTP	TE	501	57	-	4/18/38/38	0/3/3/3
56	GTP	GA	501	57	-	6/18/38/38	0/3/3/3
56	GTP	GG	501	57	-	3/18/38/38	0/3/3/3
56	GTP	SI	501	57	-	2/18/38/38	0/3/3/3
56	GTP	OA	501	57	-	3/18/38/38	0/3/3/3
56	GTP	QG	501	57	-	6/18/38/38	0/3/3/3
58	GDP	SM	501	-	-	2/12/32/32	0/3/3/3
58	GDP	OD	501	-	-	4/12/32/32	0/3/3/3
58	GDP	LL	501	-	-	2/12/32/32	0/3/3/3
58	GDP	KM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	AB	501	57	-	3/18/38/38	0/3/3/3
56	GTP	VA	501	57	-	3/18/38/38	0/3/3/3
56	GTP	BK	501	57	-	5/18/38/38	0/3/3/3
56	GTP	JI	501	57	-	2/18/38/38	0/3/3/3
58	GDP	HJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	FK	501	57	-	7/18/38/38	0/3/3/3
56	GTP	CM	501	57	-	4/18/38/38	0/3/3/3
56	GTP	OB	501	57	-	3/18/38/38	0/3/3/3
56	GTP	PI	501	57	-	3/18/38/38	0/3/3/3
58	GDP	BF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	CJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	TJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	NF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	RG	501	57	-	3/18/38/38	0/3/3/3
56	GTP	UI	501	57	-	3/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	GTP	NE	501	57	-	3/18/38/38	0/3/3/3
56	GTP	SK	501	57	-	3/18/38/38	0/3/3/3
56	GTP	QL	501	57,54	-	8/18/38/38	0/3/3/3
56	GTP	OG	501	57	-	3/18/38/38	0/3/3/3
58	GDP	QH	501	55	-	5/12/32/32	0/3/3/3
58	GDP	UC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	LJ	501	-	-	4/12/32/32	0/3/3/3
56	GTP	KK	501	57	-	4/18/38/38	0/3/3/3
56	GTP	WB	501	57	-	7/18/38/38	0/3/3/3
58	GDP	BD	501	-	-	3/12/32/32	0/3/3/3
58	GDP	FH	501	-	-	3/12/32/32	0/3/3/3
58	GDP	IJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	RH	501	-	-	1/12/32/32	0/3/3/3
56	GTP	MG	501	57	-	3/18/38/38	0/3/3/3
56	GTP	JA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	SH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	CF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	IL	501	-	-	2/12/32/32	0/3/3/3
58	GDP	MH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	LA	501	57	-	6/18/38/38	0/3/3/3
56	GTP	MB	501	57	-	5/18/38/38	0/3/3/3
56	GTP	IK	501	57	-	4/18/38/38	0/3/3/3
56	GTP	WE	501	57	-	4/18/38/38	0/3/3/3
58	GDP	CD	501	-	-	3/12/32/32	0/3/3/3
58	GDP	GH	501	-	-	1/12/32/32	0/3/3/3
56	GTP	JK	501	57	-	7/18/38/38	0/3/3/3
58	GDP	NK	501	-	-	1/12/32/32	0/3/3/3
56	GTP	DK	501	57	-	4/18/38/38	0/3/3/3
56	GTP	TI	501	57	-	7/18/38/38	0/3/3/3
58	GDP	GJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	EF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	BE	501	57	-	3/18/38/38	0/3/3/3
56	GTP	KA	501	57	-	2/18/38/38	0/3/3/3
58	GDP	JL	501	-	-	4/12/32/32	0/3/3/3
58	GDP	KC	501	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	GM	501	-	-	2/12/32/32	0/3/3/3
58	GDP	KJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	BB	501	57	-	4/18/38/38	0/3/3/3
56	GTP	NA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	BJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	DC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	HM	501	-	-	1/12/32/32	0/3/3/3
58	GDP	MF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	FB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	SL	501	-	-	2/12/32/32	0/3/3/3
58	GDP	EB	501	-	-	1/12/32/32	0/3/3/3
58	GDP	BC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	PM	501	-	-	2/12/32/32	0/3/3/3
56	GTP	WA	501	57	-	2/18/38/38	0/3/3/3
56	GTP	JG	501	57	-	3/18/38/38	0/3/3/3
56	GTP	UG	501	57	-	6/18/38/38	0/3/3/3
56	GTP	CB	501	57	-	2/18/38/38	0/3/3/3
56	GTP	RL	501	57,54	-	8/18/38/38	0/3/3/3
56	GTP	PB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	UH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	MA	501	57	-	3/18/38/38	0/3/3/3
56	GTP	GB	501	57	-	3/18/38/38	0/3/3/3
56	GTP	PE	501	57	-	3/18/38/38	0/3/3/3
58	GDP	FF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	DH	501	-	-	1/12/32/32	0/3/3/3
58	GDP	OC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	HE	501	57	-	6/18/38/38	0/3/3/3
58	GDP	BL	501	-	-	2/12/32/32	0/3/3/3
56	GTP	EG	501	57	-	3/18/38/38	0/3/3/3
56	GTP	CG	501	57	-	4/18/38/38	0/3/3/3
58	GDP	KL	501	-	-	2/12/32/32	0/3/3/3
58	GDP	NJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	IB	501	57	-	4/18/38/38	0/3/3/3
56	GTP	TA	501	57	-	8/18/38/38	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	SF	501	-	-	3/12/32/32	0/3/3/3
58	GDP	HC	501	-	-	5/12/32/32	0/3/3/3
56	GTP	IA	501	57	-	3/18/38/38	0/3/3/3
56	GTP	CE	501	57	-	3/18/38/38	0/3/3/3
56	GTP	AK	501	57	-	5/18/38/38	0/3/3/3
58	GDP	TC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	TL	501	-	-	2/12/32/32	0/3/3/3
58	GDP	MC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	DI	501	57	-	2/18/38/38	0/3/3/3
56	GTP	MI	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	NM	501	-	-	2/12/32/32	0/3/3/3
58	GDP	JF	501	-	-	2/12/32/32	0/3/3/3
56	GTP	PL	501	57	-	3/18/38/38	0/3/3/3
58	GDP	LD	501	-	-	2/12/32/32	0/3/3/3
58	GDP	FD	501	-	-	1/12/32/32	0/3/3/3
58	GDP	FL	501	-	-	2/12/32/32	0/3/3/3
58	GDP	HF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	WL	501	-	-	2/12/32/32	0/3/3/3
56	GTP	OL	501	57	-	7/18/38/38	0/3/3/3
58	GDP	RM	501	-	-	2/12/32/32	0/3/3/3
58	GDP	AC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	RB	501	57	-	6/18/38/38	0/3/3/3
58	GDP	HH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	WI	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	PD	501	-	-	1/12/32/32	0/3/3/3
56	GTP	UB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	JJ	501	-	-	3/12/32/32	0/3/3/3
56	GTP	TK	501	57	-	4/18/38/38	0/3/3/3
56	GTP	SE	501	57	-	6/18/38/38	0/3/3/3
58	GDP	RD	501	-	-	2/12/32/32	0/3/3/3
56	GTP	BM	501	57	-	9/18/38/38	0/3/3/3
56	GTP	DB	501	57	-	1/18/38/38	0/3/3/3
58	GDP	SD	501	-	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	DL	501	-	-	0/12/32/32	0/3/3/3
58	GDP	GD	501	-	-	1/12/32/32	0/3/3/3
56	GTP	FM	501	57	-	4/18/38/38	0/3/3/3
58	GDP	UL	501	-	-	3/12/32/32	0/3/3/3
58	GDP	HL	501	-	-	3/12/32/32	0/3/3/3
56	GTP	DM	501	57	-	3/18/38/38	0/3/3/3
56	GTP	CI	501	57	-	2/18/38/38	0/3/3/3
56	GTP	CA	501	57	-	3/18/38/38	0/3/3/3
58	GDP	MJ	501	-	-	2/12/32/32	0/3/3/3
56	GTP	HI	501	57	-	6/18/38/38	0/3/3/3
56	GTP	OI	501	57	-	4/18/38/38	0/3/3/3
58	GDP	RC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	LB	501	57	-	3/18/38/38	0/3/3/3
56	GTP	AG	501	57	-	4/18/38/38	0/3/3/3
56	GTP	AM	501	57	-	6/18/38/38	0/3/3/3
56	GTP	IM	501	57	-	7/18/38/38	0/3/3/3
56	GTP	DA	501	57	-	3/18/38/38	0/3/3/3
56	GTP	EC	501	57	-	3/18/38/38	0/3/3/3
58	GDP	DD	501	-	-	4/12/32/32	0/3/3/3
58	GDP	FC	501	-	-	2/12/32/32	0/3/3/3
56	GTP	EA	501	57	-	3/18/38/38	0/3/3/3
56	GTP	JB	501	57	-	3/18/38/38	0/3/3/3
58	GDP	PF	501	55	-	1/12/32/32	0/3/3/3
58	GDP	SC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	LH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	PA	501	57	-	3/18/38/38	0/3/3/3
56	GTP	HG	501	57	-	3/18/38/38	0/3/3/3
56	GTP	WK	501	57	-	6/18/38/38	0/3/3/3
58	GDP	AD	501	-	-	5/12/32/32	0/3/3/3
58	GDP	AH	501	-	-	3/12/32/32	0/3/3/3
58	GDP	UF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	VC	501	-	-	1/12/32/32	0/3/3/3
58	GDP	OJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	PJ	501	-	-	2/12/32/32	0/3/3/3
58	GDP	GC	501	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GDP	WF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	GL	501	-	-	1/12/32/32	0/3/3/3
56	GTP	FE	501	57	-	8/18/38/38	0/3/3/3
58	GDP	EH	501	-	-	2/12/32/32	0/3/3/3
58	GDP	UM	501	55	-	2/12/32/32	0/3/3/3
58	GDP	PH	501	-	-	2/12/32/32	0/3/3/3
56	GTP	SA	502	57	-	4/18/38/38	0/3/3/3
58	GDP	JH	501	-	-	1/12/32/32	0/3/3/3
58	GDP	NC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	VF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	WD	501	-	-	1/12/32/32	0/3/3/3
56	GTP	SB	501	57	-	2/18/38/38	0/3/3/3
58	GDP	VH	501	-	-	3/12/32/32	0/3/3/3
56	GTP	SG	501	57	-	7/18/38/38	0/3/3/3
56	GTP	VG	501	57	-	4/18/38/38	0/3/3/3
58	GDP	CL	501	-	-	2/12/32/32	0/3/3/3
56	GTP	EE	501	57	-	2/18/38/38	0/3/3/3
58	GDP	OF	501	-	-	2/12/32/32	0/3/3/3
58	GDP	CC	501	-	-	2/12/32/32	0/3/3/3
58	GDP	ID	501	-	-	2/12/32/32	0/3/3/3
56	GTP	GI	501	57	-	3/18/38/38	0/3/3/3

All (445) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	PA	501	GTP	C5-C6	-4.40	1.38	1.47
56	RE	501	GTP	C5-C6	-4.28	1.38	1.47
56	RG	501	GTP	C5-C6	-4.18	1.38	1.47
56	EE	501	GTP	C5-C6	-4.17	1.38	1.47
56	KG	501	GTP	C5-C6	-4.17	1.38	1.47
56	EA	501	GTP	C5-C6	-4.17	1.38	1.47
56	OK	501	GTP	C5-C6	-4.16	1.39	1.47
56	TA	501	GTP	C5-C6	-4.16	1.39	1.47
56	SK	501	GTP	C5-C6	-4.16	1.39	1.47
56	QB	501	GTP	C5-C6	-4.16	1.39	1.47
56	GE	501	GTP	C5-C6	-4.16	1.39	1.47
56	RK	501	GTP	C5-C6	-4.16	1.39	1.47
56	RA	501	GTP	C5-C6	-4.16	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	PI	501	GTP	C5-C6	-4.15	1.39	1.47
56	IB	501	GTP	C5-C6	-4.15	1.39	1.47
56	HB	501	GTP	C5-C6	-4.15	1.39	1.47
56	TE	501	GTP	C5-C6	-4.15	1.39	1.47
56	QA	501	GTP	C5-C6	-4.14	1.39	1.47
56	WI	501	GTP	C5-C6	-4.14	1.39	1.47
56	AG	501	GTP	C5-C6	-4.13	1.39	1.47
56	AK	501	GTP	C5-C6	-4.13	1.39	1.47
56	BA	501	GTP	C5-C6	-4.13	1.39	1.47
56	LK	501	GTP	C5-C6	-4.13	1.39	1.47
56	QI	501	GTP	C5-C6	-4.13	1.39	1.47
56	TI	501	GTP	C5-C6	-4.13	1.39	1.47
56	EI	501	GTP	C5-C6	-4.13	1.39	1.47
56	KK	501	GTP	C5-C6	-4.12	1.39	1.47
56	SB	501	GTP	C5-C6	-4.12	1.39	1.47
56	KB	501	GTP	C5-C6	-4.12	1.39	1.47
56	WG	501	GTP	C5-C6	-4.12	1.39	1.47
56	FI	501	GTP	C5-C6	-4.11	1.39	1.47
56	KI	501	GTP	C5-C6	-4.11	1.39	1.47
56	IK	501	GTP	C5-C6	-4.11	1.39	1.47
56	DB	501	GTP	C5-C6	-4.11	1.39	1.47
56	SE	501	GTP	C5-C6	-4.11	1.39	1.47
56	EC	501	GTP	C5-C6	-4.11	1.39	1.47
56	MG	501	GTP	C5-C6	-4.11	1.39	1.47
56	SI	501	GTP	C5-C6	-4.11	1.39	1.47
56	GB	501	GTP	C5-C6	-4.10	1.39	1.47
56	RI	501	GTP	C5-C6	-4.10	1.39	1.47
56	WA	501	GTP	C5-C6	-4.10	1.39	1.47
56	AB	501	GTP	C5-C6	-4.10	1.39	1.47
56	TB	501	GTP	C5-C6	-4.10	1.39	1.47
56	FM	501	GTP	C5-C6	-4.10	1.39	1.47
56	PL	501	GTP	C5-C6	-4.10	1.39	1.47
56	IA	501	GTP	C5-C6	-4.10	1.39	1.47
56	LI	501	GTP	C5-C6	-4.10	1.39	1.47
56	QG	501	GTP	C5-C6	-4.10	1.39	1.47
56	MK	501	GTP	C5-C6	-4.10	1.39	1.47
56	LG	501	GTP	C5-C6	-4.10	1.39	1.47
56	EK	501	GTP	C5-C6	-4.10	1.39	1.47
56	JK	501	GTP	C5-C6	-4.10	1.39	1.47
56	SG	501	GTP	C5-C6	-4.10	1.39	1.47
56	MA	501	GTP	C5-C6	-4.10	1.39	1.47
56	HE	501	GTP	C5-C6	-4.10	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	QK	501	GTP	C5-C6	-4.09	1.39	1.47
56	JA	501	GTP	C5-C6	-4.09	1.39	1.47
56	JG	501	GTP	C5-C6	-4.09	1.39	1.47
56	CB	501	GTP	C5-C6	-4.09	1.39	1.47
56	TK	501	GTP	C5-C6	-4.09	1.39	1.47
56	ME	501	GTP	C5-C6	-4.09	1.39	1.47
56	JE	501	GTP	C5-C6	-4.09	1.39	1.47
56	KE	501	GTP	C5-C6	-4.09	1.39	1.47
56	ML	501	GTP	C5-C6	-4.09	1.39	1.47
56	VB	501	GTP	C5-C6	-4.09	1.39	1.47
56	DI	501	GTP	C5-C6	-4.08	1.39	1.47
56	JI	501	GTP	C5-C6	-4.08	1.39	1.47
56	BM	501	GTP	C5-C6	-4.08	1.39	1.47
56	VE	501	GTP	C5-C6	-4.08	1.39	1.47
56	UK	501	GTP	C5-C6	-4.08	1.39	1.47
56	VG	501	GTP	C5-C6	-4.08	1.39	1.47
56	FE	501	GTP	C5-C6	-4.08	1.39	1.47
56	AE	501	GTP	C5-C6	-4.08	1.39	1.47
56	SA	502	GTP	C5-C6	-4.08	1.39	1.47
56	BI	501	GTP	C5-C6	-4.08	1.39	1.47
56	RB	501	GTP	C5-C6	-4.07	1.39	1.47
56	LB	501	GTP	C5-C6	-4.07	1.39	1.47
56	CG	501	GTP	C5-C6	-4.07	1.39	1.47
56	NG	501	GTP	C5-C6	-4.07	1.39	1.47
56	AM	501	GTP	C5-C6	-4.07	1.39	1.47
56	HG	501	GTP	C5-C6	-4.07	1.39	1.47
56	OG	501	GTP	C5-C6	-4.07	1.39	1.47
56	JB	501	GTP	C5-C6	-4.07	1.39	1.47
56	OA	501	GTP	C5-C6	-4.07	1.39	1.47
56	EG	501	GTP	C5-C6	-4.07	1.39	1.47
56	FK	501	GTP	C5-C6	-4.07	1.39	1.47
56	QE	501	GTP	C5-C6	-4.07	1.39	1.47
56	NL	501	GTP	C5-C6	-4.07	1.39	1.47
56	HK	501	GTP	C5-C6	-4.07	1.39	1.47
56	AI	501	GTP	C5-C6	-4.06	1.39	1.47
56	HA	501	GTP	C5-C6	-4.06	1.39	1.47
56	NI	501	GTP	C5-C6	-4.06	1.39	1.47
56	UG	501	GTP	C5-C6	-4.06	1.39	1.47
56	DE	501	GTP	C5-C6	-4.06	1.39	1.47
56	DA	501	GTP	C5-C6	-4.06	1.39	1.47
56	IG	501	GTP	C5-C6	-4.06	1.39	1.47
56	GK	501	GTP	C5-C6	-4.05	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	MI	501	GTP	C5-C6	-4.05	1.39	1.47
56	HI	501	GTP	C5-C6	-4.05	1.39	1.47
56	PK	501	GTP	C5-C6	-4.05	1.39	1.47
56	NE	501	GTP	C5-C6	-4.05	1.39	1.47
56	NA	501	GTP	C5-C6	-4.05	1.39	1.47
56	OB	501	GTP	C5-C6	-4.05	1.39	1.47
56	VK	501	GTP	C5-C6	-4.05	1.39	1.47
56	II	501	GTP	C5-C6	-4.05	1.39	1.47
56	FG	501	GTP	C5-C6	-4.04	1.39	1.47
56	UE	501	GTP	C5-C6	-4.04	1.39	1.47
56	MB	501	GTP	C5-C6	-4.04	1.39	1.47
56	BB	501	GTP	C5-C6	-4.04	1.39	1.47
56	IM	501	GTP	C5-C6	-4.04	1.39	1.47
56	WE	501	GTP	C5-C6	-4.04	1.39	1.47
56	GG	501	GTP	C5-C6	-4.04	1.39	1.47
56	UB	501	GTP	C5-C6	-4.04	1.39	1.47
56	VA	501	GTP	C5-C6	-4.04	1.39	1.47
56	FB	501	GTP	C5-C6	-4.04	1.39	1.47
56	VI	501	GTP	C5-C6	-4.04	1.39	1.47
56	LA	501	GTP	C5-C6	-4.04	1.39	1.47
56	DM	501	GTP	C5-C6	-4.03	1.39	1.47
56	KA	501	GTP	C5-C6	-4.03	1.39	1.47
56	WK	501	GTP	C5-C6	-4.03	1.39	1.47
56	CK	501	GTP	C5-C6	-4.03	1.39	1.47
56	DG	501	GTP	C5-C6	-4.03	1.39	1.47
56	LE	501	GTP	C5-C6	-4.03	1.39	1.47
56	OI	501	GTP	C5-C6	-4.03	1.39	1.47
56	BE	501	GTP	C5-C6	-4.02	1.39	1.47
56	TG	501	GTP	C5-C6	-4.02	1.39	1.47
56	OE	501	GTP	C5-C6	-4.02	1.39	1.47
56	AA	501	GTP	C5-C6	-4.02	1.39	1.47
56	BG	501	GTP	C5-C6	-4.02	1.39	1.47
56	UI	501	GTP	C5-C6	-4.01	1.39	1.47
56	OL	501	GTP	C5-C6	-4.01	1.39	1.47
56	CM	501	GTP	C5-C6	-4.01	1.39	1.47
56	PG	501	GTP	C5-C6	-4.01	1.39	1.47
56	CI	501	GTP	C5-C6	-4.01	1.39	1.47
56	NB	501	GTP	C5-C6	-4.00	1.39	1.47
56	CA	501	GTP	C5-C6	-4.00	1.39	1.47
56	PE	501	GTP	C5-C6	-4.00	1.39	1.47
56	WB	501	GTP	C5-C6	-4.00	1.39	1.47
56	IE	501	GTP	C5-C6	-4.00	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	RL	501	GTP	C5-C6	-3.99	1.39	1.47
56	QL	501	GTP	C5-C6	-3.99	1.39	1.47
56	CE	501	GTP	C5-C6	-3.98	1.39	1.47
56	PB	501	GTP	C5-C6	-3.98	1.39	1.47
56	UA	501	GTP	C5-C6	-3.98	1.39	1.47
56	GI	501	GTP	C5-C6	-3.97	1.39	1.47
56	DK	501	GTP	C5-C6	-3.97	1.39	1.47
56	BK	501	GTP	C5-C6	-3.96	1.39	1.47
56	GA	501	GTP	C5-C6	-3.96	1.39	1.47
58	AD	501	GDP	C6-N1	-2.83	1.33	1.37
58	HC	501	GDP	C6-N1	-2.81	1.33	1.37
58	VL	501	GDP	C6-N1	-2.79	1.33	1.37
58	DD	501	GDP	C6-N1	-2.76	1.33	1.37
58	JL	501	GDP	C6-N1	-2.73	1.33	1.37
58	CF	501	GDP	C6-N1	-2.67	1.33	1.37
58	NF	501	GDP	C6-N1	-2.65	1.33	1.37
58	QF	501	GDP	C6-N1	-2.63	1.34	1.37
58	TH	501	GDP	C6-N1	-2.63	1.34	1.37
58	FL	501	GDP	C6-N1	-2.61	1.34	1.37
58	WD	501	GDP	C6-N1	-2.59	1.34	1.37
58	NJ	501	GDP	C6-N1	-2.59	1.34	1.37
58	EM	501	GDP	C6-N1	-2.57	1.34	1.37
58	BF	501	GDP	C6-N1	-2.57	1.34	1.37
58	SJ	501	GDP	C6-N1	-2.57	1.34	1.37
58	RC	501	GDP	C6-N1	-2.57	1.34	1.37
58	LH	501	GDP	C6-N1	-2.56	1.34	1.37
58	LL	501	GDP	C6-N1	-2.55	1.34	1.37
58	SC	501	GDP	C6-N1	-2.55	1.34	1.37
58	FF	501	GDP	C6-N1	-2.54	1.34	1.37
58	WF	501	GDP	C6-N1	-2.54	1.34	1.37
58	RM	501	GDP	C6-N1	-2.54	1.34	1.37
58	RD	501	GDP	C6-N1	-2.53	1.34	1.37
58	UF	501	GDP	C6-N1	-2.53	1.34	1.37
58	OH	501	GDP	C6-N1	-2.53	1.34	1.37
58	AJ	501	GDP	C6-N1	-2.53	1.34	1.37
58	UH	501	GDP	C6-N1	-2.53	1.34	1.37
58	IL	501	GDP	C6-N1	-2.53	1.34	1.37
58	AC	501	GDP	C6-N1	-2.52	1.34	1.37
58	RH	501	GDP	C6-N1	-2.52	1.34	1.37
58	JH	501	GDP	C6-N1	-2.52	1.34	1.37
58	GF	501	GDP	C6-N1	-2.52	1.34	1.37
58	EL	501	GDP	C6-N1	-2.52	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	IJ	501	GDP	C6-N1	-2.52	1.34	1.37
58	PD	501	GDP	C6-N1	-2.51	1.34	1.37
58	PM	501	GDP	C6-N1	-2.51	1.34	1.37
58	RJ	501	GDP	C6-N1	-2.51	1.34	1.37
58	BC	501	GDP	C6-N1	-2.51	1.34	1.37
58	FM	502	GDP	C6-N1	-2.51	1.34	1.37
58	UC	501	GDP	C6-N1	-2.50	1.34	1.37
58	HL	501	GDP	C6-N1	-2.50	1.34	1.37
58	SL	501	GDP	C6-N1	-2.50	1.34	1.37
58	LC	501	GDP	C6-N1	-2.50	1.34	1.37
58	NC	501	GDP	C6-N1	-2.50	1.34	1.37
58	AF	501	GDP	C6-N1	-2.50	1.34	1.37
58	MH	501	GDP	C6-N1	-2.50	1.34	1.37
58	DJ	501	GDP	C6-N1	-2.50	1.34	1.37
58	MC	501	GDP	C6-N1	-2.50	1.34	1.37
58	CD	501	GDP	C6-N1	-2.50	1.34	1.37
58	GD	501	GDP	C6-N1	-2.49	1.34	1.37
58	GH	501	GDP	C6-N1	-2.49	1.34	1.37
58	PC	501	GDP	C6-N1	-2.49	1.34	1.37
58	QC	501	GDP	C6-N1	-2.49	1.34	1.37
58	EB	501	GDP	C6-N1	-2.49	1.34	1.37
58	KF	501	GDP	C6-N1	-2.49	1.34	1.37
58	KC	501	GDP	C6-N1	-2.49	1.34	1.37
58	LJ	501	GDP	C6-N1	-2.49	1.34	1.37
58	JC	501	GDP	C6-N1	-2.49	1.34	1.37
58	BL	501	GDP	C6-N1	-2.49	1.34	1.37
58	AL	501	GDP	C6-N1	-2.48	1.34	1.37
58	MF	501	GDP	C6-N1	-2.48	1.34	1.37
58	LF	501	GDP	C6-N1	-2.48	1.34	1.37
58	NM	501	GDP	C6-N1	-2.48	1.34	1.37
58	JM	501	GDP	C6-N1	-2.48	1.34	1.37
58	TF	501	GDP	C6-N1	-2.48	1.34	1.37
58	IF	501	GDP	C6-N1	-2.48	1.34	1.37
58	MJ	501	GDP	C6-N1	-2.48	1.34	1.37
58	NH	501	GDP	C6-N1	-2.48	1.34	1.37
58	TC	501	GDP	C6-N1	-2.47	1.34	1.37
58	KJ	501	GDP	C6-N1	-2.47	1.34	1.37
58	OJ	501	GDP	C6-N1	-2.47	1.34	1.37
58	CJ	501	GDP	C6-N1	-2.47	1.34	1.37
58	VF	501	GDP	C6-N1	-2.47	1.34	1.37
58	DL	501	GDP	C6-N1	-2.47	1.34	1.37
58	MD	501	GDP	C6-N1	-2.47	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	SH	501	GDP	C6-N1	-2.47	1.34	1.37
58	UL	501	GDP	C6-N1	-2.47	1.34	1.37
58	VD	501	GDP	C6-N1	-2.47	1.34	1.37
58	QM	501	GDP	C6-N1	-2.47	1.34	1.37
58	JJ	501	GDP	C6-N1	-2.46	1.34	1.37
58	PH	501	GDP	C6-N1	-2.46	1.34	1.37
58	QJ	501	GDP	C6-N1	-2.46	1.34	1.37
58	UJ	501	GDP	C6-N1	-2.46	1.34	1.37
58	KL	501	GDP	C6-N1	-2.46	1.34	1.37
58	KH	501	GDP	C6-N1	-2.46	1.34	1.37
58	FD	501	GDP	C6-N1	-2.46	1.34	1.37
58	GC	501	GDP	C6-N1	-2.46	1.34	1.37
58	VJ	501	GDP	C6-N1	-2.46	1.34	1.37
58	DH	501	GDP	C6-N1	-2.46	1.34	1.37
58	JD	501	GDP	C6-N1	-2.46	1.34	1.37
58	HH	501	GDP	C6-N1	-2.46	1.34	1.37
58	HJ	501	GDP	C6-N1	-2.46	1.34	1.37
58	FH	501	GDP	C6-N1	-2.45	1.34	1.37
58	IC	501	GDP	C6-N1	-2.45	1.34	1.37
58	VM	501	GDP	C6-N1	-2.45	1.34	1.37
58	TL	501	GDP	C6-N1	-2.45	1.34	1.37
58	IH	501	GDP	C6-N1	-2.45	1.34	1.37
58	GJ	501	GDP	C6-N1	-2.45	1.34	1.37
58	OF	501	GDP	C6-N1	-2.45	1.34	1.37
58	FC	501	GDP	C6-N1	-2.44	1.34	1.37
58	QD	501	GDP	C6-N1	-2.44	1.34	1.37
58	ID	501	GDP	C6-N1	-2.44	1.34	1.37
58	DC	501	GDP	C6-N1	-2.44	1.34	1.37
58	JF	501	GDP	C6-N1	-2.44	1.34	1.37
58	QH	501	GDP	C6-N1	-2.44	1.34	1.37
58	KD	501	GDP	C6-N1	-2.44	1.34	1.37
58	WC	501	GDP	C6-N1	-2.44	1.34	1.37
58	ND	501	GDP	C6-N1	-2.44	1.34	1.37
58	OC	501	GDP	C6-N1	-2.44	1.34	1.37
58	BJ	501	GDP	C6-N1	-2.44	1.34	1.37
58	PJ	501	GDP	C6-N1	-2.43	1.34	1.37
58	VC	501	GDP	C6-N1	-2.43	1.34	1.37
58	EJ	501	GDP	C6-N1	-2.43	1.34	1.37
58	WH	501	GDP	C6-N1	-2.43	1.34	1.37
58	EF	501	GDP	C6-N1	-2.43	1.34	1.37
58	WJ	501	GDP	C6-N1	-2.43	1.34	1.37
58	AH	501	GDP	C6-N1	-2.43	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	LD	501	GDP	C6-N1	-2.43	1.34	1.37
58	HF	501	GDP	C6-N1	-2.42	1.34	1.37
58	MM	501	GDP	C6-N1	-2.42	1.34	1.37
58	GL	501	GDP	C6-N1	-2.42	1.34	1.37
58	OM	501	GDP	C6-N1	-2.42	1.34	1.37
58	EH	501	GDP	C6-N1	-2.41	1.34	1.37
58	SM	501	GDP	C6-N1	-2.41	1.34	1.37
58	HD	501	GDP	C6-N1	-2.41	1.34	1.37
58	TM	501	GDP	C6-N1	-2.41	1.34	1.37
58	CC	501	GDP	C6-N1	-2.41	1.34	1.37
58	BD	501	GDP	C6-N1	-2.41	1.34	1.37
58	NK	501	GDP	C6-N1	-2.41	1.34	1.37
58	WL	501	GDP	C6-N1	-2.41	1.34	1.37
58	OD	501	GDP	C6-N1	-2.41	1.34	1.37
58	TJ	501	GDP	C6-N1	-2.40	1.34	1.37
58	BH	501	GDP	C6-N1	-2.40	1.34	1.37
58	ED	501	GDP	C6-N1	-2.40	1.34	1.37
58	GM	501	GDP	C6-N1	-2.39	1.34	1.37
58	CL	501	GDP	C6-N1	-2.39	1.34	1.37
58	FJ	501	GDP	C6-N1	-2.39	1.34	1.37
58	CH	501	GDP	C6-N1	-2.38	1.34	1.37
58	SD	501	GDP	C6-N1	-2.38	1.34	1.37
58	LM	501	GDP	C6-N1	-2.38	1.34	1.37
58	VH	501	GDP	C6-N1	-2.38	1.34	1.37
58	UM	501	GDP	C6-N1	-2.37	1.34	1.37
58	SF	501	GDP	C6-N1	-2.37	1.34	1.37
58	KM	501	GDP	C6-N1	-2.34	1.34	1.37
58	HM	501	GDP	C6-N1	-2.30	1.34	1.37
56	TG	501	GTP	C2-N3	2.30	1.38	1.33
56	CK	501	GTP	C2-N3	2.28	1.38	1.33
56	RL	501	GTP	C2-N3	2.27	1.38	1.33
56	BK	501	GTP	C2-N3	2.27	1.38	1.33
56	TA	501	GTP	C2-N3	2.26	1.38	1.33
56	LA	501	GTP	C2-N3	2.23	1.38	1.33
56	IA	501	GTP	C2-N3	2.23	1.38	1.33
56	GB	501	GTP	C2-N3	2.22	1.38	1.33
56	PL	501	GTP	C2-N3	2.22	1.38	1.33
56	UA	501	GTP	C2-N3	2.22	1.38	1.33
56	PI	501	GTP	C2-N3	2.21	1.38	1.33
56	ML	501	GTP	C2-N3	2.21	1.38	1.33
56	TI	501	GTP	C2-N3	2.21	1.38	1.33
56	PK	501	GTP	C2-N3	2.21	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	SK	501	GTP	C2-N3	2.20	1.38	1.33
56	TB	501	GTP	C2-N3	2.20	1.38	1.33
56	NB	501	GTP	C2-N3	2.19	1.38	1.33
56	FI	501	GTP	C2-N3	2.19	1.38	1.33
56	MA	501	GTP	C2-N3	2.19	1.38	1.33
56	AE	501	GTP	C2-N3	2.19	1.38	1.33
56	IM	501	GTP	C2-N3	2.19	1.38	1.33
56	GE	501	GTP	C2-N3	2.19	1.38	1.33
56	HI	501	GTP	C2-N3	2.18	1.38	1.33
56	AK	501	GTP	C2-N3	2.18	1.38	1.33
56	FB	501	GTP	C2-N3	2.18	1.38	1.33
56	GI	501	GTP	C2-N3	2.18	1.38	1.33
56	QL	501	GTP	C2-N3	2.18	1.38	1.33
58	RF	501	GDP	C6-N1	-2.18	1.34	1.37
56	SG	501	GTP	C2-N3	2.18	1.38	1.33
56	BI	501	GTP	C2-N3	2.18	1.38	1.33
58	DF	501	GDP	C6-N1	-2.18	1.34	1.37
56	KA	501	GTP	C2-N3	2.18	1.38	1.33
56	OA	501	GTP	C2-N3	2.18	1.38	1.33
56	OG	501	GTP	C2-N3	2.17	1.38	1.33
56	BG	501	GTP	C2-N3	2.17	1.38	1.33
56	UI	501	GTP	C2-N3	2.17	1.38	1.33
56	IE	501	GTP	C2-N3	2.17	1.38	1.33
56	UE	501	GTP	C2-N3	2.17	1.38	1.33
56	IK	501	GTP	C2-N3	2.17	1.38	1.33
56	VA	501	GTP	C2-N3	2.17	1.38	1.33
56	HA	501	GTP	C2-N3	2.17	1.38	1.33
56	BA	501	GTP	C2-N3	2.17	1.38	1.33
56	EC	501	GTP	C2-N3	2.17	1.38	1.33
56	EK	501	GTP	C2-N3	2.17	1.38	1.33
56	OB	501	GTP	C2-N3	2.17	1.38	1.33
56	GA	501	GTP	C2-N3	2.17	1.38	1.33
56	DK	501	GTP	C2-N3	2.17	1.38	1.33
56	HB	501	GTP	C2-N3	2.17	1.38	1.33
56	OI	501	GTP	C2-N3	2.17	1.38	1.33
56	SI	501	GTP	C2-N3	2.17	1.38	1.33
56	II	501	GTP	C2-N3	2.17	1.38	1.33
56	NE	501	GTP	C2-N3	2.17	1.38	1.33
56	FG	501	GTP	C2-N3	2.16	1.38	1.33
56	QK	501	GTP	C2-N3	2.16	1.38	1.33
56	CM	501	GTP	C2-N3	2.16	1.38	1.33
56	AG	501	GTP	C2-N3	2.16	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	GG	501	GTP	C2-N3	2.16	1.38	1.33
56	NG	501	GTP	C2-N3	2.16	1.38	1.33
56	RA	501	GTP	C2-N3	2.16	1.38	1.33
56	AM	501	GTP	C2-N3	2.16	1.38	1.33
56	EA	501	GTP	C2-N3	2.16	1.38	1.33
56	IB	501	GTP	C2-N3	2.16	1.38	1.33
56	WK	501	GTP	C2-N3	2.16	1.38	1.33
56	JB	501	GTP	C2-N3	2.16	1.38	1.33
56	OL	501	GTP	C2-N3	2.16	1.38	1.33
56	SB	501	GTP	C2-N3	2.16	1.38	1.33
56	CA	501	GTP	C2-N3	2.16	1.38	1.33
56	NA	501	GTP	C2-N3	2.16	1.38	1.33
56	PB	501	GTP	C2-N3	2.16	1.38	1.33
56	VI	501	GTP	C2-N3	2.16	1.38	1.33
56	JG	501	GTP	C2-N3	2.15	1.38	1.33
56	SA	502	GTP	C2-N3	2.15	1.38	1.33
56	FM	501	GTP	C2-N3	2.15	1.38	1.33
56	OE	501	GTP	C2-N3	2.15	1.38	1.33
56	TK	501	GTP	C2-N3	2.15	1.38	1.33
56	WG	501	GTP	C2-N3	2.15	1.38	1.33
56	PG	501	GTP	C2-N3	2.15	1.38	1.33
56	HE	501	GTP	C2-N3	2.15	1.38	1.33
56	FE	501	GTP	C2-N3	2.15	1.38	1.33
56	JE	501	GTP	C2-N3	2.15	1.38	1.33
56	RE	501	GTP	C2-N3	2.15	1.38	1.33
56	VE	501	GTP	C2-N3	2.15	1.38	1.33
56	PA	501	GTP	C2-N3	2.15	1.38	1.33
56	CB	501	GTP	C2-N3	2.15	1.38	1.33
56	RI	501	GTP	C2-N3	2.15	1.38	1.33
56	QI	501	GTP	C2-N3	2.15	1.38	1.33
56	WI	501	GTP	C2-N3	2.15	1.38	1.33
56	VK	501	GTP	C2-N3	2.15	1.38	1.33
56	GK	501	GTP	C2-N3	2.15	1.38	1.33
56	PE	501	GTP	C2-N3	2.15	1.38	1.33
56	NL	501	GTP	C2-N3	2.15	1.38	1.33
56	HG	501	GTP	C2-N3	2.14	1.38	1.33
56	AA	501	GTP	C2-N3	2.14	1.38	1.33
56	LB	501	GTP	C2-N3	2.14	1.38	1.33
56	KK	501	GTP	C2-N3	2.14	1.38	1.33
56	VB	501	GTP	C2-N3	2.14	1.38	1.33
56	DI	501	GTP	C2-N3	2.14	1.38	1.33
56	SE	501	GTP	C2-N3	2.14	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	EI	501	GTP	C2-N3	2.14	1.38	1.33
56	CI	501	GTP	C2-N3	2.14	1.38	1.33
56	WB	501	GTP	C2-N3	2.14	1.38	1.33
56	EG	501	GTP	C2-N3	2.14	1.38	1.33
56	JA	501	GTP	C2-N3	2.14	1.38	1.33
56	BB	501	GTP	C2-N3	2.14	1.38	1.33
56	NI	501	GTP	C2-N3	2.14	1.38	1.33
56	WA	501	GTP	C2-N3	2.14	1.38	1.33
56	LI	501	GTP	C2-N3	2.14	1.38	1.33
56	AB	501	GTP	C2-N3	2.14	1.38	1.33
56	JK	501	GTP	C2-N3	2.14	1.38	1.33
56	UB	501	GTP	C2-N3	2.14	1.38	1.33
56	LG	501	GTP	C2-N3	2.14	1.38	1.33
56	MG	501	GTP	C2-N3	2.14	1.38	1.33
56	WE	501	GTP	C2-N3	2.13	1.38	1.33
56	LK	501	GTP	C2-N3	2.13	1.38	1.33
56	RK	501	GTP	C2-N3	2.13	1.38	1.33
58	UD	501	GDP	C6-N1	-2.13	1.34	1.37
56	KB	501	GTP	C2-N3	2.13	1.38	1.33
56	FK	501	GTP	C2-N3	2.13	1.38	1.33
56	RG	501	GTP	C2-N3	2.13	1.38	1.33
56	DG	501	GTP	C2-N3	2.13	1.38	1.33
56	DA	501	GTP	C2-N3	2.13	1.38	1.33
56	AI	501	GTP	C2-N3	2.12	1.38	1.33
56	IG	501	GTP	C2-N3	2.12	1.38	1.33
56	TE	501	GTP	C2-N3	2.12	1.38	1.33
56	ME	501	GTP	C2-N3	2.12	1.38	1.33
56	KI	501	GTP	C2-N3	2.12	1.38	1.33
56	BM	501	GTP	C2-N3	2.12	1.38	1.33
56	VG	501	GTP	C2-N3	2.12	1.38	1.33
56	QG	501	GTP	C2-N3	2.12	1.38	1.33
56	QE	501	GTP	C2-N3	2.11	1.38	1.33
56	KE	501	GTP	C2-N3	2.11	1.38	1.33
56	UG	501	GTP	C2-N3	2.11	1.38	1.33
56	QA	501	GTP	C2-N3	2.11	1.38	1.33
56	HK	501	GTP	C2-N3	2.11	1.38	1.33
56	UK	501	GTP	C2-N3	2.11	1.38	1.33
56	DE	501	GTP	C2-N3	2.11	1.38	1.33
56	EE	501	GTP	C2-N3	2.11	1.38	1.33
56	MK	501	GTP	C2-N3	2.11	1.38	1.33
56	KG	501	GTP	C2-N3	2.11	1.38	1.33
56	JI	501	GTP	C2-N3	2.10	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	QB	501	GTP	C2-N3	2.10	1.38	1.33
56	RB	501	GTP	C2-N3	2.10	1.38	1.33
56	LE	501	GTP	C2-N3	2.10	1.38	1.33
56	MI	501	GTP	C2-N3	2.09	1.38	1.33
56	DM	501	GTP	C2-N3	2.09	1.38	1.33
58	TD	501	GDP	C6-N1	-2.09	1.34	1.37
56	MB	501	GTP	C2-N3	2.09	1.38	1.33
56	DB	501	GTP	C2-N3	2.09	1.38	1.33
56	CG	501	GTP	C2-N3	2.09	1.38	1.33
56	CE	501	GTP	C2-N3	2.09	1.38	1.33
56	OK	501	GTP	C2-N3	2.08	1.38	1.33
56	BE	501	GTP	C2-N3	2.06	1.38	1.33

All (1642) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	TE	501	GTP	PA-O3A-PB	-4.96	115.82	132.83
56	GK	501	GTP	PA-O3A-PB	-4.70	116.68	132.83
56	UE	501	GTP	PA-O3A-PB	-4.70	116.70	132.83
56	BB	501	GTP	PA-O3A-PB	-4.57	117.13	132.83
56	AI	501	GTP	PA-O3A-PB	-4.52	117.30	132.83
58	RM	501	GDP	PA-O3A-PB	-4.49	117.40	132.83
56	BE	501	GTP	PA-O3A-PB	-4.47	117.50	132.83
56	NA	501	GTP	PA-O3A-PB	-4.44	117.58	132.83
56	GG	501	GTP	PA-O3A-PB	-4.42	117.65	132.83
56	GB	501	GTP	PA-O3A-PB	-4.42	117.66	132.83
56	EG	501	GTP	PA-O3A-PB	-4.39	117.78	132.83
56	IB	501	GTP	PA-O3A-PB	-4.37	117.81	132.83
56	PB	501	GTP	PA-O3A-PB	-4.37	117.83	132.83
56	AB	501	GTP	PA-O3A-PB	-4.35	117.91	132.83
56	CE	501	GTP	PA-O3A-PB	-4.34	117.93	132.83
56	QK	501	GTP	PA-O3A-PB	-4.32	118.00	132.83
58	FC	501	GDP	PA-O3A-PB	-4.31	118.02	132.83
56	JI	501	GTP	PA-O3A-PB	-4.31	118.04	132.83
56	OB	501	GTP	PA-O3A-PB	-4.30	118.06	132.83
56	CI	501	GTP	PA-O3A-PB	-4.29	118.11	132.83
58	QJ	501	GDP	PA-O3A-PB	-4.29	118.11	132.83
56	EE	501	GTP	PA-O3A-PB	-4.28	118.13	132.83
56	KA	501	GTP	PA-O3A-PB	-4.28	118.13	132.83
56	TK	501	GTP	PA-O3A-PB	-4.28	118.13	132.83
56	UE	501	GTP	PB-O3B-PG	-4.28	118.15	132.83
56	OA	501	GTP	PA-O3A-PB	-4.27	118.16	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	JB	501	GTP	PA-O3A-PB	-4.27	118.18	132.83
58	VD	501	GDP	PA-O3A-PB	-4.26	118.22	132.83
56	AG	501	GTP	PA-O3A-PB	-4.25	118.23	132.83
58	QM	501	GDP	PA-O3A-PB	-4.25	118.23	132.83
56	MA	501	GTP	PA-O3A-PB	-4.25	118.26	132.83
56	KE	501	GTP	PA-O3A-PB	-4.23	118.31	132.83
56	CA	501	GTP	PB-O3B-PG	-4.23	118.32	132.83
58	OM	501	GDP	PA-O3A-PB	-4.22	118.34	132.83
58	TD	501	GDP	PA-O3A-PB	-4.21	118.37	132.83
56	FM	501	GTP	PA-O3A-PB	-4.21	118.38	132.83
56	RE	501	GTP	PA-O3A-PB	-4.20	118.41	132.83
56	DA	501	GTP	PA-O3A-PB	-4.20	118.41	132.83
56	GE	501	GTP	PA-O3A-PB	-4.20	118.42	132.83
56	DM	501	GTP	PA-O3A-PB	-4.19	118.45	132.83
58	TJ	501	GDP	PA-O3A-PB	-4.18	118.47	132.83
56	KB	501	GTP	PA-O3A-PB	-4.17	118.50	132.83
58	PC	501	GDP	PA-O3A-PB	-4.17	118.53	132.83
58	FJ	501	GDP	PA-O3A-PB	-4.16	118.54	132.83
58	KD	501	GDP	PA-O3A-PB	-4.16	118.55	132.83
56	OI	501	GTP	PA-O3A-PB	-4.16	118.56	132.83
58	TL	501	GDP	PA-O3A-PB	-4.16	118.56	132.83
56	KG	501	GTP	PA-O3A-PB	-4.16	118.57	132.83
56	UB	501	GTP	PA-O3A-PB	-4.14	118.62	132.83
56	QB	501	GTP	PA-O3A-PB	-4.13	118.64	132.83
56	FE	501	GTP	PB-O3B-PG	-4.13	118.65	132.83
56	FB	501	GTP	PA-O3A-PB	-4.13	118.65	132.83
56	RG	501	GTP	PA-O3A-PB	-4.13	118.66	132.83
56	FI	501	GTP	PB-O3B-PG	-4.12	118.69	132.83
56	HE	501	GTP	PB-O3B-PG	-4.12	118.70	132.83
56	RA	501	GTP	PA-O3A-PB	-4.12	118.70	132.83
58	CF	501	GDP	PA-O3A-PB	-4.12	118.70	132.83
58	MJ	501	GDP	PA-O3A-PB	-4.11	118.71	132.83
58	EH	501	GDP	PA-O3A-PB	-4.11	118.72	132.83
58	JC	501	GDP	PA-O3A-PB	-4.11	118.73	132.83
58	DC	501	GDP	PA-O3A-PB	-4.11	118.73	132.83
56	HK	501	GTP	PA-O3A-PB	-4.11	118.74	132.83
56	SB	501	GTP	PA-O3A-PB	-4.10	118.74	132.83
58	BL	501	GDP	PA-O3A-PB	-4.10	118.77	132.83
56	RK	501	GTP	PA-O3A-PB	-4.09	118.79	132.83
58	UF	501	GDP	PA-O3A-PB	-4.09	118.81	132.83
56	WK	501	GTP	PA-O3A-PB	-4.09	118.81	132.83
58	CC	501	GDP	PA-O3A-PB	-4.08	118.81	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	FF	501	GDP	PA-O3A-PB	-4.08	118.81	132.83
58	ID	501	GDP	PA-O3A-PB	-4.08	118.83	132.83
56	HA	501	GTP	PA-O3A-PB	-4.07	118.87	132.83
58	HJ	501	GDP	PA-O3A-PB	-4.06	118.88	132.83
58	HH	501	GDP	PA-O3A-PB	-4.06	118.88	132.83
58	VJ	501	GDP	PA-O3A-PB	-4.06	118.89	132.83
58	MH	501	GDP	PA-O3A-PB	-4.06	118.90	132.83
56	NE	501	GTP	PA-O3A-PB	-4.06	118.90	132.83
56	VG	501	GTP	PA-O3A-PB	-4.06	118.91	132.83
56	LI	501	GTP	PA-O3A-PB	-4.05	118.92	132.83
58	JF	501	GDP	PA-O3A-PB	-4.05	118.94	132.83
56	UA	501	GTP	PA-O3A-PB	-4.04	118.95	132.83
58	HL	501	GDP	PA-O3A-PB	-4.03	118.99	132.83
58	EM	501	GDP	PA-O3A-PB	-4.03	118.99	132.83
58	HF	501	GDP	PA-O3A-PB	-4.02	119.02	132.83
56	RL	501	GTP	PA-O3A-PB	-4.02	119.03	132.83
56	TI	501	GTP	PA-O3A-PB	-4.02	119.04	132.83
58	AL	501	GDP	PA-O3A-PB	-4.02	119.05	132.83
58	KC	501	GDP	PA-O3A-PB	-4.00	119.08	132.83
58	BJ	501	GDP	PA-O3A-PB	-4.00	119.09	132.83
56	KI	501	GTP	PA-O3A-PB	-4.00	119.10	132.83
58	RH	501	GDP	PA-O3A-PB	-4.00	119.10	132.83
58	CJ	501	GDP	PA-O3A-PB	-4.00	119.11	132.83
58	ND	501	GDP	PA-O3A-PB	-4.00	119.11	132.83
56	WA	501	GTP	PB-O3B-PG	-4.00	119.11	132.83
56	OG	501	GTP	PA-O3A-PB	-3.99	119.12	132.83
58	PM	501	GDP	PA-O3A-PB	-3.99	119.12	132.83
58	BH	501	GDP	PA-O3A-PB	-3.99	119.14	132.83
56	TE	501	GTP	PB-O3B-PG	-3.99	119.15	132.83
58	MC	501	GDP	PA-O3A-PB	-3.99	119.15	132.83
56	FG	501	GTP	PB-O3B-PG	-3.98	119.16	132.83
58	VC	501	GDP	PA-O3A-PB	-3.98	119.17	132.83
58	VF	501	GDP	PA-O3A-PB	-3.98	119.17	132.83
58	EF	501	GDP	PA-O3A-PB	-3.98	119.17	132.83
58	EJ	501	GDP	PA-O3A-PB	-3.98	119.17	132.83
56	BK	501	GTP	PA-O3A-PB	-3.97	119.19	132.83
58	GF	501	GDP	PA-O3A-PB	-3.97	119.21	132.83
56	UK	501	GTP	PA-O3A-PB	-3.97	119.22	132.83
56	LG	501	GTP	PA-O3A-PB	-3.96	119.23	132.83
56	EC	501	GTP	PA-O3A-PB	-3.96	119.24	132.83
56	UG	501	GTP	PB-O3B-PG	-3.96	119.24	132.83
58	GC	501	GDP	PA-O3A-PB	-3.96	119.25	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AC	501	GDP	PA-O3A-PB	-3.96	119.25	132.83
58	UH	501	GDP	PA-O3A-PB	-3.96	119.25	132.83
56	MI	501	GTP	PA-O3A-PB	-3.96	119.25	132.83
58	FL	501	GDP	PA-O3A-PB	-3.96	119.25	132.83
56	BE	501	GTP	PB-O3B-PG	-3.95	119.27	132.83
56	JG	501	GTP	PA-O3A-PB	-3.95	119.27	132.83
58	IL	501	GDP	PA-O3A-PB	-3.95	119.27	132.83
58	SH	501	GDP	PA-O3A-PB	-3.95	119.28	132.83
56	GG	501	GTP	PB-O3B-PG	-3.95	119.29	132.83
58	PJ	501	GDP	PA-O3A-PB	-3.94	119.29	132.83
56	WA	501	GTP	PA-O3A-PB	-3.94	119.30	132.83
58	UC	501	GDP	PA-O3A-PB	-3.94	119.31	132.83
58	CH	501	GDP	PA-O3A-PB	-3.94	119.31	132.83
56	DE	501	GTP	PA-O3A-PB	-3.94	119.31	132.83
58	LC	501	GDP	PA-O3A-PB	-3.94	119.32	132.83
56	LE	501	GTP	PA-O3A-PB	-3.93	119.33	132.83
56	VB	501	GTP	PB-O3B-PG	-3.93	119.33	132.83
56	DI	501	GTP	PA-O3A-PB	-3.93	119.34	132.83
56	NL	501	GTP	PB-O3B-PG	-3.93	119.34	132.83
56	PE	501	GTP	PA-O3A-PB	-3.93	119.34	132.83
56	ML	501	GTP	PA-O3A-PB	-3.93	119.35	132.83
58	SC	501	GDP	PA-O3A-PB	-3.92	119.36	132.83
58	LH	501	GDP	PA-O3A-PB	-3.92	119.37	132.83
56	UA	501	GTP	PB-O3B-PG	-3.92	119.38	132.83
58	FH	501	GDP	PA-O3A-PB	-3.92	119.39	132.83
58	WF	501	GDP	PA-O3A-PB	-3.91	119.40	132.83
58	NF	501	GDP	PA-O3A-PB	-3.91	119.41	132.83
56	EA	501	GTP	PA-O3A-PB	-3.91	119.41	132.83
58	TC	501	GDP	PA-O3A-PB	-3.91	119.41	132.83
56	UK	501	GTP	PB-O3B-PG	-3.91	119.42	132.83
56	GE	501	GTP	PB-O3B-PG	-3.91	119.42	132.83
56	HI	501	GTP	PB-O3B-PG	-3.91	119.42	132.83
58	UJ	501	GDP	PA-O3A-PB	-3.91	119.42	132.83
56	OK	501	GTP	PB-O3B-PG	-3.90	119.43	132.83
56	BI	501	GTP	PB-O3B-PG	-3.90	119.44	132.83
56	VA	501	GTP	PA-O3A-PB	-3.90	119.45	132.83
58	SM	501	GDP	PA-O3A-PB	-3.90	119.45	132.83
58	RC	501	GDP	PA-O3A-PB	-3.89	119.47	132.83
58	PF	501	GDP	O6-C6-C5	-3.89	116.77	124.37
58	SL	501	GDP	PA-O3A-PB	-3.89	119.48	132.83
56	PK	501	GTP	PA-O3A-PB	-3.89	119.49	132.83
58	WD	501	GDP	PA-O3A-PB	-3.89	119.49	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	JH	501	GDP	PA-O3A-PB	-3.89	119.49	132.83
56	TB	501	GTP	PA-O3A-PB	-3.89	119.49	132.83
58	GL	501	GDP	PA-O3A-PB	-3.88	119.51	132.83
56	JA	501	GTP	PA-O3A-PB	-3.88	119.51	132.83
58	IJ	501	GDP	PA-O3A-PB	-3.88	119.52	132.83
56	FK	501	GTP	PA-O3A-PB	-3.88	119.53	132.83
56	EK	501	GTP	PA-O3A-PB	-3.87	119.53	132.83
56	CG	501	GTP	PB-O3B-PG	-3.87	119.54	132.83
56	IE	501	GTP	PB-O3B-PG	-3.86	119.57	132.83
56	SI	501	GTP	PA-O3A-PB	-3.86	119.57	132.83
58	QC	501	GDP	PA-O3A-PB	-3.86	119.57	132.83
56	QE	501	GTP	PA-O3A-PB	-3.86	119.57	132.83
58	EL	501	GDP	PA-O3A-PB	-3.86	119.58	132.83
56	HG	501	GTP	PA-O3A-PB	-3.86	119.58	132.83
56	SE	501	GTP	PB-O3B-PG	-3.86	119.59	132.83
56	PL	501	GTP	PA-O3A-PB	-3.85	119.61	132.83
58	MF	501	GDP	PA-O3A-PB	-3.85	119.61	132.83
58	GJ	501	GDP	PA-O3A-PB	-3.85	119.61	132.83
56	VI	501	GTP	PA-O3A-PB	-3.85	119.61	132.83
56	EI	501	GTP	PA-O3A-PB	-3.85	119.62	132.83
58	WC	501	GDP	PA-O3A-PB	-3.85	119.62	132.83
58	FM	502	GDP	PA-O3A-PB	-3.84	119.64	132.83
56	FM	501	GTP	PB-O3B-PG	-3.84	119.64	132.83
58	SJ	501	GDP	PA-O3A-PB	-3.84	119.65	132.83
56	KG	501	GTP	PB-O3B-PG	-3.84	119.66	132.83
56	IA	501	GTP	PA-O3A-PB	-3.83	119.68	132.83
58	WJ	501	GDP	PA-O3A-PB	-3.83	119.68	132.83
58	BF	501	GDP	PA-O3A-PB	-3.83	119.68	132.83
58	RD	501	GDP	PA-O3A-PB	-3.83	119.70	132.83
58	OH	501	GDP	PA-O3A-PB	-3.82	119.70	132.83
56	TG	501	GTP	PA-O3A-PB	-3.82	119.70	132.83
58	KF	501	GDP	PA-O3A-PB	-3.82	119.71	132.83
58	JD	501	GDP	PA-O3A-PB	-3.82	119.72	132.83
56	VE	501	GTP	PB-O3B-PG	-3.82	119.72	132.83
56	NI	501	GTP	PB-O3B-PG	-3.82	119.72	132.83
56	QA	501	GTP	PB-O3B-PG	-3.82	119.73	132.83
58	NH	501	GDP	PA-O3A-PB	-3.81	119.75	132.83
56	WG	501	GTP	PB-O3B-PG	-3.81	119.76	132.83
58	GH	501	GDP	PA-O3A-PB	-3.81	119.76	132.83
58	VH	501	GDP	PA-O3A-PB	-3.81	119.76	132.83
58	IC	501	GDP	PA-O3A-PB	-3.81	119.77	132.83
58	IH	501	GDP	PA-O3A-PB	-3.81	119.77	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	EE	501	GTP	PB-O3B-PG	-3.80	119.77	132.83
56	IM	501	GTP	PB-O3B-PG	-3.80	119.77	132.83
58	MD	501	GDP	PA-O3A-PB	-3.80	119.78	132.83
58	TH	501	GDP	PA-O3A-PB	-3.80	119.78	132.83
58	CL	501	GDP	PA-O3A-PB	-3.80	119.79	132.83
58	KL	501	GDP	PA-O3A-PB	-3.80	119.80	132.83
58	JM	501	GDP	PA-O3A-PB	-3.80	119.80	132.83
56	MB	501	GTP	PB-O3B-PG	-3.80	119.80	132.83
56	BA	501	GTP	PA-O3A-PB	-3.79	119.80	132.83
56	HB	501	GTP	PA-O3A-PB	-3.79	119.81	132.83
56	JE	501	GTP	PA-O3A-PB	-3.79	119.82	132.83
58	WL	501	GDP	PA-O3A-PB	-3.79	119.82	132.83
58	NM	501	GDP	PA-O3A-PB	-3.79	119.83	132.83
58	SD	501	GDP	PA-O3A-PB	-3.79	119.83	132.83
56	IG	501	GTP	PB-O3B-PG	-3.79	119.83	132.83
56	SA	502	GTP	PB-O3B-PG	-3.79	119.83	132.83
58	KH	501	GDP	PA-O3A-PB	-3.78	119.84	132.83
56	FB	501	GTP	PB-O3B-PG	-3.78	119.86	132.83
58	BD	501	GDP	PA-O3A-PB	-3.78	119.87	132.83
58	TF	501	GDP	PA-O3A-PB	-3.78	119.87	132.83
58	LD	501	GDP	PA-O3A-PB	-3.77	119.89	132.83
56	SG	501	GTP	PB-O3B-PG	-3.77	119.89	132.83
58	QD	501	GDP	PA-O3A-PB	-3.77	119.89	132.83
56	NG	501	GTP	PA-O3A-PB	-3.77	119.90	132.83
56	QI	501	GTP	PA-O3A-PB	-3.76	119.92	132.83
58	AF	501	GDP	PA-O3A-PB	-3.76	119.92	132.83
58	AJ	501	GDP	PA-O3A-PB	-3.76	119.92	132.83
56	KI	501	GTP	PB-O3B-PG	-3.76	119.92	132.83
56	LB	501	GTP	PA-O3A-PB	-3.76	119.92	132.83
58	HD	501	GDP	PA-O3A-PB	-3.76	119.93	132.83
56	WE	501	GTP	PA-O3A-PB	-3.76	119.94	132.83
56	CB	501	GTP	PA-O3A-PB	-3.75	119.95	132.83
56	CA	501	GTP	PA-O3A-PB	-3.75	119.95	132.83
56	UI	501	GTP	PA-O3A-PB	-3.75	119.95	132.83
58	EB	501	GDP	PA-O3A-PB	-3.75	119.95	132.83
58	OC	501	GDP	PA-O3A-PB	-3.75	119.97	132.83
56	TK	501	GTP	PB-O3B-PG	-3.75	119.97	132.83
58	LJ	501	GDP	PA-O3A-PB	-3.74	119.99	132.83
56	WB	501	GTP	PB-O3B-PG	-3.74	119.99	132.83
56	OB	501	GTP	PB-O3B-PG	-3.73	120.01	132.83
56	SB	501	GTP	PB-O3B-PG	-3.73	120.01	132.83
58	RJ	501	GDP	PA-O3A-PB	-3.73	120.01	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	DH	501	GDP	PA-O3A-PB	-3.73	120.02	132.83
56	SK	501	GTP	PA-O3A-PB	-3.73	120.02	132.83
56	KK	501	GTP	PB-O3B-PG	-3.73	120.03	132.83
56	IK	501	GTP	PA-O3A-PB	-3.73	120.03	132.83
58	DD	501	GDP	PA-O3A-PB	-3.73	120.03	132.83
56	VK	501	GTP	PB-O3B-PG	-3.73	120.04	132.83
56	AG	501	GTP	PB-O3B-PG	-3.72	120.05	132.83
58	NJ	501	GDP	PA-O3A-PB	-3.72	120.05	132.83
56	PA	501	GTP	PA-O3A-PB	-3.72	120.07	132.83
56	AM	501	GTP	PA-O3A-PB	-3.72	120.07	132.83
56	WG	501	GTP	PA-O3A-PB	-3.72	120.07	132.83
58	OJ	501	GDP	PA-O3A-PB	-3.71	120.09	132.83
56	PB	501	GTP	PB-O3B-PG	-3.71	120.09	132.83
56	HG	501	GTP	PB-O3B-PG	-3.71	120.09	132.83
56	LA	501	GTP	PB-O3B-PG	-3.71	120.10	132.83
56	DB	501	GTP	PA-O3A-PB	-3.71	120.11	132.83
56	RA	501	GTP	PB-O3B-PG	-3.70	120.12	132.83
56	KB	501	GTP	PB-O3B-PG	-3.70	120.12	132.83
56	AI	501	GTP	PB-O3B-PG	-3.70	120.13	132.83
56	QK	501	GTP	PB-O3B-PG	-3.70	120.14	132.83
56	LK	501	GTP	PA-O3A-PB	-3.70	120.14	132.83
56	LA	501	GTP	PA-O3A-PB	-3.70	120.14	132.83
56	IA	501	GTP	PB-O3B-PG	-3.69	120.17	132.83
56	VB	501	GTP	PA-O3A-PB	-3.69	120.17	132.83
56	EI	501	GTP	PB-O3B-PG	-3.69	120.17	132.83
56	UI	501	GTP	PB-O3B-PG	-3.69	120.17	132.83
56	CM	501	GTP	PA-O3A-PB	-3.68	120.18	132.83
56	KE	501	GTP	PB-O3B-PG	-3.68	120.18	132.83
58	CD	501	GDP	PA-O3A-PB	-3.68	120.19	132.83
56	LG	501	GTP	PB-O3B-PG	-3.68	120.21	132.83
58	DF	501	GDP	PA-O3A-PB	-3.67	120.22	132.83
56	ME	501	GTP	PB-O3B-PG	-3.67	120.22	132.83
56	QB	501	GTP	PB-O3B-PG	-3.67	120.23	132.83
56	OE	501	GTP	PA-O3A-PB	-3.67	120.24	132.83
58	PH	501	GDP	PA-O3A-PB	-3.66	120.25	132.83
58	TM	501	GDP	PA-O3A-PB	-3.66	120.25	132.83
56	UB	501	GTP	PB-O3B-PG	-3.66	120.26	132.83
58	JJ	501	GDP	PA-O3A-PB	-3.66	120.26	132.83
56	II	501	GTP	PB-O3B-PG	-3.66	120.27	132.83
56	AE	501	GTP	PB-O3B-PG	-3.66	120.28	132.83
56	FK	501	GTP	PB-O3B-PG	-3.65	120.29	132.83
56	AA	501	GTP	PA-O3A-PB	-3.65	120.29	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	EK	501	GTP	PB-O3B-PG	-3.65	120.29	132.83
56	OG	501	GTP	PB-O3B-PG	-3.65	120.29	132.83
56	PA	501	GTP	PB-O3B-PG	-3.65	120.30	132.83
56	VI	501	GTP	PB-O3B-PG	-3.65	120.31	132.83
56	NG	501	GTP	PB-O3B-PG	-3.65	120.31	132.83
56	NB	501	GTP	PA-O3A-PB	-3.64	120.33	132.83
56	VG	501	GTP	PB-O3B-PG	-3.64	120.34	132.83
56	WE	501	GTP	PB-O3B-PG	-3.64	120.34	132.83
58	OF	501	GDP	PA-O3A-PB	-3.64	120.35	132.83
58	GM	501	GDP	PA-O3A-PB	-3.64	120.35	132.83
56	PI	501	GTP	PB-O3B-PG	-3.63	120.36	132.83
56	RE	501	GTP	PB-O3B-PG	-3.63	120.36	132.83
58	FD	501	GDP	PA-O3A-PB	-3.63	120.36	132.83
58	QF	501	GDP	C3'-C2'-C1'	3.63	106.45	100.98
58	VM	501	GDP	PA-O3A-PB	-3.63	120.36	132.83
56	SK	501	GTP	PB-O3B-PG	-3.63	120.37	132.83
56	GB	501	GTP	PB-O3B-PG	-3.63	120.38	132.83
56	NE	501	GTP	PB-O3B-PG	-3.63	120.38	132.83
56	VK	501	GTP	PA-O3A-PB	-3.62	120.40	132.83
58	SF	501	GDP	PA-O3A-PB	-3.62	120.40	132.83
56	PI	501	GTP	PA-O3A-PB	-3.62	120.41	132.83
56	OK	501	GTP	PA-O3A-PB	-3.62	120.41	132.83
56	AK	501	GTP	PB-O3B-PG	-3.62	120.41	132.83
56	PE	501	GTP	PB-O3B-PG	-3.62	120.42	132.83
56	OE	501	GTP	PB-O3B-PG	-3.61	120.44	132.83
56	LE	501	GTP	PB-O3B-PG	-3.61	120.45	132.83
56	QA	501	GTP	PA-O3A-PB	-3.60	120.46	132.83
58	UD	501	GDP	PA-O3A-PB	-3.60	120.47	132.83
58	GD	501	GDP	PA-O3A-PB	-3.60	120.48	132.83
56	ML	501	GTP	PB-O3B-PG	-3.59	120.49	132.83
56	VA	501	GTP	PB-O3B-PG	-3.59	120.49	132.83
56	MI	501	GTP	PB-O3B-PG	-3.59	120.49	132.83
58	IF	501	GDP	PA-O3A-PB	-3.59	120.50	132.83
56	OA	501	GTP	PB-O3B-PG	-3.59	120.50	132.83
58	LM	501	GDP	PA-O3A-PB	-3.59	120.51	132.83
56	PL	501	GTP	PB-O3B-PG	-3.59	120.51	132.83
56	TI	501	GTP	PB-O3B-PG	-3.59	120.51	132.83
56	AB	501	GTP	PB-O3B-PG	-3.59	120.51	132.83
56	MG	501	GTP	PB-O3B-PG	-3.59	120.52	132.83
56	HE	501	GTP	PA-O3A-PB	-3.58	120.54	132.83
56	CM	501	GTP	PB-O3B-PG	-3.58	120.54	132.83
56	IB	501	GTP	PB-O3B-PG	-3.58	120.54	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	QE	501	GTP	PB-O3B-PG	-3.58	120.55	132.83
56	BA	501	GTP	PB-O3B-PG	-3.58	120.55	132.83
58	LL	501	GDP	PA-O3A-PB	-3.58	120.55	132.83
58	AH	501	GDP	PA-O3A-PB	-3.58	120.56	132.83
58	PD	501	GDP	PA-O3A-PB	-3.58	120.56	132.83
56	DI	501	GTP	PB-O3B-PG	-3.57	120.57	132.83
56	JK	501	GTP	PB-O3B-PG	-3.57	120.58	132.83
56	SI	501	GTP	PB-O3B-PG	-3.57	120.58	132.83
58	PF	501	GDP	C3'-C2'-C1'	3.57	106.35	100.98
56	WB	501	GTP	PA-O3A-PB	-3.56	120.60	132.83
56	GA	501	GTP	PB-O3B-PG	-3.56	120.61	132.83
56	LI	501	GTP	PB-O3B-PG	-3.56	120.61	132.83
56	MA	501	GTP	PB-O3B-PG	-3.56	120.61	132.83
56	MK	501	GTP	PB-O3B-PG	-3.56	120.61	132.83
56	AE	501	GTP	PA-O3A-PB	-3.56	120.61	132.83
56	RK	501	GTP	PB-O3B-PG	-3.56	120.61	132.83
58	HC	501	GDP	PA-O3A-PB	-3.56	120.62	132.83
56	DG	501	GTP	PA-O3A-PB	-3.55	120.63	132.83
56	LB	501	GTP	PB-O3B-PG	-3.55	120.63	132.83
56	RB	501	GTP	PB-O3B-PG	-3.55	120.64	132.83
58	ED	501	GDP	C3'-C2'-C1'	3.55	106.32	100.98
56	PG	501	GTP	PB-O3B-PG	-3.55	120.65	132.83
56	AA	501	GTP	PB-O3B-PG	-3.54	120.66	132.83
56	OL	501	GTP	PA-O3A-PB	-3.54	120.67	132.83
56	EA	501	GTP	PB-O3B-PG	-3.54	120.68	132.83
58	UM	501	GDP	PA-O3A-PB	-3.54	120.69	132.83
56	JE	501	GTP	PB-O3B-PG	-3.54	120.69	132.83
56	JG	501	GTP	PB-O3B-PG	-3.53	120.71	132.83
56	RI	501	GTP	PB-O3B-PG	-3.53	120.71	132.83
58	HM	501	GDP	PA-O3A-PB	-3.53	120.72	132.83
56	TA	501	GTP	PB-O3B-PG	-3.53	120.73	132.83
56	AM	501	GTP	PB-O3B-PG	-3.52	120.73	132.83
56	CE	501	GTP	PB-O3B-PG	-3.52	120.74	132.83
58	GH	501	GDP	C3'-C2'-C1'	3.52	106.28	100.98
56	EC	501	GTP	PB-O3B-PG	-3.52	120.75	132.83
56	LK	501	GTP	PB-O3B-PG	-3.52	120.75	132.83
58	DL	501	GDP	PA-O3A-PB	-3.51	120.77	132.83
58	DD	501	GDP	C3'-C2'-C1'	3.51	106.27	100.98
58	AD	501	GDP	PA-O3A-PB	-3.51	120.77	132.83
56	HK	501	GTP	PB-O3B-PG	-3.51	120.77	132.83
56	DB	501	GTP	PB-O3B-PG	-3.51	120.78	132.83
56	KA	501	GTP	PB-O3B-PG	-3.51	120.78	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	PK	501	GTP	PB-O3B-PG	-3.51	120.79	132.83
56	CK	501	GTP	PB-O3B-PG	-3.51	120.79	132.83
56	FE	501	GTP	PA-O3A-PB	-3.50	120.80	132.83
58	DJ	501	GDP	C3'-C2'-C1'	3.50	106.25	100.98
56	JI	501	GTP	PB-O3B-PG	-3.50	120.83	132.83
56	HA	501	GTP	PB-O3B-PG	-3.50	120.83	132.83
56	JA	501	GTP	PB-O3B-PG	-3.49	120.83	132.83
56	FI	501	GTP	PA-O3A-PB	-3.49	120.84	132.83
56	UG	501	GTP	PA-O3A-PB	-3.49	120.85	132.83
56	OI	501	GTP	PB-O3B-PG	-3.49	120.85	132.83
56	CG	501	GTP	PA-O3A-PB	-3.49	120.85	132.83
56	WI	501	GTP	PA-O3A-PB	-3.49	120.86	132.83
56	II	501	GTP	PA-O3A-PB	-3.49	120.86	132.83
58	VH	501	GDP	C3'-C2'-C1'	3.49	106.23	100.98
58	ED	501	GDP	PA-O3A-PB	-3.49	120.87	132.83
56	QI	501	GTP	PB-O3B-PG	-3.48	120.88	132.83
56	NI	501	GTP	PA-O3A-PB	-3.48	120.89	132.83
56	PG	501	GTP	PA-O3A-PB	-3.47	120.90	132.83
56	DE	501	GTP	PB-O3B-PG	-3.47	120.91	132.83
56	HI	501	GTP	PA-O3A-PB	-3.47	120.94	132.83
58	RF	501	GDP	PA-O3A-PB	-3.46	120.94	132.83
56	DA	501	GTP	PB-O3B-PG	-3.46	120.95	132.83
56	JB	501	GTP	PB-O3B-PG	-3.46	120.96	132.83
58	NK	501	GDP	PA-O3A-PB	-3.46	120.97	132.83
56	WI	501	GTP	PB-O3B-PG	-3.46	120.97	132.83
56	EG	501	GTP	PB-O3B-PG	-3.46	120.97	132.83
56	EE	501	GTP	C5-C6-N1	3.45	120.05	113.95
56	NA	501	GTP	PB-O3B-PG	-3.45	120.99	132.83
56	SE	501	GTP	PA-O3A-PB	-3.45	121.00	132.83
58	OH	501	GDP	C3'-C2'-C1'	3.45	106.17	100.98
56	JK	501	GTP	PA-O3A-PB	-3.44	121.01	132.83
58	BC	501	GDP	PA-O3A-PB	-3.44	121.02	132.83
58	VL	501	GDP	PA-O3A-PB	-3.44	121.03	132.83
58	QF	501	GDP	PA-O3A-PB	-3.43	121.04	132.83
56	OL	501	GTP	PB-O3B-PG	-3.43	121.04	132.83
56	DM	501	GTP	PB-O3B-PG	-3.43	121.05	132.83
56	CB	501	GTP	C5-C6-N1	3.43	120.00	113.95
58	IC	501	GDP	C3'-C2'-C1'	3.42	106.13	100.98
56	CB	501	GTP	PB-O3B-PG	-3.42	121.08	132.83
58	KJ	501	GDP	PA-O3A-PB	-3.42	121.11	132.83
56	GI	501	GTP	PB-O3B-PG	-3.41	121.11	132.83
56	BM	501	GTP	PA-O3A-PB	-3.41	121.14	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	HM	501	GDP	C3'-C2'-C1'	3.40	106.10	100.98
58	VM	501	GDP	C3'-C2'-C1'	3.40	106.10	100.98
58	JL	501	GDP	PA-O3A-PB	-3.40	121.17	132.83
56	GI	501	GTP	PA-O3A-PB	-3.40	121.18	132.83
56	TG	501	GTP	PB-O3B-PG	-3.40	121.18	132.83
56	KK	501	GTP	PA-O3A-PB	-3.39	121.18	132.83
58	WH	501	GDP	PA-O3A-PB	-3.39	121.19	132.83
56	WK	501	GTP	PB-O3B-PG	-3.39	121.19	132.83
56	PB	501	GTP	C5-C6-N1	3.39	119.94	113.95
58	NM	501	GDP	C3'-C2'-C1'	3.39	106.08	100.98
58	LM	501	GDP	C3'-C2'-C1'	3.38	106.07	100.98
56	OL	501	GTP	C5-C6-N1	3.38	119.93	113.95
58	KJ	501	GDP	C3'-C2'-C1'	3.38	106.07	100.98
56	BE	501	GTP	C5-C6-N1	3.38	119.92	113.95
56	BI	501	GTP	PA-O3A-PB	-3.38	121.23	132.83
56	FB	501	GTP	C5-C6-N1	3.37	119.91	113.95
56	IK	501	GTP	PB-O3B-PG	-3.37	121.26	132.83
56	LE	501	GTP	C5-C6-N1	3.37	119.90	113.95
58	EF	501	GDP	C3'-C2'-C1'	3.36	106.04	100.98
56	IA	501	GTP	C5-C6-N1	3.36	119.89	113.95
58	OD	501	GDP	C3'-C2'-C1'	3.36	106.04	100.98
56	IE	501	GTP	PA-O3A-PB	-3.36	121.30	132.83
56	GK	501	GTP	PB-O3B-PG	-3.36	121.31	132.83
56	EG	501	GTP	C5-C6-N1	3.35	119.88	113.95
56	TB	501	GTP	PB-O3B-PG	-3.35	121.32	132.83
58	KL	501	GDP	C3'-C2'-C1'	3.35	106.03	100.98
56	SG	501	GTP	C5-C6-N1	3.35	119.87	113.95
56	EC	501	GTP	C5-C6-N1	3.35	119.87	113.95
58	PF	501	GDP	PA-O3A-PB	-3.35	121.33	132.83
56	CE	501	GTP	C5-C6-N1	3.35	119.86	113.95
56	RG	501	GTP	C5-C6-N1	3.35	119.86	113.95
56	DK	501	GTP	PB-O3B-PG	-3.34	121.37	132.83
56	NB	501	GTP	PB-O3B-PG	-3.34	121.37	132.83
56	OA	501	GTP	C5-C6-N1	3.34	119.84	113.95
56	GB	501	GTP	C5-C6-N1	3.34	119.84	113.95
58	KH	501	GDP	C3'-C2'-C1'	3.34	106.00	100.98
56	WB	501	GTP	C5-C6-N1	3.33	119.84	113.95
56	RL	501	GTP	C5-C6-N1	3.33	119.83	113.95
56	KK	501	GTP	C5-C6-N1	3.33	119.83	113.95
56	RG	501	GTP	PB-O3B-PG	-3.33	121.41	132.83
56	JA	501	GTP	C5-C6-N1	3.32	119.82	113.95
56	FM	501	GTP	C5-C6-N1	3.32	119.82	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	TB	501	GTP	C5-C6-N1	3.32	119.82	113.95
56	JB	501	GTP	C5-C6-N1	3.32	119.82	113.95
56	BI	501	GTP	C5-C6-N1	3.32	119.81	113.95
56	IB	501	GTP	C5-C6-N1	3.32	119.81	113.95
56	PE	501	GTP	C5-C6-N1	3.32	119.81	113.95
56	PL	501	GTP	C5-C6-N1	3.32	119.81	113.95
56	OE	501	GTP	C5-C6-N1	3.32	119.81	113.95
56	HB	501	GTP	PB-O3B-PG	-3.32	121.44	132.83
56	LK	501	GTP	C5-C6-N1	3.32	119.81	113.95
56	MG	501	GTP	C5-C6-N1	3.32	119.81	113.95
58	AJ	501	GDP	C3'-C2'-C1'	3.31	105.97	100.98
58	MF	501	GDP	C3'-C2'-C1'	3.31	105.97	100.98
56	KB	501	GTP	C5-C6-N1	3.31	119.80	113.95
56	HE	501	GTP	C5-C6-N1	3.31	119.80	113.95
56	SB	501	GTP	C5-C6-N1	3.31	119.80	113.95
58	UM	501	GDP	C3'-C2'-C1'	3.31	105.97	100.98
56	KA	501	GTP	C5-C6-N1	3.31	119.80	113.95
56	HK	501	GTP	C5-C6-N1	3.31	119.80	113.95
58	GM	501	GDP	C3'-C2'-C1'	3.31	105.96	100.98
56	TK	501	GTP	C5-C6-N1	3.31	119.79	113.95
58	TF	501	GDP	C3'-C2'-C1'	3.30	105.95	100.98
56	IE	501	GTP	C5-C6-N1	3.30	119.79	113.95
56	NB	501	GTP	C5-C6-N1	3.30	119.78	113.95
56	WE	501	GTP	C5-C6-N1	3.30	119.78	113.95
58	OC	501	GDP	C3'-C2'-C1'	3.30	105.95	100.98
56	GK	501	GTP	C5-C6-N1	3.30	119.78	113.95
56	VK	501	GTP	C5-C6-N1	3.30	119.78	113.95
56	UE	501	GTP	C5-C6-N1	3.30	119.78	113.95
56	DA	501	GTP	C5-C6-N1	3.30	119.78	113.95
56	SA	502	GTP	C5-C6-N1	3.30	119.78	113.95
56	SK	501	GTP	C5-C6-N1	3.30	119.78	113.95
56	AI	501	GTP	C5-C6-N1	3.30	119.78	113.95
56	JG	501	GTP	C5-C6-N1	3.30	119.77	113.95
56	SI	501	GTP	C5-C6-N1	3.30	119.77	113.95
56	OI	501	GTP	C5-C6-N1	3.29	119.77	113.95
56	LA	501	GTP	C5-C6-N1	3.29	119.77	113.95
56	QL	501	GTP	C5-C6-N1	3.29	119.77	113.95
56	MK	501	GTP	PA-O3A-PB	-3.29	121.53	132.83
56	DE	501	GTP	C5-C6-N1	3.29	119.77	113.95
56	PI	501	GTP	C5-C6-N1	3.29	119.76	113.95
56	MK	501	GTP	C5-C6-N1	3.29	119.76	113.95
56	RB	501	GTP	C5-C6-N1	3.29	119.76	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BG	501	GTP	C5-C6-N1	3.29	119.76	113.95
56	DB	501	GTP	C5-C6-N1	3.29	119.76	113.95
56	CA	501	GTP	C5-C6-N1	3.29	119.75	113.95
56	HB	501	GTP	C5-C6-N1	3.29	119.75	113.95
56	SE	501	GTP	C5-C6-N1	3.28	119.75	113.95
56	JE	501	GTP	C5-C6-N1	3.28	119.75	113.95
56	WK	501	GTP	C5-C6-N1	3.28	119.75	113.95
56	AM	501	GTP	C5-C6-N1	3.28	119.75	113.95
56	FI	501	GTP	C5-C6-N1	3.28	119.75	113.95
56	QA	501	GTP	C5-C6-N1	3.28	119.75	113.95
58	RH	501	GDP	C3'-C2'-C1'	3.28	105.92	100.98
56	WG	501	GTP	C5-C6-N1	3.28	119.75	113.95
56	NE	501	GTP	C5-C6-N1	3.28	119.74	113.95
56	RE	501	GTP	C5-C6-N1	3.28	119.74	113.95
56	KG	501	GTP	C5-C6-N1	3.28	119.74	113.95
56	TG	501	GTP	C5-C6-N1	3.28	119.74	113.95
56	FK	501	GTP	C5-C6-N1	3.28	119.74	113.95
56	PK	501	GTP	C5-C6-N1	3.28	119.74	113.95
58	BC	501	GDP	C3'-C2'-C1'	3.27	105.91	100.98
56	QG	501	GTP	C5-C6-N1	3.27	119.73	113.95
56	RI	501	GTP	C5-C6-N1	3.27	119.73	113.95
56	IK	501	GTP	C5-C6-N1	3.27	119.73	113.95
56	MB	501	GTP	C5-C6-N1	3.27	119.73	113.95
56	NG	501	GTP	C5-C6-N1	3.27	119.73	113.95
56	EK	501	GTP	C5-C6-N1	3.27	119.73	113.95
56	QK	501	GTP	C5-C6-N1	3.27	119.73	113.95
56	UA	501	GTP	C5-C6-N1	3.27	119.73	113.95
56	DG	501	GTP	PB-O3B-PG	-3.27	121.60	132.83
56	VA	501	GTP	C5-C6-N1	3.27	119.73	113.95
58	TM	501	GDP	C3'-C2'-C1'	3.27	105.90	100.98
56	GG	501	GTP	C5-C6-N1	3.27	119.72	113.95
56	TA	501	GTP	C5-C6-N1	3.27	119.72	113.95
56	TE	501	GTP	C5-C6-N1	3.27	119.72	113.95
56	KI	501	GTP	C5-C6-N1	3.27	119.72	113.95
56	BB	501	GTP	C5-C6-N1	3.27	119.72	113.95
56	FG	501	GTP	C5-C6-N1	3.27	119.72	113.95
58	WF	501	GDP	C3'-C2'-C1'	3.27	105.90	100.98
56	PG	501	GTP	C5-C6-N1	3.27	119.72	113.95
56	AB	501	GTP	C5-C6-N1	3.27	119.72	113.95
56	HI	501	GTP	C5-C6-N1	3.27	119.72	113.95
56	EI	501	GTP	C5-C6-N1	3.26	119.72	113.95
56	ME	501	GTP	C5-C6-N1	3.26	119.72	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	NA	501	GTP	C5-C6-N1	3.26	119.71	113.95
56	RA	501	GTP	C5-C6-N1	3.26	119.71	113.95
58	GC	501	GDP	C3'-C2'-C1'	3.26	105.89	100.98
56	HA	501	GTP	C5-C6-N1	3.26	119.71	113.95
56	GA	501	GTP	PA-O3A-PB	-3.26	121.63	132.83
56	II	501	GTP	C5-C6-N1	3.26	119.71	113.95
56	VE	501	GTP	C5-C6-N1	3.26	119.71	113.95
58	HD	501	GDP	C3'-C2'-C1'	3.26	105.89	100.98
56	AK	501	GTP	C5-C6-N1	3.26	119.71	113.95
56	DG	501	GTP	C5-C6-N1	3.26	119.71	113.95
56	MA	501	GTP	C5-C6-N1	3.26	119.71	113.95
56	OG	501	GTP	C5-C6-N1	3.26	119.71	113.95
58	LJ	501	GDP	C3'-C2'-C1'	3.26	105.88	100.98
56	GA	501	GTP	C3'-C2'-C1'	3.26	105.88	100.98
58	HF	501	GDP	C3'-C2'-C1'	3.26	105.88	100.98
58	MC	501	GDP	C3'-C2'-C1'	3.26	105.88	100.98
58	UD	501	GDP	C3'-C2'-C1'	3.26	105.88	100.98
56	GE	501	GTP	C5-C6-N1	3.26	119.70	113.95
56	LB	501	GTP	C5-C6-N1	3.26	119.70	113.95
56	IM	501	GTP	C5-C6-N1	3.25	119.70	113.95
58	KC	501	GDP	C3'-C2'-C1'	3.25	105.88	100.98
56	BA	501	GTP	C5-C6-N1	3.25	119.69	113.95
56	IM	501	GTP	PA-O3A-PB	-3.25	121.67	132.83
56	CM	501	GTP	C5-C6-N1	3.25	119.69	113.95
56	NI	501	GTP	C5-C6-N1	3.25	119.69	113.95
56	AA	501	GTP	C5-C6-N1	3.25	119.69	113.95
56	UB	501	GTP	C5-C6-N1	3.25	119.69	113.95
56	CI	501	GTP	C5-C6-N1	3.25	119.69	113.95
56	JI	501	GTP	C5-C6-N1	3.25	119.69	113.95
58	CH	501	GDP	C3'-C2'-C1'	3.25	105.87	100.98
56	RK	501	GTP	C5-C6-N1	3.25	119.69	113.95
58	AH	501	GDP	C3'-C2'-C1'	3.25	105.87	100.98
56	VB	501	GTP	C5-C6-N1	3.25	119.69	113.95
56	HG	501	GTP	C5-C6-N1	3.25	119.68	113.95
56	LG	501	GTP	C5-C6-N1	3.25	119.68	113.95
56	DI	501	GTP	C5-C6-N1	3.24	119.68	113.95
58	WJ	501	GDP	C3'-C2'-C1'	3.24	105.86	100.98
56	IG	501	GTP	PA-O3A-PB	-3.24	121.70	132.83
56	SG	501	GTP	PA-O3A-PB	-3.24	121.70	132.83
56	FE	501	GTP	C5-C6-N1	3.24	119.68	113.95
56	LI	501	GTP	C5-C6-N1	3.24	119.68	113.95
56	ML	501	GTP	C5-C6-N1	3.24	119.68	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AC	501	GDP	C3'-C2'-C1'	3.24	105.86	100.98
58	SH	501	GDP	C3'-C2'-C1'	3.24	105.86	100.98
58	KM	501	GDP	C3'-C2'-C1'	3.24	105.86	100.98
56	OB	501	GTP	C5-C6-N1	3.24	119.67	113.95
56	VI	501	GTP	C5-C6-N1	3.24	119.67	113.95
56	WI	501	GTP	C5-C6-N1	3.24	119.67	113.95
56	NL	501	GTP	C5-C6-N1	3.24	119.67	113.95
56	JK	501	GTP	C5-C6-N1	3.24	119.67	113.95
56	MI	501	GTP	C5-C6-N1	3.23	119.66	113.95
58	KM	501	GDP	PA-O3A-PB	-3.23	121.73	132.83
56	DM	501	GTP	C5-C6-N1	3.23	119.66	113.95
56	UK	501	GTP	C5-C6-N1	3.23	119.66	113.95
56	EA	501	GTP	C5-C6-N1	3.23	119.66	113.95
56	AE	501	GTP	C5-C6-N1	3.23	119.66	113.95
56	BM	501	GTP	C5-C6-N1	3.23	119.66	113.95
56	BK	501	GTP	C5-C6-N1	3.23	119.66	113.95
56	IG	501	GTP	C5-C6-N1	3.23	119.65	113.95
56	OK	501	GTP	C5-C6-N1	3.23	119.65	113.95
58	GF	501	GDP	C3'-C2'-C1'	3.23	105.84	100.98
56	TA	501	GTP	PA-O3A-PB	-3.23	121.75	132.83
58	BL	501	GDP	C3'-C2'-C1'	3.22	105.83	100.98
58	IF	501	GDP	C3'-C2'-C1'	3.22	105.83	100.98
56	KE	501	GTP	C5-C6-N1	3.22	119.64	113.95
56	AG	501	GTP	C5-C6-N1	3.22	119.63	113.95
58	SF	501	GDP	C3'-C2'-C1'	3.22	105.82	100.98
58	MM	501	GDP	PA-O3A-PB	-3.22	121.79	132.83
58	QH	501	GDP	PA-O3A-PB	-3.21	121.80	132.83
58	FF	501	GDP	C3'-C2'-C1'	3.21	105.81	100.98
58	UF	501	GDP	C3'-C2'-C1'	3.21	105.81	100.98
58	NK	501	GDP	C3'-C2'-C1'	3.21	105.81	100.98
58	LF	501	GDP	PA-O3A-PB	-3.21	121.82	132.83
56	VG	501	GTP	C5-C6-N1	3.21	119.61	113.95
56	UG	501	GTP	C5-C6-N1	3.20	119.61	113.95
56	CK	501	GTP	C5-C6-N1	3.20	119.61	113.95
56	QB	501	GTP	C5-C6-N1	3.20	119.60	113.95
58	SJ	501	GDP	C3'-C2'-C1'	3.20	105.79	100.98
56	QG	501	GTP	PB-O3B-PG	-3.20	121.86	132.83
58	NC	501	GDP	PA-O3A-PB	-3.20	121.86	132.83
56	GI	501	GTP	C5-C6-N1	3.20	119.60	113.95
56	WA	501	GTP	C5-C6-N1	3.20	119.60	113.95
56	UE	501	GTP	C3'-C2'-C1'	3.19	105.78	100.98
56	DK	501	GTP	C5-C6-N1	3.19	119.58	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	QE	501	GTP	C5-C6-N1	3.19	119.58	113.95
56	GA	501	GTP	C5-C6-N1	3.18	119.56	113.95
58	TC	501	GDP	C3'-C2'-C1'	3.18	105.76	100.98
56	QL	501	GTP	PB-O3B-PG	-3.17	121.94	132.83
58	CL	501	GDP	C3'-C2'-C1'	3.17	105.75	100.98
58	PH	501	GDP	C3'-C2'-C1'	3.17	105.75	100.98
56	OG	501	GTP	C3'-C2'-C1'	3.17	105.75	100.98
56	UI	501	GTP	C5-C6-N1	3.17	119.54	113.95
58	LH	501	GDP	C3'-C2'-C1'	3.16	105.74	100.98
58	MJ	501	GDP	C3'-C2'-C1'	3.16	105.74	100.98
56	GI	501	GTP	C3'-C2'-C1'	3.16	105.73	100.98
56	TI	501	GTP	C5-C6-N1	3.16	119.53	113.95
56	CI	501	GTP	PB-O3B-PG	-3.15	122.00	132.83
58	JM	501	GDP	C3'-C2'-C1'	3.15	105.72	100.98
56	VE	501	GTP	PA-O3A-PB	-3.15	122.02	132.83
56	CK	501	GTP	PA-O3A-PB	-3.15	122.02	132.83
56	QL	501	GTP	C3'-C2'-C1'	3.15	105.72	100.98
56	SA	502	GTP	PA-O3A-PB	-3.15	122.03	132.83
58	CC	501	GDP	C3'-C2'-C1'	3.14	105.71	100.98
56	BB	501	GTP	C3'-C2'-C1'	3.14	105.71	100.98
58	AL	501	GDP	C3'-C2'-C1'	3.14	105.71	100.98
56	AK	501	GTP	PA-O3A-PB	-3.14	122.05	132.83
56	BE	501	GTP	C3'-C2'-C1'	3.14	105.70	100.98
58	AF	501	GDP	C3'-C2'-C1'	3.13	105.69	100.98
56	IA	501	GTP	C3'-C2'-C1'	3.13	105.69	100.98
56	NE	501	GTP	C3'-C2'-C1'	3.13	105.69	100.98
58	FD	501	GDP	C3'-C2'-C1'	3.13	105.69	100.98
56	CG	501	GTP	C5-C6-N1	3.13	119.47	113.95
56	BK	501	GTP	C3'-C2'-C1'	3.13	105.69	100.98
56	VG	501	GTP	C3'-C2'-C1'	3.13	105.68	100.98
56	BB	501	GTP	PB-O3B-PG	-3.12	122.10	132.83
58	VC	501	GDP	C3'-C2'-C1'	3.12	105.68	100.98
56	TG	501	GTP	C2-N1-C6	-3.12	119.35	125.10
56	ME	501	GTP	PA-O3A-PB	-3.12	122.12	132.83
56	WA	501	GTP	C3'-C2'-C1'	3.12	105.68	100.98
56	TG	501	GTP	C8-N7-C5	3.11	108.92	102.99
58	OD	501	GDP	PA-O3A-PB	-3.11	122.15	132.83
58	NH	501	GDP	C3'-C2'-C1'	3.11	105.66	100.98
58	PM	501	GDP	C3'-C2'-C1'	3.11	105.66	100.98
58	SC	501	GDP	C3'-C2'-C1'	3.11	105.66	100.98
56	PA	501	GTP	C5-C6-N1	3.11	119.44	113.95
58	PJ	501	GDP	C3'-C2'-C1'	3.10	105.65	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	SE	501	GTP	C8-N7-C5	3.10	108.89	102.99
56	RL	501	GTP	C3'-C2'-C1'	3.10	105.64	100.98
58	HH	501	GDP	C3'-C2'-C1'	3.09	105.64	100.98
56	GK	501	GTP	C8-N7-C5	3.09	108.88	102.99
58	VJ	501	GDP	C3'-C2'-C1'	3.09	105.63	100.98
56	CE	501	GTP	C8-N7-C5	3.09	108.88	102.99
56	LE	501	GTP	C8-N7-C5	3.09	108.88	102.99
56	DI	501	GTP	C3'-C2'-C1'	3.09	105.63	100.98
56	GG	501	GTP	C8-N7-C5	3.09	108.87	102.99
56	FI	501	GTP	C3'-C2'-C1'	3.09	105.62	100.98
56	II	501	GTP	C8-N7-C5	3.08	108.87	102.99
56	LA	501	GTP	C8-N7-C5	3.08	108.87	102.99
56	PE	501	GTP	C8-N7-C5	3.08	108.86	102.99
58	JJ	501	GDP	C3'-C2'-C1'	3.08	105.62	100.98
56	AI	501	GTP	C3'-C2'-C1'	3.08	105.61	100.98
56	AB	501	GTP	C8-N7-C5	3.08	108.85	102.99
56	FG	501	GTP	C8-N7-C5	3.08	108.85	102.99
56	PK	501	GTP	C3'-C2'-C1'	3.07	105.60	100.98
56	HE	501	GTP	C8-N7-C5	3.07	108.84	102.99
58	ND	501	GDP	C3'-C2'-C1'	3.07	105.60	100.98
56	UB	501	GTP	C8-N7-C5	3.07	108.84	102.99
56	UK	501	GTP	C8-N7-C5	3.07	108.84	102.99
56	QG	501	GTP	PA-O3A-PB	-3.07	122.30	132.83
56	UA	501	GTP	C8-N7-C5	3.07	108.83	102.99
56	OA	501	GTP	C8-N7-C5	3.07	108.83	102.99
58	IJ	501	GDP	C3'-C2'-C1'	3.07	105.59	100.98
56	OE	501	GTP	C8-N7-C5	3.07	108.83	102.99
56	BG	501	GTP	PA-O3A-PB	-3.07	122.31	132.83
56	ML	501	GTP	C3'-C2'-C1'	3.06	105.59	100.98
58	OJ	501	GDP	C3'-C2'-C1'	3.06	105.59	100.98
56	HK	501	GTP	C8-N7-C5	3.06	108.82	102.99
56	IE	501	GTP	C8-N7-C5	3.06	108.82	102.99
56	FK	501	GTP	C8-N7-C5	3.06	108.82	102.99
56	MG	501	GTP	PA-O3A-PB	-3.06	122.32	132.83
56	WG	501	GTP	C3'-C2'-C1'	3.06	105.59	100.98
56	GB	501	GTP	C3'-C2'-C1'	3.06	105.58	100.98
58	BH	501	GDP	C3'-C2'-C1'	3.06	105.58	100.98
56	NA	501	GTP	C3'-C2'-C1'	3.06	105.58	100.98
56	WK	501	GTP	C8-N7-C5	3.06	108.81	102.99
56	TA	501	GTP	C3'-C2'-C1'	3.06	105.58	100.98
56	BE	501	GTP	C2-N1-C6	-3.06	119.47	125.10
56	TK	501	GTP	C8-N7-C5	3.05	108.81	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	PL	501	GTP	C3'-C2'-C1'	3.05	105.58	100.98
56	QI	501	GTP	C5-C6-N1	3.05	119.34	113.95
56	HG	501	GTP	C8-N7-C5	3.05	108.80	102.99
56	NL	501	GTP	PA-O3A-PB	-3.05	122.36	132.83
56	RB	501	GTP	PA-O3A-PB	-3.05	122.36	132.83
56	OL	501	GTP	C8-N7-C5	3.05	108.80	102.99
56	VI	501	GTP	C8-N7-C5	3.05	108.80	102.99
56	BA	501	GTP	C3'-C2'-C1'	3.05	105.57	100.98
56	AA	501	GTP	C8-N7-C5	3.05	108.80	102.99
56	EC	501	GTP	C8-N7-C5	3.05	108.80	102.99
56	PB	501	GTP	C8-N7-C5	3.05	108.79	102.99
56	DA	501	GTP	C8-N7-C5	3.05	108.79	102.99
56	JI	501	GTP	C8-N7-C5	3.05	108.79	102.99
58	UH	501	GDP	C3'-C2'-C1'	3.04	105.56	100.98
58	WC	501	GDP	C3'-C2'-C1'	3.04	105.56	100.98
56	WB	501	GTP	C8-N7-C5	3.04	108.79	102.99
58	IL	501	GDP	C3'-C2'-C1'	3.04	105.56	100.98
58	OF	501	GDP	C3'-C2'-C1'	3.04	105.56	100.98
58	DJ	501	GDP	PA-O3A-PB	-3.04	122.38	132.83
56	GI	501	GTP	C8-N7-C5	3.04	108.78	102.99
58	FM	502	GDP	C3'-C2'-C1'	3.04	105.56	100.98
56	HI	501	GTP	C8-N7-C5	3.04	108.78	102.99
56	IM	501	GTP	C8-N7-C5	3.04	108.78	102.99
56	NI	501	GTP	C8-N7-C5	3.04	108.78	102.99
56	VK	501	GTP	C8-N7-C5	3.04	108.78	102.99
56	DE	501	GTP	C8-N7-C5	3.04	108.78	102.99
56	NL	501	GTP	C3'-C2'-C1'	3.04	105.55	100.98
58	UJ	501	GDP	C3'-C2'-C1'	3.04	105.55	100.98
56	TE	501	GTP	C8-N7-C5	3.04	108.78	102.99
56	CA	501	GTP	C8-N7-C5	3.04	108.78	102.99
56	SK	501	GTP	C8-N7-C5	3.04	108.78	102.99
56	PA	501	GTP	C3'-C2'-C1'	3.04	105.55	100.98
58	NJ	501	GDP	C3'-C2'-C1'	3.04	105.55	100.98
56	GA	501	GTP	C8-N7-C5	3.04	108.77	102.99
56	VA	501	GTP	C8-N7-C5	3.03	108.77	102.99
56	OA	501	GTP	C3'-C2'-C1'	3.03	105.55	100.98
56	LK	501	GTP	C8-N7-C5	3.03	108.77	102.99
56	SA	502	GTP	C8-N7-C5	3.03	108.77	102.99
56	QL	501	GTP	PA-O3A-PB	-3.03	122.42	132.83
56	BE	501	GTP	C8-N7-C5	3.03	108.77	102.99
56	HB	501	GTP	C3'-C2'-C1'	3.03	105.54	100.98
56	FM	501	GTP	C8-N7-C5	3.03	108.76	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	UC	501	GDP	C3'-C2'-C1'	3.03	105.54	100.98
56	FB	501	GTP	C8-N7-C5	3.03	108.76	102.99
56	VA	501	GTP	C3'-C2'-C1'	3.03	105.54	100.98
58	FL	501	GDP	C3'-C2'-C1'	3.03	105.54	100.98
56	IG	501	GTP	C8-N7-C5	3.03	108.76	102.99
56	WI	501	GTP	C3'-C2'-C1'	3.03	105.53	100.98
56	NB	501	GTP	C8-N7-C5	3.03	108.75	102.99
56	DB	501	GTP	C8-N7-C5	3.03	108.75	102.99
56	CM	501	GTP	C8-N7-C5	3.02	108.75	102.99
56	AE	501	GTP	C8-N7-C5	3.02	108.75	102.99
56	JE	501	GTP	C8-N7-C5	3.02	108.75	102.99
56	ME	501	GTP	C8-N7-C5	3.02	108.75	102.99
56	JB	501	GTP	C8-N7-C5	3.02	108.75	102.99
58	VF	501	GDP	C3'-C2'-C1'	3.02	105.53	100.98
56	DK	501	GTP	C8-N7-C5	3.02	108.75	102.99
56	MI	501	GTP	C8-N7-C5	3.02	108.75	102.99
56	SG	501	GTP	C8-N7-C5	3.02	108.75	102.99
56	OI	501	GTP	C3'-C2'-C1'	3.02	105.53	100.98
56	KB	501	GTP	C8-N7-C5	3.02	108.74	102.99
56	OG	501	GTP	C8-N7-C5	3.02	108.74	102.99
56	VE	501	GTP	C8-N7-C5	3.02	108.74	102.99
56	JB	501	GTP	C3'-C2'-C1'	3.02	105.52	100.98
56	BI	501	GTP	C8-N7-C5	3.02	108.74	102.99
56	MG	501	GTP	C8-N7-C5	3.02	108.74	102.99
56	AI	501	GTP	C8-N7-C5	3.02	108.73	102.99
56	AK	501	GTP	C8-N7-C5	3.02	108.73	102.99
56	KA	501	GTP	C8-N7-C5	3.01	108.73	102.99
56	KG	501	GTP	C8-N7-C5	3.01	108.73	102.99
58	PF	501	GDP	C5-C6-N1	3.01	119.27	113.95
56	MB	501	GTP	C8-N7-C5	3.01	108.73	102.99
56	FI	501	GTP	C8-N7-C5	3.01	108.73	102.99
56	BB	501	GTP	C8-N7-C5	3.01	108.73	102.99
56	QB	501	GTP	C8-N7-C5	3.01	108.73	102.99
56	FE	501	GTP	C8-N7-C5	3.01	108.73	102.99
56	PG	501	GTP	C8-N7-C5	3.01	108.72	102.99
56	PK	501	GTP	C8-N7-C5	3.01	108.72	102.99
56	QG	501	GTP	C8-N7-C5	3.01	108.72	102.99
56	RI	501	GTP	C8-N7-C5	3.01	108.72	102.99
56	CI	501	GTP	C8-N7-C5	3.01	108.72	102.99
56	EG	501	GTP	C8-N7-C5	3.01	108.72	102.99
56	QI	501	GTP	C8-N7-C5	3.01	108.72	102.99
58	DC	501	GDP	C3'-C2'-C1'	3.01	105.50	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	LI	501	GTP	C8-N7-C5	3.01	108.72	102.99
56	ML	501	GTP	C8-N7-C5	3.01	108.72	102.99
56	OI	501	GTP	C8-N7-C5	3.01	108.72	102.99
56	RB	501	GTP	C8-N7-C5	3.01	108.72	102.99
56	FM	501	GTP	C3'-C2'-C1'	3.00	105.50	100.98
56	DI	501	GTP	C8-N7-C5	3.00	108.71	102.99
56	OB	501	GTP	C8-N7-C5	3.00	108.71	102.99
56	DM	501	GTP	C8-N7-C5	3.00	108.71	102.99
56	BK	501	GTP	C8-N7-C5	3.00	108.71	102.99
56	EK	501	GTP	C8-N7-C5	3.00	108.71	102.99
56	QA	501	GTP	C8-N7-C5	3.00	108.71	102.99
56	PB	501	GTP	C3'-C2'-C1'	3.00	105.50	100.98
58	TH	501	GDP	C3'-C2'-C1'	3.00	105.50	100.98
56	BM	501	GTP	C8-N7-C5	3.00	108.71	102.99
56	UG	501	GTP	C8-N7-C5	3.00	108.71	102.99
56	WE	501	GTP	C8-N7-C5	3.00	108.71	102.99
56	NA	501	GTP	C8-N7-C5	3.00	108.70	102.99
56	PI	501	GTP	C8-N7-C5	3.00	108.70	102.99
56	VB	501	GTP	C8-N7-C5	3.00	108.70	102.99
56	DK	501	GTP	C3'-C2'-C1'	3.00	105.49	100.98
56	SG	501	GTP	C2-N1-C6	-3.00	119.58	125.10
56	HA	501	GTP	C8-N7-C5	3.00	108.70	102.99
56	MK	501	GTP	C8-N7-C5	3.00	108.70	102.99
58	NC	501	GDP	C3'-C2'-C1'	3.00	105.49	100.98
56	JA	501	GTP	C8-N7-C5	3.00	108.70	102.99
56	PI	501	GTP	C2-N1-C6	-3.00	119.58	125.10
56	QE	501	GTP	C8-N7-C5	3.00	108.70	102.99
56	TB	501	GTP	C8-N7-C5	3.00	108.70	102.99
56	LB	501	GTP	C3'-C2'-C1'	3.00	105.49	100.98
56	KE	501	GTP	C8-N7-C5	3.00	108.70	102.99
56	NL	501	GTP	C8-N7-C5	3.00	108.70	102.99
58	BJ	501	GDP	C3'-C2'-C1'	3.00	105.49	100.98
56	BG	501	GTP	C8-N7-C5	2.99	108.69	102.99
56	AM	501	GTP	C8-N7-C5	2.99	108.69	102.99
56	BA	501	GTP	C8-N7-C5	2.99	108.69	102.99
56	FM	501	GTP	C2-N1-C6	-2.99	119.59	125.10
56	QG	501	GTP	C2-N1-C6	-2.99	119.59	125.10
56	GB	501	GTP	C8-N7-C5	2.99	108.69	102.99
56	QK	501	GTP	C8-N7-C5	2.99	108.69	102.99
56	TA	501	GTP	C8-N7-C5	2.99	108.69	102.99
56	KE	501	GTP	C3'-C2'-C1'	2.99	105.48	100.98
56	DK	501	GTP	PA-O3A-PB	-2.99	122.57	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BM	501	GTP	C2-N1-C6	-2.99	119.59	125.10
56	EA	501	GTP	C3'-C2'-C1'	2.99	105.48	100.98
56	LI	501	GTP	C3'-C2'-C1'	2.99	105.48	100.98
56	VE	501	GTP	C3'-C2'-C1'	2.99	105.48	100.98
56	TI	501	GTP	C8-N7-C5	2.99	108.68	102.99
56	BM	501	GTP	PB-O3B-PG	-2.99	122.58	132.83
56	RG	501	GTP	C2-N1-C6	-2.99	119.60	125.10
56	KI	501	GTP	C8-N7-C5	2.99	108.68	102.99
56	WI	501	GTP	C8-N7-C5	2.99	108.68	102.99
56	UE	501	GTP	C8-N7-C5	2.98	108.68	102.99
56	CG	501	GTP	C8-N7-C5	2.98	108.67	102.99
56	PB	501	GTP	C2-N1-C6	-2.98	119.60	125.10
58	QC	501	GDP	C3'-C2'-C1'	2.98	105.47	100.98
56	IK	501	GTP	C3'-C2'-C1'	2.98	105.47	100.98
58	UL	501	GDP	PA-O3A-PB	-2.98	122.59	132.83
56	NG	501	GTP	C2-N1-C6	-2.98	119.61	125.10
56	OA	501	GTP	C2-N1-C6	-2.98	119.61	125.10
56	HB	501	GTP	C8-N7-C5	2.98	108.67	102.99
56	PI	501	GTP	C3'-C2'-C1'	2.98	105.47	100.98
56	OI	501	GTP	C2-N1-C6	-2.98	119.61	125.10
56	VB	501	GTP	C2-N1-C6	-2.98	119.61	125.10
56	NE	501	GTP	C8-N7-C5	2.98	108.67	102.99
56	IB	501	GTP	C8-N7-C5	2.98	108.66	102.99
56	IK	501	GTP	C8-N7-C5	2.98	108.66	102.99
56	JB	501	GTP	C2-N1-C6	-2.98	119.62	125.10
56	CB	501	GTP	C8-N7-C5	2.98	108.66	102.99
56	EI	501	GTP	C8-N7-C5	2.98	108.66	102.99
56	UE	501	GTP	C2-N1-C6	-2.97	119.62	125.10
56	JK	501	GTP	C8-N7-C5	2.97	108.66	102.99
56	KK	501	GTP	C8-N7-C5	2.97	108.66	102.99
56	HB	501	GTP	C2-N1-C6	-2.97	119.62	125.10
58	HC	501	GDP	C3'-C2'-C1'	2.97	105.45	100.98
56	TB	501	GTP	C2-N1-C6	-2.97	119.62	125.10
56	LB	501	GTP	C8-N7-C5	2.97	108.65	102.99
56	MA	501	GTP	C8-N7-C5	2.97	108.65	102.99
56	OL	501	GTP	C2-N1-C6	-2.97	119.63	125.10
56	LG	501	GTP	C8-N7-C5	2.97	108.65	102.99
56	KA	501	GTP	C2-N1-C6	-2.97	119.63	125.10
56	AG	501	GTP	C8-N7-C5	2.97	108.65	102.99
56	AB	501	GTP	C2-N1-C6	-2.97	119.63	125.10
56	WA	501	GTP	C8-N7-C5	2.97	108.64	102.99
56	FE	501	GTP	C3'-C2'-C1'	2.97	105.45	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	EA	501	GTP	C2-N1-C6	-2.97	119.64	125.10
56	OE	501	GTP	C2-N1-C6	-2.97	119.64	125.10
56	BI	501	GTP	C2-N1-C6	-2.97	119.64	125.10
58	LF	501	GDP	C3'-C2'-C1'	2.97	105.44	100.98
56	RA	501	GTP	C8-N7-C5	2.96	108.64	102.99
56	QL	501	GTP	C8-N7-C5	2.96	108.64	102.99
56	QL	501	GTP	C2-N1-C6	-2.96	119.64	125.10
56	UI	501	GTP	C8-N7-C5	2.96	108.64	102.99
56	IA	501	GTP	C2-N1-C6	-2.96	119.64	125.10
56	JG	501	GTP	C2-N1-C6	-2.96	119.64	125.10
56	VK	501	GTP	C3'-C2'-C1'	2.96	105.44	100.98
58	WH	501	GDP	C3'-C2'-C1'	2.96	105.44	100.98
56	JG	501	GTP	C8-N7-C5	2.96	108.63	102.99
56	FB	501	GTP	C2-N1-C6	-2.96	119.65	125.10
56	WI	501	GTP	C2-N1-C6	-2.96	119.65	125.10
56	GE	501	GTP	C8-N7-C5	2.96	108.63	102.99
56	GE	501	GTP	C3'-C2'-C1'	2.96	105.43	100.98
56	WE	501	GTP	C3'-C2'-C1'	2.96	105.43	100.98
56	VB	501	GTP	C3'-C2'-C1'	2.96	105.43	100.98
56	DI	501	GTP	C2-N1-C6	-2.96	119.65	125.10
56	TK	501	GTP	C2-N1-C6	-2.96	119.66	125.10
56	SB	501	GTP	C8-N7-C5	2.96	108.62	102.99
56	VK	501	GTP	C2-N1-C6	-2.96	119.66	125.10
56	CM	501	GTP	C3'-C2'-C1'	2.95	105.43	100.98
56	QK	501	GTP	C3'-C2'-C1'	2.95	105.43	100.98
56	IE	501	GTP	C2-N1-C6	-2.95	119.66	125.10
56	SI	501	GTP	C8-N7-C5	2.95	108.62	102.99
56	OK	501	GTP	C3'-C2'-C1'	2.95	105.43	100.98
56	SG	501	GTP	C3'-C2'-C1'	2.95	105.43	100.98
56	OK	501	GTP	C2-N1-C6	-2.95	119.66	125.10
56	JA	501	GTP	C2-N1-C6	-2.95	119.66	125.10
56	EG	501	GTP	C2-N1-C6	-2.95	119.66	125.10
56	PL	501	GTP	C8-N7-C5	2.95	108.61	102.99
56	IK	501	GTP	C2-N1-C6	-2.95	119.66	125.10
56	IA	501	GTP	C8-N7-C5	2.95	108.61	102.99
56	LE	501	GTP	C2-N1-C6	-2.95	119.66	125.10
58	AD	501	GDP	C3'-C2'-C1'	2.95	105.42	100.98
56	VG	501	GTP	C8-N7-C5	2.95	108.61	102.99
56	NE	501	GTP	C2-N1-C6	-2.95	119.67	125.10
56	AE	501	GTP	C3'-C2'-C1'	2.95	105.42	100.98
56	EA	501	GTP	C8-N7-C5	2.95	108.61	102.99
56	KA	501	GTP	C3'-C2'-C1'	2.95	105.42	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	BG	501	GTP	C2-N1-C6	-2.95	119.67	125.10
56	AK	501	GTP	C3'-C2'-C1'	2.95	105.42	100.98
56	KG	501	GTP	C3'-C2'-C1'	2.95	105.42	100.98
56	LG	501	GTP	C3'-C2'-C1'	2.95	105.42	100.98
56	BA	501	GTP	C2-N1-C6	-2.95	119.67	125.10
56	VA	501	GTP	C2-N1-C6	-2.95	119.67	125.10
56	RK	501	GTP	C8-N7-C5	2.95	108.60	102.99
58	TL	501	GDP	C3'-C2'-C1'	2.94	105.41	100.98
56	WK	501	GTP	C2-N1-C6	-2.94	119.68	125.10
56	RG	501	GTP	C8-N7-C5	2.94	108.60	102.99
56	CI	501	GTP	C3'-C2'-C1'	2.94	105.41	100.98
56	PL	501	GTP	C2-N1-C6	-2.94	119.68	125.10
56	SK	501	GTP	C2-N1-C6	-2.94	119.68	125.10
56	EK	501	GTP	C3'-C2'-C1'	2.94	105.41	100.98
56	UK	501	GTP	C3'-C2'-C1'	2.94	105.41	100.98
56	CK	501	GTP	C8-N7-C5	2.94	108.59	102.99
56	IM	501	GTP	C2-N1-C6	-2.94	119.68	125.10
56	CE	501	GTP	C2-N1-C6	-2.94	119.68	125.10
56	CM	501	GTP	C2-N1-C6	-2.94	119.68	125.10
56	UI	501	GTP	C3'-C2'-C1'	2.94	105.40	100.98
58	KD	501	GDP	C3'-C2'-C1'	2.94	105.40	100.98
56	II	501	GTP	C3'-C2'-C1'	2.94	105.40	100.98
58	PC	501	GDP	C3'-C2'-C1'	2.94	105.40	100.98
56	DG	501	GTP	C8-N7-C5	2.94	108.59	102.99
56	EK	501	GTP	C2-N1-C6	-2.94	119.69	125.10
56	WE	501	GTP	C2-N1-C6	-2.94	119.69	125.10
56	WG	501	GTP	C8-N7-C5	2.94	108.58	102.99
56	EE	501	GTP	C2-N1-C6	-2.94	119.69	125.10
56	OB	501	GTP	C2-N1-C6	-2.94	119.69	125.10
56	GG	501	GTP	C3'-C2'-C1'	2.94	105.40	100.98
56	II	501	GTP	C2-N1-C6	-2.94	119.69	125.10
56	UA	501	GTP	C2-N1-C6	-2.94	119.69	125.10
56	AG	501	GTP	C3'-C2'-C1'	2.94	105.40	100.98
56	IB	501	GTP	C2-N1-C6	-2.93	119.69	125.10
56	EC	501	GTP	C2-N1-C6	-2.93	119.69	125.10
56	PG	501	GTP	C2-N1-C6	-2.93	119.70	125.10
56	DK	501	GTP	C2-N1-C6	-2.93	119.70	125.10
56	UB	501	GTP	C2-N1-C6	-2.93	119.70	125.10
56	SB	501	GTP	C2-N1-C6	-2.93	119.70	125.10
56	RG	501	GTP	C3'-C2'-C1'	2.93	105.39	100.98
56	FI	501	GTP	C2-N1-C6	-2.93	119.70	125.10
56	IG	501	GTP	C3'-C2'-C1'	2.93	105.39	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	JD	501	GDP	C3'-C2'-C1'	2.93	105.39	100.98
56	VE	501	GTP	C2-N1-C6	-2.93	119.70	125.10
56	AA	501	GTP	C2-N1-C6	-2.93	119.71	125.10
56	JK	501	GTP	C2-N1-C6	-2.93	119.71	125.10
56	TB	501	GTP	C3'-C2'-C1'	2.93	105.39	100.98
56	JE	501	GTP	C2-N1-C6	-2.93	119.71	125.10
56	HE	501	GTP	C2-N1-C6	-2.93	119.71	125.10
56	MG	501	GTP	C2-N1-C6	-2.93	119.71	125.10
56	HA	501	GTP	C3'-C2'-C1'	2.93	105.38	100.98
56	GB	501	GTP	C2-N1-C6	-2.93	119.71	125.10
56	OG	501	GTP	C2-N1-C6	-2.92	119.71	125.10
56	RL	501	GTP	C8-N7-C5	2.92	108.56	102.99
56	DG	501	GTP	C2-N1-C6	-2.92	119.72	125.10
56	PG	501	GTP	C3'-C2'-C1'	2.92	105.38	100.98
56	NG	501	GTP	C8-N7-C5	2.92	108.56	102.99
56	JE	501	GTP	C3'-C2'-C1'	2.92	105.38	100.98
58	WD	501	GDP	C3'-C2'-C1'	2.92	105.38	100.98
56	HI	501	GTP	C2-N1-C6	-2.92	119.72	125.10
56	VI	501	GTP	C2-N1-C6	-2.92	119.72	125.10
56	KK	501	GTP	C2-N1-C6	-2.92	119.72	125.10
56	AB	501	GTP	C3'-C2'-C1'	2.92	105.38	100.98
56	BB	501	GTP	C2-N1-C6	-2.92	119.72	125.10
56	TI	501	GTP	C3'-C2'-C1'	2.92	105.37	100.98
56	OK	501	GTP	C8-N7-C5	2.92	108.55	102.99
56	AK	501	GTP	C2-N1-C6	-2.92	119.72	125.10
56	UA	501	GTP	C3'-C2'-C1'	2.92	105.37	100.98
58	EJ	501	GDP	C3'-C2'-C1'	2.92	105.37	100.98
56	BI	501	GTP	C3'-C2'-C1'	2.92	105.37	100.98
56	WB	501	GTP	C2-N1-C6	-2.92	119.72	125.10
56	EE	501	GTP	C8-N7-C5	2.92	108.55	102.99
56	IG	501	GTP	C2-N1-C6	-2.92	119.73	125.10
56	TA	501	GTP	C2-N1-C6	-2.92	119.73	125.10
58	QH	501	GDP	C3'-C2'-C1'	2.92	105.37	100.98
56	MA	501	GTP	C2-N1-C6	-2.92	119.73	125.10
56	PE	501	GTP	C2-N1-C6	-2.91	119.73	125.10
56	NB	501	GTP	C3'-C2'-C1'	2.91	105.36	100.98
56	LA	501	GTP	C2-N1-C6	-2.91	119.73	125.10
56	LK	501	GTP	C2-N1-C6	-2.91	119.73	125.10
56	PK	501	GTP	C2-N1-C6	-2.91	119.73	125.10
56	AG	501	GTP	C2-N1-C6	-2.91	119.74	125.10
56	HA	501	GTP	C2-N1-C6	-2.91	119.74	125.10
56	NI	501	GTP	C2-N1-C6	-2.91	119.74	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	NL	501	GTP	C2-N1-C6	-2.91	119.74	125.10
56	WG	501	GTP	C2-N1-C6	-2.91	119.74	125.10
58	NF	501	GDP	C3'-C2'-C1'	2.91	105.36	100.98
56	AI	501	GTP	C2-N1-C6	-2.91	119.74	125.10
56	CB	501	GTP	C2-N1-C6	-2.91	119.74	125.10
56	RA	501	GTP	C2-N1-C6	-2.91	119.75	125.10
56	DE	501	GTP	C2-N1-C6	-2.91	119.75	125.10
56	QI	501	GTP	C2-N1-C6	-2.91	119.75	125.10
56	RI	501	GTP	C2-N1-C6	-2.91	119.75	125.10
56	MK	501	GTP	C3'-C2'-C1'	2.91	105.35	100.98
56	DB	501	GTP	C2-N1-C6	-2.91	119.75	125.10
56	LG	501	GTP	C2-N1-C6	-2.91	119.75	125.10
56	MB	501	GTP	C2-N1-C6	-2.91	119.75	125.10
56	SE	501	GTP	C2-N1-C6	-2.91	119.75	125.10
56	IB	501	GTP	C3'-C2'-C1'	2.91	105.35	100.98
56	WK	501	GTP	C3'-C2'-C1'	2.91	105.35	100.98
56	SI	501	GTP	C2-N1-C6	-2.90	119.75	125.10
56	CK	501	GTP	C2-N1-C6	-2.90	119.75	125.10
58	CD	501	GDP	C3'-C2'-C1'	2.90	105.35	100.98
56	NB	501	GTP	C2-N1-C6	-2.90	119.75	125.10
56	FB	501	GTP	C3'-C2'-C1'	2.90	105.35	100.98
56	RB	501	GTP	C2-N1-C6	-2.90	119.75	125.10
56	QA	501	GTP	C2-N1-C6	-2.90	119.76	125.10
56	CA	501	GTP	C2-N1-C6	-2.90	119.76	125.10
56	FK	501	GTP	C2-N1-C6	-2.90	119.76	125.10
56	MA	501	GTP	C3'-C2'-C1'	2.90	105.34	100.98
56	BK	501	GTP	C2-N1-C6	-2.90	119.76	125.10
56	HK	501	GTP	C2-N1-C6	-2.90	119.76	125.10
56	LB	501	GTP	C2-N1-C6	-2.90	119.76	125.10
56	WA	501	GTP	C2-N1-C6	-2.90	119.76	125.10
56	FG	501	GTP	C2-N1-C6	-2.90	119.76	125.10
56	NA	501	GTP	C2-N1-C6	-2.90	119.76	125.10
56	NG	501	GTP	C3'-C2'-C1'	2.90	105.34	100.98
56	AM	501	GTP	C2-N1-C6	-2.90	119.77	125.10
56	CA	501	GTP	C3'-C2'-C1'	2.89	105.34	100.98
56	HG	501	GTP	C2-N1-C6	-2.89	119.77	125.10
56	TE	501	GTP	C3'-C2'-C1'	2.89	105.33	100.98
56	FG	501	GTP	PA-O3A-PB	-2.89	122.90	132.83
56	CK	501	GTP	C3'-C2'-C1'	2.89	105.33	100.98
56	OL	501	GTP	C3'-C2'-C1'	2.89	105.33	100.98
58	RC	501	GDP	C3'-C2'-C1'	2.89	105.33	100.98
56	CG	501	GTP	C2-N1-C6	-2.89	119.77	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	JA	501	GTP	C3'-C2'-C1'	2.89	105.33	100.98
56	EI	501	GTP	C2-N1-C6	-2.89	119.78	125.10
56	DB	501	GTP	C3'-C2'-C1'	2.89	105.33	100.98
56	FE	501	GTP	C2-N1-C6	-2.89	119.78	125.10
56	MB	501	GTP	PA-O3A-PB	-2.89	122.91	132.83
56	GG	501	GTP	C2-N1-C6	-2.89	119.78	125.10
56	JI	501	GTP	C2-N1-C6	-2.89	119.78	125.10
56	OB	501	GTP	C3'-C2'-C1'	2.89	105.33	100.98
56	CI	501	GTP	C2-N1-C6	-2.89	119.78	125.10
56	MK	501	GTP	C2-N1-C6	-2.89	119.78	125.10
56	RK	501	GTP	C2-N1-C6	-2.89	119.78	125.10
56	VI	501	GTP	C3'-C2'-C1'	2.89	105.32	100.98
56	GK	501	GTP	C2-N1-C6	-2.89	119.78	125.10
56	ML	501	GTP	C2-N1-C6	-2.89	119.78	125.10
56	RE	501	GTP	C8-N7-C5	2.89	108.49	102.99
56	TK	501	GTP	C3'-C2'-C1'	2.88	105.32	100.98
56	KI	501	GTP	C2-N1-C6	-2.88	119.79	125.10
56	GK	501	GTP	C3'-C2'-C1'	2.88	105.32	100.98
56	QG	501	GTP	C3'-C2'-C1'	2.88	105.32	100.98
56	GE	501	GTP	C2-N1-C6	-2.88	119.79	125.10
56	AE	501	GTP	C2-N1-C6	-2.88	119.79	125.10
56	BM	501	GTP	C3'-C2'-C1'	2.88	105.31	100.98
56	LI	501	GTP	C2-N1-C6	-2.88	119.80	125.10
56	ME	501	GTP	C2-N1-C6	-2.88	119.80	125.10
58	MD	501	GDP	C3'-C2'-C1'	2.88	105.31	100.98
56	UG	501	GTP	C2-N1-C6	-2.87	119.80	125.10
56	PE	501	GTP	C3'-C2'-C1'	2.87	105.30	100.98
58	LC	501	GDP	C3'-C2'-C1'	2.87	105.30	100.98
58	RM	501	GDP	C3'-C2'-C1'	2.87	105.30	100.98
56	DA	501	GTP	C2-N1-C6	-2.87	119.81	125.10
56	KG	501	GTP	C2-N1-C6	-2.87	119.81	125.10
58	IH	501	GDP	C3'-C2'-C1'	2.87	105.30	100.98
56	UK	501	GTP	C2-N1-C6	-2.87	119.82	125.10
56	KE	501	GTP	C2-N1-C6	-2.87	119.82	125.10
56	RE	501	GTP	C2-N1-C6	-2.87	119.82	125.10
56	GI	501	GTP	C2-N1-C6	-2.87	119.82	125.10
56	QK	501	GTP	C2-N1-C6	-2.87	119.82	125.10
56	UI	501	GTP	C2-N1-C6	-2.87	119.82	125.10
58	GJ	501	GDP	C3'-C2'-C1'	2.86	105.29	100.98
56	TE	501	GTP	C2-N1-C6	-2.86	119.83	125.10
56	FG	501	GTP	C3'-C2'-C1'	2.86	105.28	100.98
56	NI	501	GTP	C3'-C2'-C1'	2.86	105.28	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	KB	501	GTP	C2-N1-C6	-2.86	119.83	125.10
56	EI	501	GTP	C3'-C2'-C1'	2.86	105.28	100.98
56	HI	501	GTP	C3'-C2'-C1'	2.86	105.28	100.98
56	DM	501	GTP	C2-N1-C6	-2.86	119.84	125.10
56	MB	501	GTP	C3'-C2'-C1'	2.86	105.28	100.98
56	AA	501	GTP	C3'-C2'-C1'	2.85	105.27	100.98
56	TI	501	GTP	C2-N1-C6	-2.85	119.84	125.10
56	MG	501	GTP	C3'-C2'-C1'	2.85	105.27	100.98
56	VG	501	GTP	C2-N1-C6	-2.85	119.85	125.10
56	RK	501	GTP	C3'-C2'-C1'	2.85	105.27	100.98
58	MH	501	GDP	C3'-C2'-C1'	2.85	105.27	100.98
58	TD	501	GDP	C3'-C2'-C1'	2.85	105.26	100.98
56	SB	501	GTP	C3'-C2'-C1'	2.85	105.26	100.98
56	MI	501	GTP	C2-N1-C6	-2.84	119.86	125.10
58	LD	501	GDP	C3'-C2'-C1'	2.84	105.26	100.98
56	JG	501	GTP	C3'-C2'-C1'	2.84	105.26	100.98
56	BG	501	GTP	C3'-C2'-C1'	2.84	105.26	100.98
58	OM	501	GDP	C3'-C2'-C1'	2.84	105.26	100.98
56	DG	501	GTP	C3'-C2'-C1'	2.84	105.25	100.98
56	SA	502	GTP	C2-N1-C6	-2.84	119.87	125.10
56	QE	501	GTP	C2-N1-C6	-2.84	119.87	125.10
56	CB	501	GTP	C3'-C2'-C1'	2.84	105.25	100.98
56	PA	501	GTP	C2-N1-C6	-2.83	119.88	125.10
56	QB	501	GTP	C2-N1-C6	-2.83	119.89	125.10
56	GA	501	GTP	C2-N1-C6	-2.83	119.89	125.10
58	PF	501	GDP	C2-N1-C6	-2.82	119.90	125.10
56	UB	501	GTP	C3'-C2'-C1'	2.82	105.23	100.98
56	CG	501	GTP	C3'-C2'-C1'	2.81	105.21	100.98
56	OE	501	GTP	C3'-C2'-C1'	2.81	105.21	100.98
56	RL	501	GTP	C2-N1-C6	-2.81	119.92	125.10
56	SI	501	GTP	C3'-C2'-C1'	2.81	105.21	100.98
58	SD	501	GDP	C3'-C2'-C1'	2.81	105.21	100.98
58	SM	501	GDP	C3'-C2'-C1'	2.81	105.21	100.98
58	BF	501	GDP	C3'-C2'-C1'	2.80	105.20	100.98
56	QA	501	GTP	C3'-C2'-C1'	2.80	105.19	100.98
56	PA	501	GTP	C8-N7-C5	2.80	108.32	102.99
56	EC	501	GTP	C3'-C2'-C1'	2.79	105.19	100.98
56	KK	501	GTP	C3'-C2'-C1'	2.79	105.18	100.98
58	PF	501	GDP	O6-C6-N1	2.79	123.94	120.65
56	MI	501	GTP	C3'-C2'-C1'	2.79	105.17	100.98
56	HG	501	GTP	C3'-C2'-C1'	2.78	105.17	100.98
56	IM	501	GTP	C3'-C2'-C1'	2.78	105.16	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	CF	501	GDP	C3'-C2'-C1'	2.78	105.16	100.98
58	GD	501	GDP	C3'-C2'-C1'	2.78	105.16	100.98
58	HL	501	GDP	C3'-C2'-C1'	2.78	105.16	100.98
56	AM	501	GTP	C3'-C2'-C1'	2.77	105.16	100.98
58	JH	501	GDP	C3'-C2'-C1'	2.77	105.15	100.98
56	QB	501	GTP	C3'-C2'-C1'	2.77	105.15	100.98
56	CE	501	GTP	C3'-C2'-C1'	2.77	105.14	100.98
56	EG	501	GTP	C3'-C2'-C1'	2.77	105.14	100.98
58	FJ	501	GDP	C3'-C2'-C1'	2.76	105.14	100.98
56	QI	501	GTP	C3'-C2'-C1'	2.76	105.13	100.98
58	WL	501	GDP	C3'-C2'-C1'	2.76	105.13	100.98
58	RJ	501	GDP	C3'-C2'-C1'	2.75	105.12	100.98
56	WB	501	GTP	C3'-C2'-C1'	2.75	105.12	100.98
56	SA	502	GTP	C3'-C2'-C1'	2.75	105.12	100.98
56	IE	501	GTP	C3'-C2'-C1'	2.74	105.11	100.98
56	RA	501	GTP	C3'-C2'-C1'	2.74	105.11	100.98
58	CJ	501	GDP	C3'-C2'-C1'	2.74	105.11	100.98
56	BM	501	GTP	O3G-PG-O3B	2.74	113.82	104.64
56	RI	501	GTP	C3'-C2'-C1'	2.74	105.10	100.98
58	QH	501	GDP	C5-C6-N1	2.74	118.79	113.95
58	VL	501	GDP	C3'-C2'-C1'	2.74	105.10	100.98
56	HK	501	GTP	C3'-C2'-C1'	2.74	105.10	100.98
56	JK	501	GTP	C3'-C2'-C1'	2.74	105.10	100.98
58	FC	501	GDP	C3'-C2'-C1'	2.73	105.09	100.98
58	KF	501	GDP	C3'-C2'-C1'	2.73	105.09	100.98
56	SK	501	GTP	C3'-C2'-C1'	2.72	105.07	100.98
58	HJ	501	GDP	C3'-C2'-C1'	2.72	105.07	100.98
56	DA	501	GTP	C3'-C2'-C1'	2.71	105.06	100.98
56	LA	501	GTP	C3'-C2'-C1'	2.71	105.06	100.98
58	MM	501	GDP	C3'-C2'-C1'	2.71	105.06	100.98
58	LL	501	GDP	C3'-C2'-C1'	2.71	105.06	100.98
58	EH	501	GDP	C3'-C2'-C1'	2.71	105.05	100.98
56	BG	501	GTP	PB-O3B-PG	-2.70	123.55	132.83
56	QE	501	GTP	C3'-C2'-C1'	2.69	105.03	100.98
58	EM	501	GDP	C3'-C2'-C1'	2.69	105.03	100.98
56	EE	501	GTP	C3'-C2'-C1'	2.68	105.02	100.98
56	KB	501	GTP	C3'-C2'-C1'	2.68	105.01	100.98
56	RI	501	GTP	PA-O3A-PB	-2.68	123.63	132.83
56	KI	501	GTP	C3'-C2'-C1'	2.68	105.01	100.98
58	JF	501	GDP	C3'-C2'-C1'	2.67	105.00	100.98
56	ME	501	GTP	C3'-C2'-C1'	2.67	105.00	100.98
58	SL	501	GDP	C3'-C2'-C1'	2.66	104.98	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DE	501	GTP	C3'-C2'-C1'	2.64	104.95	100.98
58	RD	501	GDP	C3'-C2'-C1'	2.64	104.95	100.98
56	LK	501	GTP	C3'-C2'-C1'	2.64	104.95	100.98
58	VD	501	GDP	C5-C6-N1	2.64	118.61	113.95
58	DH	501	GDP	C3'-C2'-C1'	2.62	104.93	100.98
56	SE	501	GTP	C3'-C2'-C1'	2.61	104.91	100.98
56	TG	501	GTP	C3'-C2'-C1'	2.61	104.91	100.98
56	FK	501	GTP	C3'-C2'-C1'	2.61	104.91	100.98
56	RL	501	GTP	PB-O3B-PG	-2.61	123.88	132.83
58	TJ	501	GDP	C3'-C2'-C1'	2.59	104.88	100.98
56	RB	501	GTP	C3'-C2'-C1'	2.58	104.87	100.98
58	EB	501	GDP	C3'-C2'-C1'	2.58	104.86	100.98
56	JI	501	GTP	C3'-C2'-C1'	2.58	104.86	100.98
56	DM	501	GTP	C3'-C2'-C1'	2.56	104.84	100.98
56	HE	501	GTP	C3'-C2'-C1'	2.56	104.83	100.98
56	RE	501	GTP	C3'-C2'-C1'	2.56	104.83	100.98
58	QJ	501	GDP	C3'-C2'-C1'	2.56	104.83	100.98
56	UG	501	GTP	C3'-C2'-C1'	2.56	104.83	100.98
56	BG	501	GTP	O3G-PG-O3B	2.55	113.19	104.64
58	ID	501	GDP	C3'-C2'-C1'	2.53	104.79	100.98
58	PD	501	GDP	C3'-C2'-C1'	2.53	104.78	100.98
58	EL	501	GDP	C3'-C2'-C1'	2.52	104.78	100.98
58	FH	501	GDP	C3'-C2'-C1'	2.52	104.77	100.98
58	CF	501	GDP	C5-C6-N1	2.49	118.36	113.95
58	BD	501	GDP	C3'-C2'-C1'	2.49	104.73	100.98
58	UD	501	GDP	C5-C6-N1	2.49	118.34	113.95
58	JC	501	GDP	C5-C6-N1	2.48	118.33	113.95
56	RL	501	GTP	O3G-PG-O3B	2.47	112.92	104.64
58	QD	501	GDP	C3'-C2'-C1'	2.47	104.69	100.98
58	RM	501	GDP	C5-C6-N1	2.46	118.30	113.95
58	NF	501	GDP	C5-C6-N1	2.45	118.29	113.95
58	LL	501	GDP	C5-C6-N1	2.45	118.28	113.95
58	PC	501	GDP	C8-N7-C5	2.45	107.66	102.99
58	EB	501	GDP	C8-N7-C5	2.45	107.65	102.99
56	BK	501	GTP	PB-O3B-PG	-2.44	124.44	132.83
58	EM	501	GDP	C5-C6-N1	2.44	118.27	113.95
58	FM	502	GDP	C5-C6-N1	2.44	118.26	113.95
58	WD	501	GDP	C8-N7-C5	2.44	107.63	102.99
58	JL	501	GDP	C3'-C2'-C1'	2.43	104.63	100.98
58	QM	501	GDP	C3'-C2'-C1'	2.42	104.63	100.98
56	RE	501	GTP	O6-C6-C5	-2.42	119.64	124.37
58	IC	501	GDP	C8-N7-C5	2.42	107.60	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	VC	501	GDP	C8-N7-C5	2.42	107.60	102.99
56	QI	501	GTP	O6-C6-C5	-2.42	119.65	124.37
58	FL	501	GDP	C8-N7-C5	2.42	107.59	102.99
58	FH	501	GDP	C5-C6-N1	2.41	118.21	113.95
58	GL	501	GDP	C5-C6-N1	2.41	118.20	113.95
58	EL	501	GDP	C8-N7-C5	2.41	107.58	102.99
58	RD	501	GDP	C5-C6-N1	2.41	118.20	113.95
56	EA	501	GTP	O6-C6-C5	-2.40	119.67	124.37
58	PM	501	GDP	C5-C6-N1	2.40	118.19	113.95
58	FF	501	GDP	C8-N7-C5	2.40	107.56	102.99
58	LC	501	GDP	C5-C6-N1	2.40	118.19	113.95
58	EM	501	GDP	C8-N7-C5	2.40	107.56	102.99
58	ID	501	GDP	C8-N7-C5	2.40	107.56	102.99
58	OM	501	GDP	C8-N7-C5	2.39	107.55	102.99
58	BF	501	GDP	C8-N7-C5	2.39	107.55	102.99
58	CJ	501	GDP	C5-C6-N1	2.39	118.17	113.95
58	LC	501	GDP	C8-N7-C5	2.39	107.54	102.99
58	VD	501	GDP	C2'-C3'-C4'	2.39	107.28	102.64
58	BD	501	GDP	C8-N7-C5	2.38	107.53	102.99
58	PD	501	GDP	C8-N7-C5	2.38	107.53	102.99
58	EF	501	GDP	C8-N7-C5	2.38	107.53	102.99
58	FL	501	GDP	C5-C6-N1	2.38	118.16	113.95
58	QD	501	GDP	C8-N7-C5	2.38	107.53	102.99
58	OJ	501	GDP	C5-C6-N1	2.38	118.16	113.95
58	UC	501	GDP	C8-N7-C5	2.38	107.53	102.99
58	JC	501	GDP	C3'-C2'-C1'	2.38	104.56	100.98
58	TF	501	GDP	C5-C6-N1	2.38	118.16	113.95
58	TH	501	GDP	C8-N7-C5	2.38	107.52	102.99
58	BL	501	GDP	C5-C6-N1	2.38	118.15	113.95
58	GL	501	GDP	C8-N7-C5	2.37	107.51	102.99
58	LL	501	GDP	C8-N7-C5	2.37	107.51	102.99
58	NC	501	GDP	C8-N7-C5	2.37	107.51	102.99
58	TL	501	GDP	C8-N7-C5	2.37	107.51	102.99
58	UL	501	GDP	C8-N7-C5	2.37	107.51	102.99
58	CJ	501	GDP	C8-N7-C5	2.37	107.51	102.99
58	EB	501	GDP	C5-C6-N1	2.37	118.14	113.95
58	SL	501	GDP	C8-N7-C5	2.37	107.51	102.99
58	ID	501	GDP	C5-C6-N1	2.37	118.14	113.95
58	JC	501	GDP	C8-N7-C5	2.37	107.50	102.99
58	EJ	501	GDP	C5-C6-N1	2.37	118.13	113.95
58	UL	501	GDP	C3'-C2'-C1'	2.37	104.54	100.98
58	AJ	501	GDP	C8-N7-C5	2.37	107.50	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	WD	501	GDP	C5-C6-N1	2.37	118.13	113.95
58	BH	501	GDP	C8-N7-C5	2.36	107.50	102.99
58	NH	501	GDP	C8-N7-C5	2.36	107.50	102.99
58	FC	501	GDP	C8-N7-C5	2.36	107.49	102.99
58	BF	501	GDP	C5-C6-N1	2.36	118.12	113.95
58	WC	501	GDP	C8-N7-C5	2.36	107.49	102.99
58	UH	501	GDP	C8-N7-C5	2.36	107.49	102.99
58	LH	501	GDP	C8-N7-C5	2.36	107.49	102.99
58	NF	501	GDP	C8-N7-C5	2.36	107.49	102.99
58	UJ	501	GDP	C8-N7-C5	2.36	107.49	102.99
58	GJ	501	GDP	C5-C6-N1	2.36	118.12	113.95
58	LH	501	GDP	C5-C6-N1	2.36	118.12	113.95
58	DH	501	GDP	C8-N7-C5	2.36	107.48	102.99
58	JF	501	GDP	C8-N7-C5	2.36	107.48	102.99
58	EH	501	GDP	C5-C6-N1	2.36	118.12	113.95
58	UH	501	GDP	C5-C6-N1	2.36	118.12	113.95
58	DL	501	GDP	C8-N7-C5	2.36	107.48	102.99
58	FJ	501	GDP	C8-N7-C5	2.36	107.48	102.99
58	VH	501	GDP	C8-N7-C5	2.36	107.48	102.99
58	BJ	501	GDP	C8-N7-C5	2.35	107.48	102.99
58	LJ	501	GDP	C8-N7-C5	2.35	107.48	102.99
56	SK	501	GTP	O6-C6-C5	-2.35	119.77	124.37
58	HH	501	GDP	C8-N7-C5	2.35	107.47	102.99
58	UM	501	GDP	C8-N7-C5	2.35	107.47	102.99
58	KD	501	GDP	C8-N7-C5	2.35	107.47	102.99
58	PH	501	GDP	C5-C6-N1	2.35	118.11	113.95
58	ED	501	GDP	C5-C6-N1	2.35	118.11	113.95
58	IL	501	GDP	C5-C6-N1	2.35	118.10	113.95
58	GD	501	GDP	C8-N7-C5	2.35	107.47	102.99
58	ND	501	GDP	C8-N7-C5	2.35	107.47	102.99
58	JJ	501	GDP	C8-N7-C5	2.35	107.46	102.99
58	WJ	501	GDP	C5-C6-N1	2.35	118.10	113.95
58	KM	501	GDP	C8-N7-C5	2.35	107.46	102.99
58	NK	501	GDP	C8-N7-C5	2.35	107.46	102.99
58	WH	501	GDP	C8-N7-C5	2.35	107.46	102.99
58	HJ	501	GDP	C8-N7-C5	2.34	107.46	102.99
58	OM	501	GDP	C5-C6-N1	2.34	118.09	113.95
58	FH	501	GDP	C8-N7-C5	2.34	107.45	102.99
58	GM	501	GDP	C8-N7-C5	2.34	107.45	102.99
58	TJ	501	GDP	C5-C6-N1	2.34	118.09	113.95
58	CH	501	GDP	C8-N7-C5	2.34	107.45	102.99
58	BD	501	GDP	C5-C6-N1	2.34	118.08	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AF	501	GDP	C8-N7-C5	2.34	107.45	102.99
58	BJ	501	GDP	C5-C6-N1	2.34	118.08	113.95
58	IJ	501	GDP	C8-N7-C5	2.34	107.45	102.99
58	RJ	501	GDP	C5-C6-N1	2.34	118.08	113.95
58	QC	501	GDP	C8-N7-C5	2.34	107.44	102.99
58	HF	501	GDP	C8-N7-C5	2.34	107.44	102.99
58	HL	501	GDP	C8-N7-C5	2.34	107.44	102.99
58	JD	501	GDP	C8-N7-C5	2.34	107.44	102.99
58	AF	501	GDP	C5-C6-N1	2.34	118.08	113.95
58	OF	501	GDP	C8-N7-C5	2.34	107.44	102.99
58	SJ	501	GDP	C5-C6-N1	2.34	118.08	113.95
58	EJ	501	GDP	C8-N7-C5	2.34	107.44	102.99
58	EL	501	GDP	C5-C6-N1	2.33	118.08	113.95
58	IH	501	GDP	C5-C6-N1	2.33	118.08	113.95
58	LF	501	GDP	C5-C6-N1	2.33	118.08	113.95
58	QM	501	GDP	C8-N7-C5	2.33	107.44	102.99
58	VF	501	GDP	C5-C6-N1	2.33	118.07	113.95
58	IL	501	GDP	C8-N7-C5	2.33	107.43	102.99
58	LF	501	GDP	C8-N7-C5	2.33	107.43	102.99
58	PM	501	GDP	C8-N7-C5	2.33	107.43	102.99
58	HH	501	GDP	C5-C6-N1	2.33	118.07	113.95
58	TM	501	GDP	C8-N7-C5	2.33	107.43	102.99
58	RC	501	GDP	C5-C6-N1	2.33	118.07	113.95
58	CC	501	GDP	C8-N7-C5	2.33	107.43	102.99
58	UF	501	GDP	C8-N7-C5	2.33	107.43	102.99
58	NC	501	GDP	C5-C6-N1	2.33	118.07	113.95
58	FJ	501	GDP	C5-C6-N1	2.33	118.06	113.95
58	SM	501	GDP	C8-N7-C5	2.33	107.43	102.99
58	IJ	501	GDP	C5-C6-N1	2.33	118.06	113.95
58	TL	501	GDP	C5-C6-N1	2.33	118.06	113.95
58	WF	501	GDP	C8-N7-C5	2.33	107.42	102.99
58	FD	501	GDP	C8-N7-C5	2.33	107.42	102.99
58	UF	501	GDP	C5-C6-N1	2.33	118.06	113.95
58	AJ	501	GDP	C5-C6-N1	2.33	118.06	113.95
58	WC	501	GDP	C5-C6-N1	2.33	118.06	113.95
58	DH	501	GDP	C5-C6-N1	2.32	118.06	113.95
58	OC	501	GDP	C8-N7-C5	2.32	107.42	102.99
58	SD	501	GDP	C8-N7-C5	2.32	107.42	102.99
58	TF	501	GDP	C8-N7-C5	2.32	107.42	102.99
58	AC	501	GDP	C5-C6-N1	2.32	118.05	113.95
58	JF	501	GDP	C5-C6-N1	2.32	118.05	113.95
58	MH	501	GDP	C5-C6-N1	2.32	118.05	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	VF	501	GDP	C8-N7-C5	2.32	107.41	102.99
58	ND	501	GDP	C5-C6-N1	2.32	118.05	113.95
58	GF	501	GDP	C5-C6-N1	2.32	118.05	113.95
58	VC	501	GDP	C5-C6-N1	2.32	118.05	113.95
58	WH	501	GDP	C5-C6-N1	2.32	118.05	113.95
58	EH	501	GDP	C8-N7-C5	2.32	107.41	102.99
58	MH	501	GDP	C8-N7-C5	2.32	107.41	102.99
58	GD	501	GDP	C5-C6-N1	2.32	118.04	113.95
58	QM	501	GDP	C5-C6-N1	2.32	118.04	113.95
58	TC	501	GDP	C5-C6-N1	2.32	118.04	113.95
58	KJ	501	GDP	C8-N7-C5	2.32	107.40	102.99
58	MD	501	GDP	C8-N7-C5	2.32	107.40	102.99
58	NJ	501	GDP	C8-N7-C5	2.32	107.40	102.99
58	NM	501	GDP	C5-C6-N1	2.32	118.04	113.95
56	BK	501	GTP	O3G-PG-O3B	2.32	112.40	104.64
58	CF	501	GDP	C8-N7-C5	2.32	107.40	102.99
58	IH	501	GDP	C8-N7-C5	2.32	107.40	102.99
58	LM	501	GDP	C8-N7-C5	2.32	107.40	102.99
58	VJ	501	GDP	C8-N7-C5	2.31	107.40	102.99
58	TH	501	GDP	C5-C6-N1	2.31	118.04	113.95
58	WL	501	GDP	C8-N7-C5	2.31	107.40	102.99
58	FC	501	GDP	C5-C6-N1	2.31	118.04	113.95
58	DC	501	GDP	C8-N7-C5	2.31	107.40	102.99
58	HD	501	GDP	C8-N7-C5	2.31	107.40	102.99
58	SF	501	GDP	C8-N7-C5	2.31	107.40	102.99
58	SC	501	GDP	C5-C6-N1	2.31	118.04	113.95
58	KC	501	GDP	C5-C6-N1	2.31	118.04	113.95
58	JM	501	GDP	C8-N7-C5	2.31	107.39	102.99
58	RJ	501	GDP	C8-N7-C5	2.31	107.39	102.99
58	VJ	501	GDP	C5-C6-N1	2.31	118.03	113.95
58	OH	501	GDP	C5-C6-N1	2.31	118.03	113.95
58	GF	501	GDP	C8-N7-C5	2.31	107.39	102.99
58	RC	501	GDP	C8-N7-C5	2.31	107.39	102.99
58	JH	501	GDP	C5-C6-N1	2.31	118.03	113.95
58	NH	501	GDP	C5-C6-N1	2.31	118.03	113.95
58	SH	501	GDP	C8-N7-C5	2.31	107.39	102.99
58	IF	501	GDP	C8-N7-C5	2.31	107.39	102.99
58	KL	501	GDP	C8-N7-C5	2.31	107.39	102.99
58	JD	501	GDP	C5-C6-N1	2.31	118.03	113.95
58	BC	501	GDP	C8-N7-C5	2.31	107.39	102.99
58	KF	501	GDP	C5-C6-N1	2.31	118.03	113.95
58	BL	501	GDP	C8-N7-C5	2.31	107.39	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	LD	501	GDP	C8-N7-C5	2.31	107.39	102.99
58	MM	501	GDP	C8-N7-C5	2.31	107.39	102.99
58	QJ	501	GDP	C8-N7-C5	2.31	107.39	102.99
58	FD	501	GDP	C5-C6-N1	2.31	118.03	113.95
58	SJ	501	GDP	C8-N7-C5	2.31	107.39	102.99
58	AC	501	GDP	C8-N7-C5	2.31	107.38	102.99
58	GC	501	GDP	C8-N7-C5	2.31	107.38	102.99
58	PH	501	GDP	C8-N7-C5	2.31	107.38	102.99
58	RH	501	GDP	C8-N7-C5	2.31	107.38	102.99
58	PD	501	GDP	C5-C6-N1	2.31	118.02	113.95
58	AH	501	GDP	C8-N7-C5	2.31	107.38	102.99
58	TC	501	GDP	C8-N7-C5	2.30	107.38	102.99
58	AD	501	GDP	C5-C6-N1	2.30	118.02	113.95
58	GC	501	GDP	C5-C6-N1	2.30	118.02	113.95
58	QC	501	GDP	C5-C6-N1	2.30	118.02	113.95
58	HM	501	GDP	C8-N7-C5	2.30	107.38	102.99
58	TJ	501	GDP	C8-N7-C5	2.30	107.38	102.99
58	OC	501	GDP	C5-C6-N1	2.30	118.02	113.95
58	RH	501	GDP	C5-C6-N1	2.30	118.02	113.95
58	UC	501	GDP	C5-C6-N1	2.30	118.02	113.95
58	DC	501	GDP	C5-C6-N1	2.30	118.02	113.95
58	CD	501	GDP	C5-C6-N1	2.30	118.02	113.95
58	KD	501	GDP	C5-C6-N1	2.30	118.02	113.95
58	BH	501	GDP	C5-C6-N1	2.30	118.01	113.95
58	HD	501	GDP	C5-C6-N1	2.30	118.01	113.95
58	OF	501	GDP	C5-C6-N1	2.30	118.01	113.95
58	KF	501	GDP	C8-N7-C5	2.30	107.37	102.99
58	PJ	501	GDP	C8-N7-C5	2.30	107.37	102.99
58	MJ	501	GDP	C8-N7-C5	2.30	107.37	102.99
58	VH	501	GDP	C5-C6-N1	2.30	118.01	113.95
58	WJ	501	GDP	C8-N7-C5	2.30	107.37	102.99
58	MM	501	GDP	C5-C6-N1	2.30	118.01	113.95
58	AL	501	GDP	C8-N7-C5	2.30	107.37	102.99
58	CH	501	GDP	C5-C6-N1	2.30	118.01	113.95
58	HJ	501	GDP	C5-C6-N1	2.30	118.01	113.95
56	UE	501	GTP	O6-C6-C5	-2.30	119.89	124.37
58	HF	501	GDP	C5-C6-N1	2.30	118.00	113.95
58	SM	501	GDP	C5-C6-N1	2.30	118.00	113.95
58	KL	501	GDP	C5-C6-N1	2.29	118.00	113.95
58	NM	501	GDP	C8-N7-C5	2.29	107.36	102.99
58	AL	501	GDP	C5-C6-N1	2.29	118.00	113.95
58	KC	501	GDP	C8-N7-C5	2.29	107.36	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	KH	501	GDP	C8-N7-C5	2.29	107.35	102.99
58	FF	501	GDP	C5-C6-N1	2.29	118.00	113.95
58	EF	501	GDP	C5-C6-N1	2.29	117.99	113.95
58	QD	501	GDP	C5-C6-N1	2.29	117.99	113.95
58	SH	501	GDP	C5-C6-N1	2.29	117.99	113.95
56	EI	501	GTP	O6-C6-C5	-2.29	119.91	124.37
58	JM	501	GDP	C5-C6-N1	2.29	117.99	113.95
58	NJ	501	GDP	C5-C6-N1	2.29	117.99	113.95
58	UJ	501	GDP	C5-C6-N1	2.29	117.99	113.95
56	JG	501	GTP	O6-C6-C5	-2.29	119.91	124.37
58	LD	501	GDP	C5-C6-N1	2.29	117.99	113.95
58	GJ	501	GDP	C8-N7-C5	2.28	107.34	102.99
58	OJ	501	GDP	C8-N7-C5	2.28	107.34	102.99
58	CC	501	GDP	C5-C6-N1	2.28	117.99	113.95
58	KJ	501	GDP	C5-C6-N1	2.28	117.99	113.95
58	MC	501	GDP	C5-C6-N1	2.28	117.98	113.95
58	OH	501	GDP	C8-N7-C5	2.28	107.34	102.99
58	LM	501	GDP	C5-C6-N1	2.28	117.98	113.95
58	BC	501	GDP	C5-C6-N1	2.28	117.98	113.95
58	MJ	501	GDP	C5-C6-N1	2.28	117.98	113.95
58	CL	501	GDP	C5-C6-N1	2.28	117.98	113.95
58	CD	501	GDP	C8-N7-C5	2.28	107.33	102.99
58	ED	501	GDP	C8-N7-C5	2.28	107.33	102.99
58	MF	501	GDP	C8-N7-C5	2.28	107.33	102.99
58	RD	501	GDP	C8-N7-C5	2.28	107.33	102.99
58	TM	501	GDP	C5-C6-N1	2.28	117.98	113.95
58	OD	501	GDP	C5-C6-N1	2.28	117.97	113.95
58	MD	501	GDP	C5-C6-N1	2.28	117.97	113.95
58	SF	501	GDP	C5-C6-N1	2.28	117.97	113.95
56	TK	501	GTP	O6-C6-C5	-2.28	119.93	124.37
58	NK	501	GDP	C5-C6-N1	2.27	117.97	113.95
58	MC	501	GDP	C8-N7-C5	2.27	107.32	102.99
58	TD	501	GDP	O6-C6-C5	-2.27	119.93	124.37
56	EE	501	GTP	O6-C6-C5	-2.27	119.94	124.37
58	JJ	501	GDP	C5-C6-N1	2.27	117.96	113.95
56	TG	501	GTP	O6-C6-C5	-2.27	119.94	124.37
58	IC	501	GDP	C5-C6-N1	2.27	117.96	113.95
58	DJ	501	GDP	C8-N7-C5	2.27	107.31	102.99
58	PJ	501	GDP	C5-C6-N1	2.27	117.95	113.95
56	MA	501	GTP	O6-C6-C5	-2.27	119.95	124.37
58	AH	501	GDP	C5-C6-N1	2.26	117.95	113.95
58	QJ	501	GDP	C5-C6-N1	2.26	117.95	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	RM	501	GDP	C8-N7-C5	2.26	107.30	102.99
56	LK	501	GTP	O6-C6-C5	-2.26	119.95	124.37
58	OD	501	GDP	C8-N7-C5	2.26	107.30	102.99
58	UM	501	GDP	C5-C6-N1	2.26	117.94	113.95
58	LJ	501	GDP	C5-C6-N1	2.26	117.94	113.95
58	SC	501	GDP	C8-N7-C5	2.26	107.29	102.99
58	KH	501	GDP	C5-C6-N1	2.25	117.93	113.95
58	GM	501	GDP	C5-C6-N1	2.25	117.93	113.95
58	UL	501	GDP	C5-C6-N1	2.25	117.93	113.95
58	WF	501	GDP	C5-C6-N1	2.25	117.93	113.95
56	SA	502	GTP	O6-C6-C5	-2.25	119.97	124.37
58	SL	501	GDP	C5-C6-N1	2.25	117.93	113.95
58	KM	501	GDP	C5-C6-N1	2.25	117.93	113.95
56	QL	501	GTP	O6-C6-C5	-2.25	119.98	124.37
58	GH	501	GDP	C5-C6-N1	2.25	117.92	113.95
56	MG	501	GTP	O6-C6-C5	-2.25	119.98	124.37
58	FM	502	GDP	C8-N7-C5	2.25	107.27	102.99
56	FM	501	GTP	O6-C6-C5	-2.25	119.98	124.37
58	HM	501	GDP	C5-C6-N1	2.25	117.92	113.95
56	SB	501	GTP	O6-C6-C5	-2.25	119.98	124.37
56	SE	501	GTP	O6-C6-C5	-2.25	119.98	124.37
56	JE	501	GTP	O6-C6-C5	-2.25	119.98	124.37
58	QF	501	GDP	C5-C6-N1	2.25	117.92	113.95
56	IB	501	GTP	O6-C6-C5	-2.24	119.99	124.37
58	JH	501	GDP	C8-N7-C5	2.24	107.26	102.99
56	TB	501	GTP	O6-C6-C5	-2.24	119.99	124.37
56	RI	501	GTP	O6-C6-C5	-2.24	120.00	124.37
58	CL	501	GDP	C8-N7-C5	2.24	107.26	102.99
58	DJ	501	GDP	C5-C6-N1	2.24	117.91	113.95
56	LI	501	GTP	O6-C6-C5	-2.24	120.00	124.37
58	PC	501	GDP	C5-C6-N1	2.23	117.90	113.95
56	RK	501	GTP	O6-C6-C5	-2.23	120.01	124.37
56	PI	501	GTP	O6-C6-C5	-2.23	120.01	124.37
56	EK	501	GTP	O6-C6-C5	-2.23	120.02	124.37
56	AB	501	GTP	O6-C6-C5	-2.23	120.02	124.37
56	NG	501	GTP	O6-C6-C5	-2.23	120.02	124.37
58	VD	501	GDP	C8-N7-C5	2.23	107.23	102.99
56	JK	501	GTP	O6-C6-C5	-2.23	120.03	124.37
56	AM	501	GTP	O6-C6-C5	-2.22	120.03	124.37
58	MF	501	GDP	C5-C6-N1	2.22	117.88	113.95
58	HL	501	GDP	C5-C6-N1	2.22	117.87	113.95
56	RA	501	GTP	O6-C6-C5	-2.22	120.04	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	HA	501	GTP	O6-C6-C5	-2.22	120.04	124.37
58	IF	501	GDP	C5-C6-N1	2.22	117.87	113.95
58	SD	501	GDP	C5-C6-N1	2.22	117.87	113.95
56	HB	501	GTP	O6-C6-C5	-2.22	120.04	124.37
58	TD	501	GDP	C8-N7-C5	2.22	107.21	102.99
56	BE	501	GTP	O6-C6-C5	-2.21	120.05	124.37
56	SI	501	GTP	O6-C6-C5	-2.21	120.05	124.37
56	FI	501	GTP	O6-C6-C5	-2.21	120.05	124.37
56	KI	501	GTP	O6-C6-C5	-2.21	120.05	124.37
58	WL	501	GDP	C5-C6-N1	2.21	117.86	113.95
56	BA	501	GTP	O6-C6-C5	-2.21	120.06	124.37
56	LG	501	GTP	O6-C6-C5	-2.21	120.06	124.37
56	TE	501	GTP	O6-C6-C5	-2.21	120.06	124.37
58	DL	501	GDP	C5-C6-N1	2.21	117.85	113.95
58	GH	501	GDP	C8-N7-C5	2.20	107.19	102.99
56	FE	501	GTP	O6-C6-C5	-2.20	120.07	124.37
58	VM	501	GDP	C5-C6-N1	2.20	117.84	113.95
56	WI	501	GTP	O6-C6-C5	-2.20	120.07	124.37
56	AK	501	GTP	O6-C6-C5	-2.20	120.08	124.37
56	BI	501	GTP	O6-C6-C5	-2.20	120.08	124.37
56	NL	501	GTP	O6-C6-C5	-2.20	120.08	124.37
58	AD	501	GDP	C2'-C3'-C4'	2.20	106.91	102.64
56	RB	501	GTP	O6-C6-C5	-2.20	120.08	124.37
56	TI	501	GTP	O6-C6-C5	-2.20	120.08	124.37
56	IG	501	GTP	O6-C6-C5	-2.20	120.08	124.37
56	HG	501	GTP	O6-C6-C5	-2.19	120.08	124.37
56	CB	501	GTP	O6-C6-C5	-2.19	120.09	124.37
56	VA	501	GTP	O6-C6-C5	-2.19	120.09	124.37
56	KG	501	GTP	O6-C6-C5	-2.19	120.09	124.37
56	WG	501	GTP	O6-C6-C5	-2.19	120.09	124.37
56	PL	501	GTP	O6-C6-C5	-2.19	120.09	124.37
56	SG	501	GTP	O6-C6-C5	-2.19	120.10	124.37
56	CK	501	GTP	O6-C6-C5	-2.19	120.10	124.37
56	EC	501	GTP	O6-C6-C5	-2.19	120.10	124.37
56	QA	501	GTP	O6-C6-C5	-2.19	120.10	124.37
56	FG	501	GTP	O6-C6-C5	-2.19	120.10	124.37
56	KE	501	GTP	O6-C6-C5	-2.19	120.10	124.37
56	HI	501	GTP	O6-C6-C5	-2.19	120.10	124.37
56	LB	501	GTP	O6-C6-C5	-2.19	120.10	124.37
56	QK	501	GTP	O6-C6-C5	-2.19	120.10	124.37
56	NE	501	GTP	O6-C6-C5	-2.19	120.10	124.37
56	IM	501	GTP	O6-C6-C5	-2.18	120.11	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	MB	501	GTP	O6-C6-C5	-2.18	120.11	124.37
56	UG	501	GTP	O6-C6-C5	-2.18	120.11	124.37
56	UK	501	GTP	O6-C6-C5	-2.18	120.12	124.37
56	AE	501	GTP	O6-C6-C5	-2.18	120.12	124.37
56	LA	501	GTP	O6-C6-C5	-2.18	120.12	124.37
56	WA	501	GTP	O6-C6-C5	-2.18	120.12	124.37
56	RG	501	GTP	O6-C6-C5	-2.18	120.12	124.37
56	AA	501	GTP	O6-C6-C5	-2.17	120.12	124.37
56	OK	501	GTP	O6-C6-C5	-2.17	120.13	124.37
58	VM	501	GDP	C8-N7-C5	2.17	107.13	102.99
56	AG	501	GTP	O6-C6-C5	-2.17	120.13	124.37
56	JB	501	GTP	O6-C6-C5	-2.17	120.13	124.37
58	RM	501	GDP	C2'-C3'-C4'	2.17	106.86	102.64
56	DM	501	GTP	O6-C6-C5	-2.17	120.14	124.37
56	BM	501	GTP	O6-C6-C5	-2.17	120.14	124.37
56	IK	501	GTP	O6-C6-C5	-2.16	120.14	124.37
56	II	501	GTP	O6-C6-C5	-2.16	120.15	124.37
56	JA	501	GTP	O6-C6-C5	-2.16	120.15	124.37
56	VB	501	GTP	O6-C6-C5	-2.16	120.15	124.37
56	UA	501	GTP	O6-C6-C5	-2.16	120.16	124.37
56	WK	501	GTP	O6-C6-C5	-2.16	120.16	124.37
56	FK	501	GTP	O6-C6-C5	-2.16	120.16	124.37
56	GE	501	GTP	O6-C6-C5	-2.16	120.16	124.37
56	DA	501	GTP	O6-C6-C5	-2.16	120.16	124.37
56	UI	501	GTP	O6-C6-C5	-2.15	120.17	124.37
58	GL	501	GDP	C3'-C2'-C1'	2.15	104.22	100.98
56	IA	501	GTP	O6-C6-C5	-2.15	120.17	124.37
56	TA	501	GTP	O6-C6-C5	-2.15	120.17	124.37
58	HC	501	GDP	C2'-C3'-C4'	2.15	106.82	102.64
56	KA	501	GTP	O6-C6-C5	-2.15	120.18	124.37
56	VE	501	GTP	O6-C6-C5	-2.15	120.18	124.37
56	VK	501	GTP	O6-C6-C5	-2.15	120.18	124.37
58	QH	501	GDP	O2B-PB-O3A	2.14	111.83	104.64
56	ML	501	GTP	O6-C6-C5	-2.14	120.18	124.37
56	DK	501	GTP	O6-C6-C5	-2.14	120.19	124.37
56	VG	501	GTP	O6-C6-C5	-2.14	120.19	124.37
56	QB	501	GTP	O6-C6-C5	-2.14	120.19	124.37
56	QE	501	GTP	O6-C6-C5	-2.14	120.19	124.37
56	KK	501	GTP	O6-C6-C5	-2.14	120.19	124.37
58	UL	501	GDP	C2'-C3'-C4'	2.14	106.80	102.64
58	VL	501	GDP	C5-C6-N1	2.14	117.73	113.95
56	ME	501	GTP	O6-C6-C5	-2.14	120.20	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	DE	501	GTP	O6-C6-C5	-2.13	120.20	124.37
56	UB	501	GTP	O6-C6-C5	-2.13	120.20	124.37
56	DG	501	GTP	O6-C6-C5	-2.13	120.21	124.37
56	PA	501	GTP	O6-C6-C5	-2.13	120.22	124.37
56	KB	501	GTP	O6-C6-C5	-2.13	120.22	124.37
58	RF	501	GDP	C8-N7-C5	2.13	107.04	102.99
56	CI	501	GTP	O6-C6-C5	-2.12	120.23	124.37
56	GB	501	GTP	O6-C6-C5	-2.12	120.24	124.37
56	OE	501	GTP	O6-C6-C5	-2.12	120.24	124.37
56	EG	501	GTP	O6-C6-C5	-2.12	120.24	124.37
56	GK	501	GTP	O6-C6-C5	-2.12	120.24	124.37
56	OL	501	GTP	O6-C6-C5	-2.11	120.24	124.37
56	HE	501	GTP	O6-C6-C5	-2.11	120.25	124.37
58	VD	501	GDP	O6-C6-C5	-2.11	120.25	124.37
56	PG	501	GTP	O6-C6-C5	-2.11	120.25	124.37
56	IE	501	GTP	O6-C6-C5	-2.11	120.25	124.37
58	EH	501	GDP	C2'-C3'-C4'	2.11	106.74	102.64
58	RF	501	GDP	C5-C6-N1	2.11	117.67	113.95
58	DD	501	GDP	C5-C6-N1	2.10	117.67	113.95
56	OI	501	GTP	O6-C6-C5	-2.10	120.26	124.37
56	BG	501	GTP	O6-C6-C5	-2.10	120.27	124.37
56	AI	501	GTP	O6-C6-C5	-2.10	120.27	124.37
56	NB	501	GTP	O6-C6-C5	-2.10	120.28	124.37
56	OG	501	GTP	O6-C6-C5	-2.10	120.28	124.37
58	UD	501	GDP	C8-N7-C5	2.10	106.98	102.99
56	QG	501	GTP	O6-C6-C5	-2.09	120.28	124.37
58	DF	501	GDP	C5-C6-N1	2.09	117.65	113.95
58	JC	501	GDP	C2'-C3'-C4'	2.09	106.71	102.64
56	VI	501	GTP	O6-C6-C5	-2.09	120.30	124.37
56	FB	501	GTP	O6-C6-C5	-2.09	120.30	124.37
56	PK	501	GTP	O6-C6-C5	-2.09	120.30	124.37
56	WE	501	GTP	O6-C6-C5	-2.09	120.30	124.37
56	NI	501	GTP	O6-C6-C5	-2.08	120.30	124.37
58	TD	501	GDP	C5-C6-N1	2.08	117.63	113.95
56	NA	501	GTP	O6-C6-C5	-2.08	120.32	124.37
56	BK	501	GTP	O6-C6-C5	-2.08	120.32	124.37
56	OA	501	GTP	O6-C6-C5	-2.08	120.32	124.37
56	JI	501	GTP	O6-C6-C5	-2.07	120.32	124.37
58	BD	501	GDP	C2'-C3'-C4'	2.07	106.67	102.64
58	PF	501	GDP	C8-N7-C5	2.07	106.94	102.99
56	OB	501	GTP	O6-C6-C5	-2.07	120.33	124.37
56	CM	501	GTP	O6-C6-C5	-2.07	120.33	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	CG	501	GTP	O6-C6-C5	-2.07	120.34	124.37
58	JF	501	GDP	C2'-C3'-C4'	2.07	106.66	102.64
58	DF	501	GDP	C8-N7-C5	2.06	106.92	102.99
56	DB	501	GTP	O6-C6-C5	-2.06	120.35	124.37
56	DI	501	GTP	O6-C6-C5	-2.05	120.36	124.37
56	MI	501	GTP	O6-C6-C5	-2.05	120.37	124.37
58	VD	501	GDP	C3'-C2'-C1'	2.05	104.06	100.98
56	BB	501	GTP	O6-C6-C5	-2.05	120.37	124.37
58	WL	501	GDP	C2'-C3'-C4'	2.04	106.61	102.64
56	WB	501	GTP	O6-C6-C5	-2.04	120.39	124.37
56	LE	501	GTP	O6-C6-C5	-2.04	120.39	124.37
56	GI	501	GTP	O6-C6-C5	-2.03	120.40	124.37
58	QJ	501	GDP	C2'-C3'-C4'	2.03	106.58	102.64
56	CK	501	GTP	O3G-PG-O3B	2.02	111.42	104.64
56	PE	501	GTP	O6-C6-C5	-2.02	120.42	124.37
56	HK	501	GTP	O6-C6-C5	-2.02	120.43	124.37
56	PB	501	GTP	O6-C6-C5	-2.02	120.43	124.37
58	OM	501	GDP	C2'-C3'-C4'	2.01	106.55	102.64
58	DD	501	GDP	C8-N7-C5	2.00	106.81	102.99
58	FM	502	GDP	O6-C6-C5	-2.00	120.46	124.37

There are no chirality outliers.

All (958) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	AA	501	GTP	C5'-O5'-PA-O1A
56	AA	501	GTP	C5'-O5'-PA-O2A
56	AA	501	GTP	C3'-C4'-C5'-O5'
56	AB	501	GTP	C5'-O5'-PA-O3A
56	AE	501	GTP	C5'-O5'-PA-O3A
56	AE	501	GTP	C5'-O5'-PA-O1A
56	AE	501	GTP	C5'-O5'-PA-O2A
56	AG	501	GTP	C5'-O5'-PA-O1A
56	AG	501	GTP	C5'-O5'-PA-O2A
56	AI	501	GTP	C5'-O5'-PA-O3A
56	AI	501	GTP	C5'-O5'-PA-O2A
56	AK	501	GTP	C5'-O5'-PA-O1A
56	AM	501	GTP	C5'-O5'-PA-O1A
56	AM	501	GTP	C5'-O5'-PA-O2A
56	BA	501	GTP	C5'-O5'-PA-O3A
56	BB	501	GTP	C5'-O5'-PA-O3A
56	BE	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
56	BG	501	GTP	C5'-O5'-PA-O1A
56	BI	501	GTP	C5'-O5'-PA-O1A
56	BI	501	GTP	C5'-O5'-PA-O2A
56	BK	501	GTP	PB-O3B-PG-O2G
56	BK	501	GTP	C5'-O5'-PA-O3A
56	BM	501	GTP	C5'-O5'-PA-O1A
56	BM	501	GTP	C5'-O5'-PA-O2A
56	BM	501	GTP	C3'-C4'-C5'-O5'
56	CA	501	GTP	C5'-O5'-PA-O3A
56	CB	501	GTP	C5'-O5'-PA-O3A
56	CE	501	GTP	C5'-O5'-PA-O3A
56	CG	501	GTP	C5'-O5'-PA-O1A
56	CG	501	GTP	C5'-O5'-PA-O2A
56	CK	501	GTP	C5'-O5'-PA-O3A
56	CK	501	GTP	C5'-O5'-PA-O2A
56	CM	501	GTP	C5'-O5'-PA-O1A
56	CM	501	GTP	C5'-O5'-PA-O2A
56	DA	501	GTP	C5'-O5'-PA-O3A
56	DE	501	GTP	C5'-O5'-PA-O3A
56	DG	501	GTP	C5'-O5'-PA-O3A
56	DK	501	GTP	C5'-O5'-PA-O3A
56	DK	501	GTP	C5'-O5'-PA-O2A
56	DM	501	GTP	C5'-O5'-PA-O3A
56	EA	501	GTP	C5'-O5'-PA-O3A
56	EC	501	GTP	C5'-O5'-PA-O3A
56	EG	501	GTP	C5'-O5'-PA-O3A
56	FB	501	GTP	C5'-O5'-PA-O3A
56	FE	501	GTP	C5'-O5'-PA-O3A
56	FE	501	GTP	C5'-O5'-PA-O1A
56	FE	501	GTP	C5'-O5'-PA-O2A
56	FG	501	GTP	C5'-O5'-PA-O1A
56	FG	501	GTP	C5'-O5'-PA-O2A
56	FI	501	GTP	C5'-O5'-PA-O3A
56	FI	501	GTP	C5'-O5'-PA-O2A
56	FK	501	GTP	C5'-O5'-PA-O1A
56	FK	501	GTP	C5'-O5'-PA-O2A
56	FM	501	GTP	PB-O3B-PG-O3G
56	FM	501	GTP	C5'-O5'-PA-O3A
56	FM	501	GTP	C5'-O5'-PA-O2A
56	GA	501	GTP	C5'-O5'-PA-O1A
56	GA	501	GTP	C5'-O5'-PA-O2A
56	GB	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
56	GG	501	GTP	C5'-O5'-PA-O3A
56	GG	501	GTP	C5'-O5'-PA-O2A
56	GI	501	GTP	C5'-O5'-PA-O3A
56	GK	501	GTP	C5'-O5'-PA-O3A
56	GK	501	GTP	C5'-O5'-PA-O1A
56	GK	501	GTP	C5'-O5'-PA-O2A
56	HA	501	GTP	C5'-O5'-PA-O3A
56	HB	501	GTP	C5'-O5'-PA-O3A
56	HB	501	GTP	C5'-O5'-PA-O2A
56	HE	501	GTP	C5'-O5'-PA-O1A
56	HE	501	GTP	C5'-O5'-PA-O2A
56	HG	501	GTP	C5'-O5'-PA-O3A
56	HI	501	GTP	C5'-O5'-PA-O1A
56	HI	501	GTP	C5'-O5'-PA-O2A
56	HK	501	GTP	C5'-O5'-PA-O1A
56	HK	501	GTP	C3'-C4'-C5'-O5'
56	IB	501	GTP	PB-O3B-PG-O2G
56	IB	501	GTP	C5'-O5'-PA-O3A
56	IE	501	GTP	C5'-O5'-PA-O3A
56	IE	501	GTP	C5'-O5'-PA-O1A
56	IE	501	GTP	C5'-O5'-PA-O2A
56	IG	501	GTP	C5'-O5'-PA-O1A
56	IG	501	GTP	C5'-O5'-PA-O2A
56	II	501	GTP	C5'-O5'-PA-O1A
56	II	501	GTP	C5'-O5'-PA-O2A
56	IK	501	GTP	C5'-O5'-PA-O3A
56	IM	501	GTP	C5'-O5'-PA-O3A
56	IM	501	GTP	C5'-O5'-PA-O1A
56	IM	501	GTP	C5'-O5'-PA-O2A
56	JA	501	GTP	C5'-O5'-PA-O3A
56	JB	501	GTP	C5'-O5'-PA-O3A
56	JE	501	GTP	C5'-O5'-PA-O3A
56	JG	501	GTP	C5'-O5'-PA-O3A
56	JK	501	GTP	C5'-O5'-PA-O1A
56	JK	501	GTP	C5'-O5'-PA-O2A
56	JK	501	GTP	C3'-C4'-C5'-O5'
56	KB	501	GTP	C5'-O5'-PA-O3A
56	KG	501	GTP	C5'-O5'-PA-O3A
56	KK	501	GTP	C5'-O5'-PA-O1A
56	KK	501	GTP	C5'-O5'-PA-O2A
56	LA	501	GTP	C5'-O5'-PA-O1A
56	LA	501	GTP	C5'-O5'-PA-O2A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
56	LB	501	GTP	C5'-O5'-PA-O3A
56	LB	501	GTP	C5'-O5'-PA-O2A
56	LE	501	GTP	C5'-O5'-PA-O3A
56	LG	501	GTP	C5'-O5'-PA-O3A
56	LK	501	GTP	C5'-O5'-PA-O1A
56	LK	501	GTP	C5'-O5'-PA-O2A
56	MB	501	GTP	C5'-O5'-PA-O3A
56	MB	501	GTP	C5'-O5'-PA-O1A
56	MB	501	GTP	C5'-O5'-PA-O2A
56	ME	501	GTP	C5'-O5'-PA-O1A
56	ME	501	GTP	C5'-O5'-PA-O2A
56	MG	501	GTP	C5'-O5'-PA-O3A
56	MG	501	GTP	C5'-O5'-PA-O2A
56	MI	501	GTP	C5'-O5'-PA-O3A
56	MK	501	GTP	C5'-O5'-PA-O1A
56	MK	501	GTP	C5'-O5'-PA-O2A
56	ML	501	GTP	C5'-O5'-PA-O3A
56	NA	501	GTP	C5'-O5'-PA-O3A
56	NB	501	GTP	C5'-O5'-PA-O1A
56	NB	501	GTP	C5'-O5'-PA-O2A
56	NE	501	GTP	C5'-O5'-PA-O3A
56	NG	501	GTP	C5'-O5'-PA-O3A
56	NG	501	GTP	C5'-O5'-PA-O1A
56	NG	501	GTP	C5'-O5'-PA-O2A
56	NI	501	GTP	C5'-O5'-PA-O1A
56	NI	501	GTP	C5'-O5'-PA-O2A
56	NL	501	GTP	C5'-O5'-PA-O1A
56	NL	501	GTP	C5'-O5'-PA-O2A
56	OA	501	GTP	C5'-O5'-PA-O3A
56	OB	501	GTP	C5'-O5'-PA-O3A
56	OB	501	GTP	C5'-O5'-PA-O2A
56	OE	501	GTP	C5'-O5'-PA-O1A
56	OE	501	GTP	C5'-O5'-PA-O2A
56	OG	501	GTP	C5'-O5'-PA-O3A
56	OI	501	GTP	C5'-O5'-PA-O3A
56	OI	501	GTP	C5'-O5'-PA-O1A
56	OI	501	GTP	C5'-O5'-PA-O2A
56	OK	501	GTP	C5'-O5'-PA-O3A
56	OK	501	GTP	C5'-O5'-PA-O2A
56	OL	501	GTP	C5'-O5'-PA-O1A
56	OL	501	GTP	C5'-O5'-PA-O2A
56	PA	501	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
56	PA	501	GTP	C5'-O5'-PA-O2A
56	PB	501	GTP	C5'-O5'-PA-O3A
56	PB	501	GTP	C5'-O5'-PA-O2A
56	PE	501	GTP	C5'-O5'-PA-O3A
56	PE	501	GTP	C5'-O5'-PA-O2A
56	PG	501	GTP	C5'-O5'-PA-O1A
56	PG	501	GTP	C5'-O5'-PA-O2A
56	PI	501	GTP	C5'-O5'-PA-O3A
56	PI	501	GTP	C5'-O5'-PA-O2A
56	PL	501	GTP	C5'-O5'-PA-O3A
56	QA	501	GTP	C5'-O5'-PA-O3A
56	QA	501	GTP	C5'-O5'-PA-O1A
56	QA	501	GTP	C5'-O5'-PA-O2A
56	QG	501	GTP	C5'-O5'-PA-O1A
56	QG	501	GTP	C5'-O5'-PA-O2A
56	QI	501	GTP	C5'-O5'-PA-O3A
56	QK	501	GTP	C5'-O5'-PA-O3A
56	QL	501	GTP	C5'-O5'-PA-O1A
56	QL	501	GTP	C5'-O5'-PA-O2A
56	RA	501	GTP	C5'-O5'-PA-O3A
56	RB	501	GTP	C5'-O5'-PA-O1A
56	RB	501	GTP	C5'-O5'-PA-O2A
56	RI	501	GTP	C5'-O5'-PA-O3A
56	RI	501	GTP	C5'-O5'-PA-O2A
56	RL	501	GTP	C5'-O5'-PA-O3A
56	SA	502	GTP	C5'-O5'-PA-O3A
56	SA	502	GTP	C5'-O5'-PA-O2A
56	SE	501	GTP	C5'-O5'-PA-O1A
56	SE	501	GTP	C5'-O5'-PA-O2A
56	SE	501	GTP	C3'-C4'-C5'-O5'
56	SG	501	GTP	C5'-O5'-PA-O1A
56	SG	501	GTP	C5'-O5'-PA-O2A
56	SK	501	GTP	C5'-O5'-PA-O3A
56	SK	501	GTP	C5'-O5'-PA-O2A
56	TA	501	GTP	C5'-O5'-PA-O1A
56	TA	501	GTP	C5'-O5'-PA-O2A
56	TB	501	GTP	C5'-O5'-PA-O1A
56	TB	501	GTP	C5'-O5'-PA-O2A
56	TE	501	GTP	C5'-O5'-PA-O1A
56	TE	501	GTP	C5'-O5'-PA-O2A
56	TG	501	GTP	C5'-O5'-PA-O1A
56	TG	501	GTP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
56	TG	501	GTP	C3'-C4'-C5'-O5'
56	TI	501	GTP	C5'-O5'-PA-O1A
56	TI	501	GTP	O4'-C4'-C5'-O5'
56	TI	501	GTP	C3'-C4'-C5'-O5'
56	TK	501	GTP	C5'-O5'-PA-O1A
56	TK	501	GTP	C5'-O5'-PA-O2A
56	UA	501	GTP	C5'-O5'-PA-O1A
56	UA	501	GTP	C5'-O5'-PA-O2A
56	UB	501	GTP	C5'-O5'-PA-O3A
56	UE	501	GTP	C5'-O5'-PA-O3A
56	UE	501	GTP	C5'-O5'-PA-O1A
56	UE	501	GTP	C5'-O5'-PA-O2A
56	UG	501	GTP	C5'-O5'-PA-O1A
56	UG	501	GTP	C5'-O5'-PA-O2A
56	UG	501	GTP	C3'-C4'-C5'-O5'
56	UI	501	GTP	C5'-O5'-PA-O3A
56	UK	501	GTP	C5'-O5'-PA-O1A
56	UK	501	GTP	C5'-O5'-PA-O2A
56	UK	501	GTP	C3'-C4'-C5'-O5'
56	VA	501	GTP	C5'-O5'-PA-O3A
56	VB	501	GTP	C5'-O5'-PA-O1A
56	VB	501	GTP	C5'-O5'-PA-O2A
56	VE	501	GTP	C5'-O5'-PA-O3A
56	VE	501	GTP	C5'-O5'-PA-O2A
56	VG	501	GTP	C5'-O5'-PA-O3A
56	VI	501	GTP	C5'-O5'-PA-O3A
56	VK	501	GTP	C5'-O5'-PA-O1A
56	VK	501	GTP	C5'-O5'-PA-O2A
56	WB	501	GTP	C5'-O5'-PA-O1A
56	WB	501	GTP	C5'-O5'-PA-O2A
56	WE	501	GTP	C5'-O5'-PA-O3A
56	WE	501	GTP	C5'-O5'-PA-O2A
56	WI	501	GTP	C5'-O5'-PA-O3A
56	WK	501	GTP	C5'-O5'-PA-O1A
56	WK	501	GTP	C5'-O5'-PA-O2A
58	AC	501	GDP	C5'-O5'-PA-O3A
58	AD	501	GDP	C5'-O5'-PA-O1A
58	AD	501	GDP	C5'-O5'-PA-O2A
58	AD	501	GDP	O4'-C4'-C5'-O5'
58	AD	501	GDP	C3'-C4'-C5'-O5'
58	AF	501	GDP	C5'-O5'-PA-O3A
58	AH	501	GDP	C5'-O5'-PA-O3A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
58	AH	501	GDP	C5'-O5'-PA-O2A
58	AJ	501	GDP	C5'-O5'-PA-O3A
58	AJ	501	GDP	C5'-O5'-PA-O1A
58	AL	501	GDP	C5'-O5'-PA-O3A
58	AL	501	GDP	C5'-O5'-PA-O1A
58	BC	501	GDP	C5'-O5'-PA-O1A
58	BD	501	GDP	C5'-O5'-PA-O1A
58	BD	501	GDP	C5'-O5'-PA-O2A
58	BF	501	GDP	C5'-O5'-PA-O1A
58	BH	501	GDP	C5'-O5'-PA-O1A
58	BJ	501	GDP	C5'-O5'-PA-O3A
58	BJ	501	GDP	C5'-O5'-PA-O1A
58	BL	501	GDP	C5'-O5'-PA-O3A
58	BL	501	GDP	C5'-O5'-PA-O1A
58	CC	501	GDP	C5'-O5'-PA-O3A
58	CC	501	GDP	C5'-O5'-PA-O1A
58	CD	501	GDP	C5'-O5'-PA-O3A
58	CD	501	GDP	C5'-O5'-PA-O2A
58	CF	501	GDP	C5'-O5'-PA-O3A
58	CF	501	GDP	C5'-O5'-PA-O1A
58	CH	501	GDP	C5'-O5'-PA-O1A
58	CJ	501	GDP	C5'-O5'-PA-O3A
58	CJ	501	GDP	C5'-O5'-PA-O1A
58	CL	501	GDP	C5'-O5'-PA-O3A
58	DC	501	GDP	C5'-O5'-PA-O1A
58	DD	501	GDP	C5'-O5'-PA-O1A
58	DD	501	GDP	C3'-C4'-C5'-O5'
58	DF	501	GDP	C5'-O5'-PA-O1A
58	DH	501	GDP	C5'-O5'-PA-O1A
58	DJ	501	GDP	C5'-O5'-PA-O3A
58	EB	501	GDP	C5'-O5'-PA-O1A
58	ED	501	GDP	C5'-O5'-PA-O3A
58	EF	501	GDP	C5'-O5'-PA-O3A
58	EF	501	GDP	C5'-O5'-PA-O1A
58	EH	501	GDP	C5'-O5'-PA-O3A
58	EJ	501	GDP	C5'-O5'-PA-O1A
58	EM	501	GDP	C5'-O5'-PA-O3A
58	EM	501	GDP	C5'-O5'-PA-O1A
58	FC	501	GDP	C5'-O5'-PA-O3A
58	FC	501	GDP	C5'-O5'-PA-O1A
58	FF	501	GDP	C5'-O5'-PA-O3A
58	FF	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
58	FH	501	GDP	C5'-O5'-PA-O1A
58	FH	501	GDP	C5'-O5'-PA-O2A
58	FJ	501	GDP	C5'-O5'-PA-O1A
58	FL	501	GDP	C5'-O5'-PA-O3A
58	FL	501	GDP	C5'-O5'-PA-O1A
58	GC	501	GDP	C5'-O5'-PA-O3A
58	GC	501	GDP	C5'-O5'-PA-O1A
58	GF	501	GDP	C5'-O5'-PA-O3A
58	GH	501	GDP	C5'-O5'-PA-O1A
58	GJ	501	GDP	C5'-O5'-PA-O1A
58	GM	501	GDP	C5'-O5'-PA-O1A
58	HC	501	GDP	C5'-O5'-PA-O1A
58	HC	501	GDP	C5'-O5'-PA-O2A
58	HD	501	GDP	C5'-O5'-PA-O3A
58	HD	501	GDP	C5'-O5'-PA-O1A
58	HF	501	GDP	C5'-O5'-PA-O1A
58	HH	501	GDP	C5'-O5'-PA-O1A
58	HJ	501	GDP	C5'-O5'-PA-O1A
58	HL	501	GDP	C5'-O5'-PA-O3A
58	HL	501	GDP	C5'-O5'-PA-O1A
58	HM	501	GDP	C5'-O5'-PA-O1A
58	IC	501	GDP	C5'-O5'-PA-O3A
58	IC	501	GDP	C5'-O5'-PA-O1A
58	ID	501	GDP	C5'-O5'-PA-O3A
58	ID	501	GDP	C5'-O5'-PA-O1A
58	IF	501	GDP	C5'-O5'-PA-O3A
58	IH	501	GDP	C5'-O5'-PA-O3A
58	IJ	501	GDP	C5'-O5'-PA-O1A
58	IL	501	GDP	C5'-O5'-PA-O3A
58	IL	501	GDP	C5'-O5'-PA-O1A
58	JC	501	GDP	C5'-O5'-PA-O3A
58	JC	501	GDP	C5'-O5'-PA-O1A
58	JD	501	GDP	C5'-O5'-PA-O3A
58	JF	501	GDP	C5'-O5'-PA-O3A
58	JF	501	GDP	C5'-O5'-PA-O1A
58	JJ	501	GDP	C5'-O5'-PA-O3A
58	JL	501	GDP	C5'-O5'-PA-O1A
58	JL	501	GDP	O4'-C4'-C5'-O5'
58	JL	501	GDP	C3'-C4'-C5'-O5'
58	JM	501	GDP	C5'-O5'-PA-O1A
58	KC	501	GDP	C5'-O5'-PA-O3A
58	KC	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
58	KD	501	GDP	C5'-O5'-PA-O3A
58	KF	501	GDP	C5'-O5'-PA-O3A
58	KH	501	GDP	C5'-O5'-PA-O3A
58	KJ	501	GDP	C5'-O5'-PA-O3A
58	KJ	501	GDP	C5'-O5'-PA-O1A
58	KL	501	GDP	C5'-O5'-PA-O3A
58	KL	501	GDP	C5'-O5'-PA-O1A
58	KM	501	GDP	C5'-O5'-PA-O1A
58	LC	501	GDP	C5'-O5'-PA-O3A
58	LC	501	GDP	C5'-O5'-PA-O1A
58	LD	501	GDP	C5'-O5'-PA-O3A
58	LF	501	GDP	C5'-O5'-PA-O3A
58	LF	501	GDP	C5'-O5'-PA-O1A
58	LH	501	GDP	C5'-O5'-PA-O3A
58	LJ	501	GDP	C5'-O5'-PA-O3A
58	LJ	501	GDP	C5'-O5'-PA-O1A
58	LL	501	GDP	C5'-O5'-PA-O1A
58	MC	501	GDP	C5'-O5'-PA-O3A
58	MC	501	GDP	C5'-O5'-PA-O1A
58	MD	501	GDP	C5'-O5'-PA-O1A
58	MF	501	GDP	C5'-O5'-PA-O3A
58	MH	501	GDP	C5'-O5'-PA-O1A
58	MJ	501	GDP	C5'-O5'-PA-O3A
58	MM	501	GDP	C5'-O5'-PA-O3A
58	MM	501	GDP	C5'-O5'-PA-O1A
58	NC	501	GDP	C5'-O5'-PA-O3A
58	NC	501	GDP	C5'-O5'-PA-O1A
58	ND	501	GDP	C5'-O5'-PA-O1A
58	NF	501	GDP	C5'-O5'-PA-O3A
58	NF	501	GDP	C5'-O5'-PA-O1A
58	NH	501	GDP	C5'-O5'-PA-O1A
58	NJ	501	GDP	C5'-O5'-PA-O3A
58	NJ	501	GDP	C5'-O5'-PA-O1A
58	NK	501	GDP	C5'-O5'-PA-O1A
58	NM	501	GDP	C5'-O5'-PA-O1A
58	OC	501	GDP	C5'-O5'-PA-O3A
58	OD	501	GDP	C5'-O5'-PA-O3A
58	OF	501	GDP	C5'-O5'-PA-O3A
58	OH	501	GDP	C5'-O5'-PA-O3A
58	OJ	501	GDP	C5'-O5'-PA-O1A
58	OM	501	GDP	C5'-O5'-PA-O3A
58	OM	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
58	PC	501	GDP	C5'-O5'-PA-O3A
58	PC	501	GDP	C5'-O5'-PA-O1A
58	PH	501	GDP	C5'-O5'-PA-O3A
58	PH	501	GDP	C5'-O5'-PA-O1A
58	PJ	501	GDP	C5'-O5'-PA-O3A
58	PJ	501	GDP	C5'-O5'-PA-O1A
58	PM	501	GDP	C5'-O5'-PA-O1A
58	QC	501	GDP	C5'-O5'-PA-O3A
58	QC	501	GDP	C5'-O5'-PA-O1A
58	QD	501	GDP	C5'-O5'-PA-O1A
58	QF	501	GDP	C5'-O5'-PA-O3A
58	QF	501	GDP	C5'-O5'-PA-O2A
58	QH	501	GDP	PA-O3A-PB-O2B
58	QH	501	GDP	C5'-O5'-PA-O3A
58	QH	501	GDP	C5'-O5'-PA-O1A
58	QJ	501	GDP	C5'-O5'-PA-O1A
58	QM	501	GDP	C5'-O5'-PA-O1A
58	RC	501	GDP	C5'-O5'-PA-O1A
58	RD	501	GDP	C5'-O5'-PA-O3A
58	RF	501	GDP	C5'-O5'-PA-O1A
58	RF	501	GDP	C5'-O5'-PA-O2A
58	RF	501	GDP	C3'-C4'-C5'-O5'
58	RJ	501	GDP	C5'-O5'-PA-O1A
58	RM	501	GDP	C5'-O5'-PA-O3A
58	RM	501	GDP	C5'-O5'-PA-O1A
58	SC	501	GDP	C5'-O5'-PA-O3A
58	SF	501	GDP	C5'-O5'-PA-O3A
58	SH	501	GDP	C5'-O5'-PA-O3A
58	SH	501	GDP	C5'-O5'-PA-O1A
58	SJ	501	GDP	C5'-O5'-PA-O1A
58	SL	501	GDP	C5'-O5'-PA-O1A
58	SM	501	GDP	C5'-O5'-PA-O1A
58	TC	501	GDP	C5'-O5'-PA-O3A
58	TC	501	GDP	C5'-O5'-PA-O1A
58	TD	501	GDP	C5'-O5'-PA-O1A
58	TD	501	GDP	O4'-C4'-C5'-O5'
58	TD	501	GDP	C3'-C4'-C5'-O5'
58	TF	501	GDP	C5'-O5'-PA-O1A
58	TH	501	GDP	C5'-O5'-PA-O3A
58	TH	501	GDP	C5'-O5'-PA-O1A
58	TJ	501	GDP	C5'-O5'-PA-O1A
58	TL	501	GDP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
58	TL	501	GDP	C5'-O5'-PA-O1A
58	TM	501	GDP	C5'-O5'-PA-O1A
58	UC	501	GDP	C5'-O5'-PA-O1A
58	UD	501	GDP	O4'-C4'-C5'-O5'
58	UD	501	GDP	C3'-C4'-C5'-O5'
58	UF	501	GDP	C5'-O5'-PA-O3A
58	UF	501	GDP	C5'-O5'-PA-O1A
58	UH	501	GDP	C5'-O5'-PA-O3A
58	UH	501	GDP	C5'-O5'-PA-O1A
58	UJ	501	GDP	C5'-O5'-PA-O1A
58	UL	501	GDP	C5'-O5'-PA-O1A
58	UL	501	GDP	C5'-O5'-PA-O2A
58	VC	501	GDP	C5'-O5'-PA-O1A
58	VD	501	GDP	C5'-O5'-PA-O1A
58	VF	501	GDP	C5'-O5'-PA-O1A
58	VH	501	GDP	C5'-O5'-PA-O1A
58	VH	501	GDP	O4'-C4'-C5'-O5'
58	VH	501	GDP	C3'-C4'-C5'-O5'
58	VJ	501	GDP	C5'-O5'-PA-O1A
58	VL	501	GDP	C5'-O5'-PA-O2A
58	VM	501	GDP	C5'-O5'-PA-O1A
58	WC	501	GDP	C5'-O5'-PA-O1A
58	WD	501	GDP	C5'-O5'-PA-O1A
58	WF	501	GDP	C5'-O5'-PA-O3A
58	WF	501	GDP	C5'-O5'-PA-O1A
58	WH	501	GDP	C5'-O5'-PA-O1A
58	WJ	501	GDP	C5'-O5'-PA-O3A
58	WL	501	GDP	C5'-O5'-PA-O1A
56	AA	501	GTP	O4'-C4'-C5'-O5'
56	BG	501	GTP	C3'-C4'-C5'-O5'
56	BM	501	GTP	O4'-C4'-C5'-O5'
56	HK	501	GTP	O4'-C4'-C5'-O5'
56	II	501	GTP	C3'-C4'-C5'-O5'
56	JK	501	GTP	O4'-C4'-C5'-O5'
56	NB	501	GTP	O4'-C4'-C5'-O5'
56	NB	501	GTP	C3'-C4'-C5'-O5'
56	NG	501	GTP	C3'-C4'-C5'-O5'
56	NI	501	GTP	O4'-C4'-C5'-O5'
56	NI	501	GTP	C3'-C4'-C5'-O5'
56	SE	501	GTP	O4'-C4'-C5'-O5'
56	TG	501	GTP	O4'-C4'-C5'-O5'
56	UG	501	GTP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
56	UK	501	GTP	O4'-C4'-C5'-O5'
58	DD	501	GDP	O4'-C4'-C5'-O5'
58	RF	501	GDP	O4'-C4'-C5'-O5'
56	RL	501	GTP	C4'-C5'-O5'-PA
56	BG	501	GTP	O4'-C4'-C5'-O5'
56	IE	501	GTP	O4'-C4'-C5'-O5'
56	IE	501	GTP	C3'-C4'-C5'-O5'
56	II	501	GTP	O4'-C4'-C5'-O5'
56	NG	501	GTP	O4'-C4'-C5'-O5'
56	OE	501	GTP	O4'-C4'-C5'-O5'
56	OE	501	GTP	C3'-C4'-C5'-O5'
56	OK	501	GTP	O4'-C4'-C5'-O5'
56	PG	501	GTP	O4'-C4'-C5'-O5'
56	PG	501	GTP	C3'-C4'-C5'-O5'
58	DJ	501	GDP	O4'-C4'-C5'-O5'
58	DJ	501	GDP	C3'-C4'-C5'-O5'
58	HC	501	GDP	O4'-C4'-C5'-O5'
58	HC	501	GDP	C3'-C4'-C5'-O5'
56	BK	501	GTP	C4'-C5'-O5'-PA
56	GK	501	GTP	C4'-C5'-O5'-PA
56	IB	501	GTP	C4'-C5'-O5'-PA
56	OK	501	GTP	C3'-C4'-C5'-O5'
56	TB	501	GTP	C3'-C4'-C5'-O5'
56	EG	501	GTP	C4'-C5'-O5'-PA
56	HA	501	GTP	C4'-C5'-O5'-PA
56	JI	501	GTP	C4'-C5'-O5'-PA
56	KB	501	GTP	C4'-C5'-O5'-PA
56	RK	501	GTP	C4'-C5'-O5'-PA
56	VG	501	GTP	C4'-C5'-O5'-PA
56	WE	501	GTP	C4'-C5'-O5'-PA
56	BI	501	GTP	C3'-C4'-C5'-O5'
56	HE	501	GTP	C3'-C4'-C5'-O5'
56	IM	501	GTP	C3'-C4'-C5'-O5'
56	OL	501	GTP	C3'-C4'-C5'-O5'
56	TB	501	GTP	O4'-C4'-C5'-O5'
56	EI	501	GTP	C4'-C5'-O5'-PA
56	OL	501	GTP	O4'-C4'-C5'-O5'
56	SG	501	GTP	C3'-C4'-C5'-O5'
56	UA	501	GTP	C3'-C4'-C5'-O5'
58	OD	501	GDP	C3'-C4'-C5'-O5'
58	SD	501	GDP	C3'-C4'-C5'-O5'
56	CA	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
56	DE	501	GTP	C4'-C5'-O5'-PA
56	FB	501	GTP	C4'-C5'-O5'-PA
56	GE	501	GTP	C4'-C5'-O5'-PA
56	KA	501	GTP	C4'-C5'-O5'-PA
56	LE	501	GTP	C4'-C5'-O5'-PA
56	LG	501	GTP	C4'-C5'-O5'-PA
56	QB	501	GTP	C4'-C5'-O5'-PA
56	QK	501	GTP	C4'-C5'-O5'-PA
56	RA	501	GTP	C4'-C5'-O5'-PA
56	UE	501	GTP	C4'-C5'-O5'-PA
56	WG	501	GTP	C4'-C5'-O5'-PA
56	BI	501	GTP	O4'-C4'-C5'-O5'
56	HE	501	GTP	O4'-C4'-C5'-O5'
56	MK	501	GTP	C3'-C4'-C5'-O5'
56	RL	501	GTP	C3'-C4'-C5'-O5'
56	TA	501	GTP	C3'-C4'-C5'-O5'
58	LJ	501	GDP	C3'-C4'-C5'-O5'
56	GG	501	GTP	C4'-C5'-O5'-PA
56	IK	501	GTP	C4'-C5'-O5'-PA
56	KG	501	GTP	C4'-C5'-O5'-PA
56	PL	501	GTP	C4'-C5'-O5'-PA
56	QE	501	GTP	C4'-C5'-O5'-PA
56	WA	501	GTP	C4'-C5'-O5'-PA
56	HI	501	GTP	PB-O3A-PA-O1A
56	II	501	GTP	PB-O3A-PA-O1A
56	OL	501	GTP	PB-O3A-PA-O1A
56	QL	501	GTP	PB-O3A-PA-O1A
56	FK	501	GTP	C3'-C4'-C5'-O5'
56	IM	501	GTP	O4'-C4'-C5'-O5'
56	QL	501	GTP	C3'-C4'-C5'-O5'
56	VB	501	GTP	C3'-C4'-C5'-O5'
56	WB	501	GTP	C3'-C4'-C5'-O5'
56	AB	501	GTP	C4'-C5'-O5'-PA
56	AI	501	GTP	C4'-C5'-O5'-PA
56	BA	501	GTP	C4'-C5'-O5'-PA
56	BB	501	GTP	C4'-C5'-O5'-PA
56	BE	501	GTP	C4'-C5'-O5'-PA
56	CB	501	GTP	C4'-C5'-O5'-PA
56	CE	501	GTP	C4'-C5'-O5'-PA
56	CI	501	GTP	C4'-C5'-O5'-PA
56	DA	501	GTP	C4'-C5'-O5'-PA
56	DM	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
56	EA	501	GTP	C4'-C5'-O5'-PA
56	EE	501	GTP	C4'-C5'-O5'-PA
56	EK	501	GTP	C4'-C5'-O5'-PA
56	GB	501	GTP	C4'-C5'-O5'-PA
56	JA	501	GTP	C4'-C5'-O5'-PA
56	JB	501	GTP	C4'-C5'-O5'-PA
56	JE	501	GTP	C4'-C5'-O5'-PA
56	JG	501	GTP	C4'-C5'-O5'-PA
56	KE	501	GTP	C4'-C5'-O5'-PA
56	LB	501	GTP	C4'-C5'-O5'-PA
56	MA	501	GTP	C4'-C5'-O5'-PA
56	ML	501	GTP	C4'-C5'-O5'-PA
56	NA	501	GTP	C4'-C5'-O5'-PA
56	OB	501	GTP	C4'-C5'-O5'-PA
56	OG	501	GTP	C4'-C5'-O5'-PA
56	PB	501	GTP	C4'-C5'-O5'-PA
56	RE	501	GTP	C4'-C5'-O5'-PA
56	RG	501	GTP	C4'-C5'-O5'-PA
56	UI	501	GTP	C4'-C5'-O5'-PA
56	VA	501	GTP	C4'-C5'-O5'-PA
56	VI	501	GTP	C4'-C5'-O5'-PA
56	SG	501	GTP	O4'-C4'-C5'-O5'
56	AM	501	GTP	C4'-C5'-O5'-PA
56	BG	501	GTP	C4'-C5'-O5'-PA
56	CG	501	GTP	C4'-C5'-O5'-PA
56	CK	501	GTP	C4'-C5'-O5'-PA
56	DG	501	GTP	C4'-C5'-O5'-PA
56	DI	501	GTP	C4'-C5'-O5'-PA
56	EC	501	GTP	C4'-C5'-O5'-PA
56	FK	501	GTP	C4'-C5'-O5'-PA
56	GA	501	GTP	C4'-C5'-O5'-PA
56	HE	501	GTP	C4'-C5'-O5'-PA
56	HG	501	GTP	C4'-C5'-O5'-PA
56	HI	501	GTP	C4'-C5'-O5'-PA
56	HK	501	GTP	C4'-C5'-O5'-PA
56	IA	501	GTP	C4'-C5'-O5'-PA
56	KI	501	GTP	C4'-C5'-O5'-PA
56	KK	501	GTP	C4'-C5'-O5'-PA
56	LA	501	GTP	C4'-C5'-O5'-PA
56	LI	501	GTP	C4'-C5'-O5'-PA
56	MG	501	GTP	C4'-C5'-O5'-PA
56	NE	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
56	OA	501	GTP	C4'-C5'-O5'-PA
56	OE	501	GTP	C4'-C5'-O5'-PA
56	PG	501	GTP	C4'-C5'-O5'-PA
56	PI	501	GTP	C4'-C5'-O5'-PA
56	QA	501	GTP	C4'-C5'-O5'-PA
56	QG	501	GTP	C4'-C5'-O5'-PA
56	QL	501	GTP	C4'-C5'-O5'-PA
56	RB	501	GTP	C4'-C5'-O5'-PA
56	SB	501	GTP	C4'-C5'-O5'-PA
56	TA	501	GTP	C4'-C5'-O5'-PA
56	TE	501	GTP	C4'-C5'-O5'-PA
56	TK	501	GTP	C4'-C5'-O5'-PA
56	UK	501	GTP	C4'-C5'-O5'-PA
56	WB	501	GTP	C4'-C5'-O5'-PA
58	QH	501	GDP	C4'-C5'-O5'-PA
56	CK	501	GTP	PB-O3A-PA-O5'
56	TA	501	GTP	O4'-C4'-C5'-O5'
56	UA	501	GTP	O4'-C4'-C5'-O5'
56	HK	501	GTP	PB-O3B-PG-O1G
56	RL	501	GTP	PB-O3B-PG-O1G
58	GM	501	GDP	PA-O3A-PB-O1B
56	AE	501	GTP	C4'-C5'-O5'-PA
56	BI	501	GTP	C4'-C5'-O5'-PA
56	BM	501	GTP	C4'-C5'-O5'-PA
56	FE	501	GTP	C4'-C5'-O5'-PA
56	FG	501	GTP	C4'-C5'-O5'-PA
56	FI	501	GTP	C4'-C5'-O5'-PA
56	IM	501	GTP	C4'-C5'-O5'-PA
56	MK	501	GTP	C4'-C5'-O5'-PA
56	NB	501	GTP	C4'-C5'-O5'-PA
56	NI	501	GTP	C4'-C5'-O5'-PA
56	NL	501	GTP	C4'-C5'-O5'-PA
56	OK	501	GTP	C4'-C5'-O5'-PA
56	PA	501	GTP	C4'-C5'-O5'-PA
56	SA	502	GTP	C4'-C5'-O5'-PA
56	SG	501	GTP	C4'-C5'-O5'-PA
56	SK	501	GTP	C4'-C5'-O5'-PA
56	TB	501	GTP	C4'-C5'-O5'-PA
56	TG	501	GTP	C4'-C5'-O5'-PA
56	TI	501	GTP	C4'-C5'-O5'-PA
56	VB	501	GTP	C4'-C5'-O5'-PA
56	VK	501	GTP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
56	WK	501	GTP	C4'-C5'-O5'-PA
56	BB	501	GTP	PB-O3B-PG-O2G
56	BM	501	GTP	PB-O3B-PG-O3G
56	QL	501	GTP	PB-O3B-PG-O3G
56	WI	501	GTP	PB-O3B-PG-O2G
56	AA	501	GTP	C5'-O5'-PA-O3A
56	BG	501	GTP	C5'-O5'-PA-O3A
56	CM	501	GTP	C5'-O5'-PA-O3A
56	FG	501	GTP	C5'-O5'-PA-O3A
56	HK	501	GTP	C5'-O5'-PA-O3A
56	IA	501	GTP	C5'-O5'-PA-O3A
56	IG	501	GTP	C5'-O5'-PA-O3A
56	JI	501	GTP	C5'-O5'-PA-O3A
56	JK	501	GTP	C5'-O5'-PA-O3A
56	KA	501	GTP	C5'-O5'-PA-O3A
56	LA	501	GTP	C5'-O5'-PA-O3A
56	MA	501	GTP	C5'-O5'-PA-O3A
56	ME	501	GTP	C5'-O5'-PA-O3A
56	NI	501	GTP	C5'-O5'-PA-O3A
56	NL	501	GTP	C5'-O5'-PA-O3A
56	SE	501	GTP	C5'-O5'-PA-O3A
56	TB	501	GTP	C5'-O5'-PA-O3A
56	UG	501	GTP	C5'-O5'-PA-O3A
56	WG	501	GTP	C5'-O5'-PA-O3A
58	BC	501	GDP	C5'-O5'-PA-O3A
58	DC	501	GDP	C5'-O5'-PA-O3A
58	GJ	501	GDP	C5'-O5'-PA-O3A
58	MH	501	GDP	C5'-O5'-PA-O3A
58	NH	501	GDP	C5'-O5'-PA-O3A
58	PM	501	GDP	C5'-O5'-PA-O3A
58	QM	501	GDP	C5'-O5'-PA-O3A
58	RC	501	GDP	C5'-O5'-PA-O3A
58	SJ	501	GDP	C5'-O5'-PA-O3A
58	SL	501	GDP	C5'-O5'-PA-O3A
58	VL	501	GDP	C5'-O5'-PA-O3A
58	SD	501	GDP	O4'-C4'-C5'-O5'
58	VL	501	GDP	C3'-C4'-C5'-O5'
56	CK	501	GTP	PA-O3A-PB-O2B
56	FE	501	GTP	PB-O3A-PA-O1A
56	FG	501	GTP	PB-O3A-PA-O2A
56	FK	501	GTP	PB-O3A-PA-O2A
56	MB	501	GTP	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
56	OE	501	GTP	PB-O3A-PA-O1A
56	OK	501	GTP	PA-O3A-PB-O2B
56	QA	501	GTP	PB-O3A-PA-O1A
56	UK	501	GTP	PB-O3A-PA-O1A
56	VK	501	GTP	PB-O3A-PA-O1A
56	WB	501	GTP	PB-O3A-PA-O1A
56	WK	501	GTP	PB-O3A-PA-O1A
56	AA	501	GTP	C4'-C5'-O5'-PA
56	AG	501	GTP	C4'-C5'-O5'-PA
56	DB	501	GTP	C4'-C5'-O5'-PA
56	DK	501	GTP	C4'-C5'-O5'-PA
56	GI	501	GTP	C4'-C5'-O5'-PA
56	HB	501	GTP	C4'-C5'-O5'-PA
56	IE	501	GTP	C4'-C5'-O5'-PA
56	IG	501	GTP	C4'-C5'-O5'-PA
56	II	501	GTP	C4'-C5'-O5'-PA
56	JK	501	GTP	C4'-C5'-O5'-PA
56	MB	501	GTP	C4'-C5'-O5'-PA
56	ME	501	GTP	C4'-C5'-O5'-PA
56	MI	501	GTP	C4'-C5'-O5'-PA
56	NG	501	GTP	C4'-C5'-O5'-PA
56	OL	501	GTP	C4'-C5'-O5'-PA
56	PE	501	GTP	C4'-C5'-O5'-PA
56	PK	501	GTP	C4'-C5'-O5'-PA
56	QI	501	GTP	C4'-C5'-O5'-PA
56	RI	501	GTP	C4'-C5'-O5'-PA
56	SE	501	GTP	C4'-C5'-O5'-PA
56	SI	501	GTP	C4'-C5'-O5'-PA
56	UA	501	GTP	C4'-C5'-O5'-PA
56	UG	501	GTP	C4'-C5'-O5'-PA
56	VE	501	GTP	C4'-C5'-O5'-PA
56	WI	501	GTP	C4'-C5'-O5'-PA
56	AB	501	GTP	C5'-O5'-PA-O2A
56	AK	501	GTP	C5'-O5'-PA-O2A
56	BA	501	GTP	C5'-O5'-PA-O2A
56	BB	501	GTP	C5'-O5'-PA-O2A
56	BE	501	GTP	C5'-O5'-PA-O2A
56	BG	501	GTP	C5'-O5'-PA-O2A
56	BK	501	GTP	C5'-O5'-PA-O2A
56	CA	501	GTP	C5'-O5'-PA-O2A
56	CE	501	GTP	C5'-O5'-PA-O2A
56	DA	501	GTP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
56	DE	501	GTP	C5'-O5'-PA-O2A
56	DG	501	GTP	C5'-O5'-PA-O2A
56	DM	501	GTP	C5'-O5'-PA-O2A
56	EC	501	GTP	C5'-O5'-PA-O2A
56	EG	501	GTP	C5'-O5'-PA-O2A
56	FB	501	GTP	C5'-O5'-PA-O2A
56	GB	501	GTP	C5'-O5'-PA-O2A
56	GI	501	GTP	C5'-O5'-PA-O2A
56	HG	501	GTP	C5'-O5'-PA-O2A
56	HK	501	GTP	C5'-O5'-PA-O2A
56	IB	501	GTP	C5'-O5'-PA-O2A
56	IK	501	GTP	C5'-O5'-PA-O2A
56	JA	501	GTP	C5'-O5'-PA-O2A
56	JB	501	GTP	C5'-O5'-PA-O2A
56	JE	501	GTP	C5'-O5'-PA-O2A
56	JG	501	GTP	C5'-O5'-PA-O2A
56	KG	501	GTP	C5'-O5'-PA-O2A
56	LE	501	GTP	C5'-O5'-PA-O2A
56	LG	501	GTP	C5'-O5'-PA-O2A
56	MI	501	GTP	C5'-O5'-PA-O2A
56	ML	501	GTP	C5'-O5'-PA-O2A
56	NA	501	GTP	C5'-O5'-PA-O2A
56	NE	501	GTP	C5'-O5'-PA-O2A
56	OA	501	GTP	C5'-O5'-PA-O2A
56	OG	501	GTP	C5'-O5'-PA-O2A
56	PL	501	GTP	C5'-O5'-PA-O2A
56	QK	501	GTP	C5'-O5'-PA-O2A
56	RA	501	GTP	C5'-O5'-PA-O2A
56	RL	501	GTP	C5'-O5'-PA-O2A
56	TI	501	GTP	C5'-O5'-PA-O2A
56	UB	501	GTP	C5'-O5'-PA-O2A
56	UI	501	GTP	C5'-O5'-PA-O2A
56	VA	501	GTP	C5'-O5'-PA-O2A
56	VG	501	GTP	C5'-O5'-PA-O2A
56	VI	501	GTP	C5'-O5'-PA-O2A
56	WI	501	GTP	C5'-O5'-PA-O2A
58	AC	501	GDP	C5'-O5'-PA-O1A
58	AF	501	GDP	C5'-O5'-PA-O1A
58	AH	501	GDP	C5'-O5'-PA-O1A
58	CD	501	GDP	C5'-O5'-PA-O1A
58	CL	501	GDP	C5'-O5'-PA-O1A
58	DJ	501	GDP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
58	ED	501	GDP	C5'-O5'-PA-O1A
58	EH	501	GDP	C5'-O5'-PA-O1A
58	GF	501	GDP	C5'-O5'-PA-O1A
58	IF	501	GDP	C5'-O5'-PA-O1A
58	IH	501	GDP	C5'-O5'-PA-O1A
58	JD	501	GDP	C5'-O5'-PA-O1A
58	JJ	501	GDP	C5'-O5'-PA-O1A
58	KD	501	GDP	C5'-O5'-PA-O1A
58	KF	501	GDP	C5'-O5'-PA-O1A
58	KH	501	GDP	C5'-O5'-PA-O1A
58	LD	501	GDP	C5'-O5'-PA-O1A
58	LH	501	GDP	C5'-O5'-PA-O1A
58	MF	501	GDP	C5'-O5'-PA-O1A
58	MJ	501	GDP	C5'-O5'-PA-O1A
58	OC	501	GDP	C5'-O5'-PA-O1A
58	OD	501	GDP	C5'-O5'-PA-O1A
58	OF	501	GDP	C5'-O5'-PA-O1A
58	OH	501	GDP	C5'-O5'-PA-O1A
58	QF	501	GDP	C5'-O5'-PA-O1A
58	RD	501	GDP	C5'-O5'-PA-O1A
58	SC	501	GDP	C5'-O5'-PA-O1A
58	SF	501	GDP	C5'-O5'-PA-O1A
58	VL	501	GDP	C5'-O5'-PA-O1A
58	WJ	501	GDP	C5'-O5'-PA-O1A
56	CK	501	GTP	C3'-C4'-C5'-O5'
56	DG	501	GTP	C3'-C4'-C5'-O5'
56	QE	501	GTP	C3'-C4'-C5'-O5'
56	RK	501	GTP	C3'-C4'-C5'-O5'
56	VK	501	GTP	C3'-C4'-C5'-O5'
58	OD	501	GDP	O4'-C4'-C5'-O5'
56	CM	501	GTP	C4'-C5'-O5'-PA
56	FM	501	GTP	C4'-C5'-O5'-PA
56	OI	501	GTP	C4'-C5'-O5'-PA
56	UB	501	GTP	C4'-C5'-O5'-PA
56	FE	501	GTP	C3'-C4'-C5'-O5'
56	MK	501	GTP	O4'-C4'-C5'-O5'
56	QL	501	GTP	O4'-C4'-C5'-O5'
56	VB	501	GTP	O4'-C4'-C5'-O5'
56	WB	501	GTP	O4'-C4'-C5'-O5'
56	WE	501	GTP	C3'-C4'-C5'-O5'
58	LJ	501	GDP	O4'-C4'-C5'-O5'
56	BK	501	GTP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
56	LK	501	GTP	C3'-C4'-C5'-O5'
56	BG	501	GTP	PA-O3A-PB-O2B
56	DK	501	GTP	PA-O3A-PB-O2B
56	HK	501	GTP	PB-O3A-PA-O1A
56	IG	501	GTP	PB-O3A-PA-O2A
56	JK	501	GTP	PA-O3A-PB-O2B
56	LA	501	GTP	PB-O3A-PA-O2A
56	ME	501	GTP	PB-O3A-PA-O1A
56	QG	501	GTP	PB-O3A-PA-O2A
56	RB	501	GTP	PB-O3A-PA-O2A
56	RI	501	GTP	PB-O3A-PA-O2A
56	SA	502	GTP	PB-O3A-PA-O2A
56	SG	501	GTP	PB-O3A-PA-O1A
56	TA	501	GTP	PB-O3A-PA-O2A
56	TB	501	GTP	PB-O3A-PA-O2A
56	UA	501	GTP	PB-O3A-PA-O2A
56	VE	501	GTP	PB-O3A-PA-O2A
56	AK	501	GTP	C4'-C5'-O5'-PA
58	HL	501	GDP	C3'-C4'-C5'-O5'
56	LK	501	GTP	C4'-C5'-O5'-PA
56	NB	501	GTP	PB-O3B-PG-O1G
56	AE	501	GTP	PB-O3A-PA-O2A
56	BI	501	GTP	PB-O3A-PA-O1A
56	BM	501	GTP	PB-O3A-PA-O1A
56	GA	501	GTP	PB-O3A-PA-O2A
56	IM	501	GTP	PA-O3A-PB-O2B
56	ME	501	GTP	PB-O3A-PA-O2A
56	PG	501	GTP	PB-O3A-PA-O1A
56	RB	501	GTP	PB-O3A-PA-O1A
56	WI	501	GTP	PB-O3A-PA-O2A
56	CK	501	GTP	O4'-C4'-C5'-O5'
56	FK	501	GTP	O4'-C4'-C5'-O5'
56	RE	501	GTP	C3'-C4'-C5'-O5'
56	VK	501	GTP	O4'-C4'-C5'-O5'
58	LF	501	GDP	C3'-C4'-C5'-O5'
58	VL	501	GDP	O4'-C4'-C5'-O5'
56	BM	501	GTP	PB-O3B-PG-O1G
58	UD	501	GDP	PA-O3A-PB-O1B
56	AK	501	GTP	C3'-C4'-C5'-O5'
56	DG	501	GTP	O4'-C4'-C5'-O5'
56	FE	501	GTP	O4'-C4'-C5'-O5'
56	RL	501	GTP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
58	JJ	501	GDP	C3'-C4'-C5'-O5'
58	SF	501	GDP	C3'-C4'-C5'-O5'
56	AA	501	GTP	PB-O3B-PG-O2G
56	HK	501	GTP	PB-O3B-PG-O2G
56	HK	501	GTP	PB-O3B-PG-O3G
56	IK	501	GTP	PB-O3B-PG-O2G
56	MA	501	GTP	PB-O3B-PG-O2G
56	NB	501	GTP	PB-O3B-PG-O2G
56	NB	501	GTP	PB-O3B-PG-O3G
56	RL	501	GTP	PB-O3B-PG-O2G
56	RL	501	GTP	PB-O3B-PG-O3G
56	UK	501	GTP	PB-O3B-PG-O2G
58	QH	501	GDP	PA-O3A-PB-O3B
56	AG	501	GTP	C5'-O5'-PA-O3A
56	AK	501	GTP	C5'-O5'-PA-O3A
56	AM	501	GTP	C5'-O5'-PA-O3A
56	BI	501	GTP	C5'-O5'-PA-O3A
56	BM	501	GTP	C5'-O5'-PA-O3A
56	CG	501	GTP	C5'-O5'-PA-O3A
56	CI	501	GTP	C5'-O5'-PA-O3A
56	DI	501	GTP	C5'-O5'-PA-O3A
56	EE	501	GTP	C5'-O5'-PA-O3A
56	EI	501	GTP	C5'-O5'-PA-O3A
56	EK	501	GTP	C5'-O5'-PA-O3A
56	FK	501	GTP	C5'-O5'-PA-O3A
56	GA	501	GTP	C5'-O5'-PA-O3A
56	GE	501	GTP	C5'-O5'-PA-O3A
56	HE	501	GTP	C5'-O5'-PA-O3A
56	HI	501	GTP	C5'-O5'-PA-O3A
56	II	501	GTP	C5'-O5'-PA-O3A
56	KE	501	GTP	C5'-O5'-PA-O3A
56	KI	501	GTP	C5'-O5'-PA-O3A
56	KK	501	GTP	C5'-O5'-PA-O3A
56	LI	501	GTP	C5'-O5'-PA-O3A
56	LK	501	GTP	C5'-O5'-PA-O3A
56	MK	501	GTP	C5'-O5'-PA-O3A
56	NB	501	GTP	C5'-O5'-PA-O3A
56	OE	501	GTP	C5'-O5'-PA-O3A
56	OL	501	GTP	C5'-O5'-PA-O3A
56	PG	501	GTP	C5'-O5'-PA-O3A
56	QB	501	GTP	C5'-O5'-PA-O3A
56	QE	501	GTP	C5'-O5'-PA-O3A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
56	QG	501	GTP	C5'-O5'-PA-O3A
56	QL	501	GTP	C5'-O5'-PA-O3A
56	RB	501	GTP	C5'-O5'-PA-O3A
56	RE	501	GTP	C5'-O5'-PA-O3A
56	RG	501	GTP	C5'-O5'-PA-O3A
56	RK	501	GTP	C5'-O5'-PA-O3A
56	SB	501	GTP	C5'-O5'-PA-O3A
56	SG	501	GTP	C5'-O5'-PA-O3A
56	SI	501	GTP	C5'-O5'-PA-O3A
56	TA	501	GTP	C5'-O5'-PA-O3A
56	TE	501	GTP	C5'-O5'-PA-O3A
56	TG	501	GTP	C5'-O5'-PA-O3A
56	TI	501	GTP	C5'-O5'-PA-O3A
56	TK	501	GTP	C5'-O5'-PA-O3A
56	UA	501	GTP	C5'-O5'-PA-O3A
56	UK	501	GTP	C5'-O5'-PA-O3A
56	VB	501	GTP	C5'-O5'-PA-O3A
56	VK	501	GTP	C5'-O5'-PA-O3A
56	WA	501	GTP	C5'-O5'-PA-O3A
56	WB	501	GTP	C5'-O5'-PA-O3A
56	WK	501	GTP	C5'-O5'-PA-O3A
58	AD	501	GDP	C5'-O5'-PA-O3A
58	BD	501	GDP	C5'-O5'-PA-O3A
58	BF	501	GDP	C5'-O5'-PA-O3A
58	BH	501	GDP	C5'-O5'-PA-O3A
58	CH	501	GDP	C5'-O5'-PA-O3A
58	DD	501	GDP	C5'-O5'-PA-O3A
58	DF	501	GDP	C5'-O5'-PA-O3A
58	EJ	501	GDP	C5'-O5'-PA-O3A
58	FH	501	GDP	C5'-O5'-PA-O3A
58	FJ	501	GDP	C5'-O5'-PA-O3A
58	HC	501	GDP	C5'-O5'-PA-O3A
58	HF	501	GDP	C5'-O5'-PA-O3A
58	HH	501	GDP	C5'-O5'-PA-O3A
58	HJ	501	GDP	C5'-O5'-PA-O3A
58	IJ	501	GDP	C5'-O5'-PA-O3A
58	JL	501	GDP	C5'-O5'-PA-O3A
58	JM	501	GDP	C5'-O5'-PA-O3A
58	KM	501	GDP	C5'-O5'-PA-O3A
58	LL	501	GDP	C5'-O5'-PA-O3A
58	ND	501	GDP	C5'-O5'-PA-O3A
58	NM	501	GDP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
58	OJ	501	GDP	C5'-O5'-PA-O3A
58	QD	501	GDP	C5'-O5'-PA-O3A
58	RF	501	GDP	C5'-O5'-PA-O3A
58	RJ	501	GDP	C5'-O5'-PA-O3A
58	SM	501	GDP	C5'-O5'-PA-O3A
58	TJ	501	GDP	C5'-O5'-PA-O3A
58	TM	501	GDP	C5'-O5'-PA-O3A
58	UC	501	GDP	C5'-O5'-PA-O3A
58	UJ	501	GDP	C5'-O5'-PA-O3A
58	UL	501	GDP	C5'-O5'-PA-O3A
58	VD	501	GDP	C5'-O5'-PA-O3A
58	VF	501	GDP	C5'-O5'-PA-O3A
58	VJ	501	GDP	C5'-O5'-PA-O3A
58	VM	501	GDP	C5'-O5'-PA-O3A
58	WH	501	GDP	C5'-O5'-PA-O3A
58	WL	501	GDP	C5'-O5'-PA-O3A
56	HA	501	GTP	C3'-C4'-C5'-O5'
58	VM	501	GDP	C3'-C4'-C5'-O5'
56	AE	501	GTP	PB-O3A-PA-O1A
56	AM	501	GTP	PB-O3A-PA-O1A
56	AM	501	GTP	PB-O3A-PA-O2A
56	BG	501	GTP	PA-O3A-PB-O1B
56	FE	501	GTP	PB-O3A-PA-O2A
56	GA	501	GTP	PB-O3A-PA-O1A
56	HI	501	GTP	PB-O3A-PA-O2A
56	IG	501	GTP	PB-O3A-PA-O1A
56	II	501	GTP	PB-O3A-PA-O2A
56	LK	501	GTP	PB-O3A-PA-O2A
56	NB	501	GTP	PA-O3A-PB-O2B
56	QA	501	GTP	PB-O3A-PA-O2A
56	QG	501	GTP	PB-O3A-PA-O1A
56	TA	501	GTP	PB-O3A-PA-O1A
56	TB	501	GTP	PB-O3A-PA-O1A
56	TI	501	GTP	PA-O3A-PB-O2B
56	UK	501	GTP	PB-O3A-PA-O2A
56	WI	501	GTP	PB-O3A-PA-O1A
56	WK	501	GTP	PB-O3A-PA-O2A
56	EA	501	GTP	C5'-O5'-PA-O2A
56	HA	501	GTP	C5'-O5'-PA-O2A
56	IA	501	GTP	C5'-O5'-PA-O2A
56	KB	501	GTP	C5'-O5'-PA-O2A
56	QI	501	GTP	C5'-O5'-PA-O2A

*Continued on next page...*

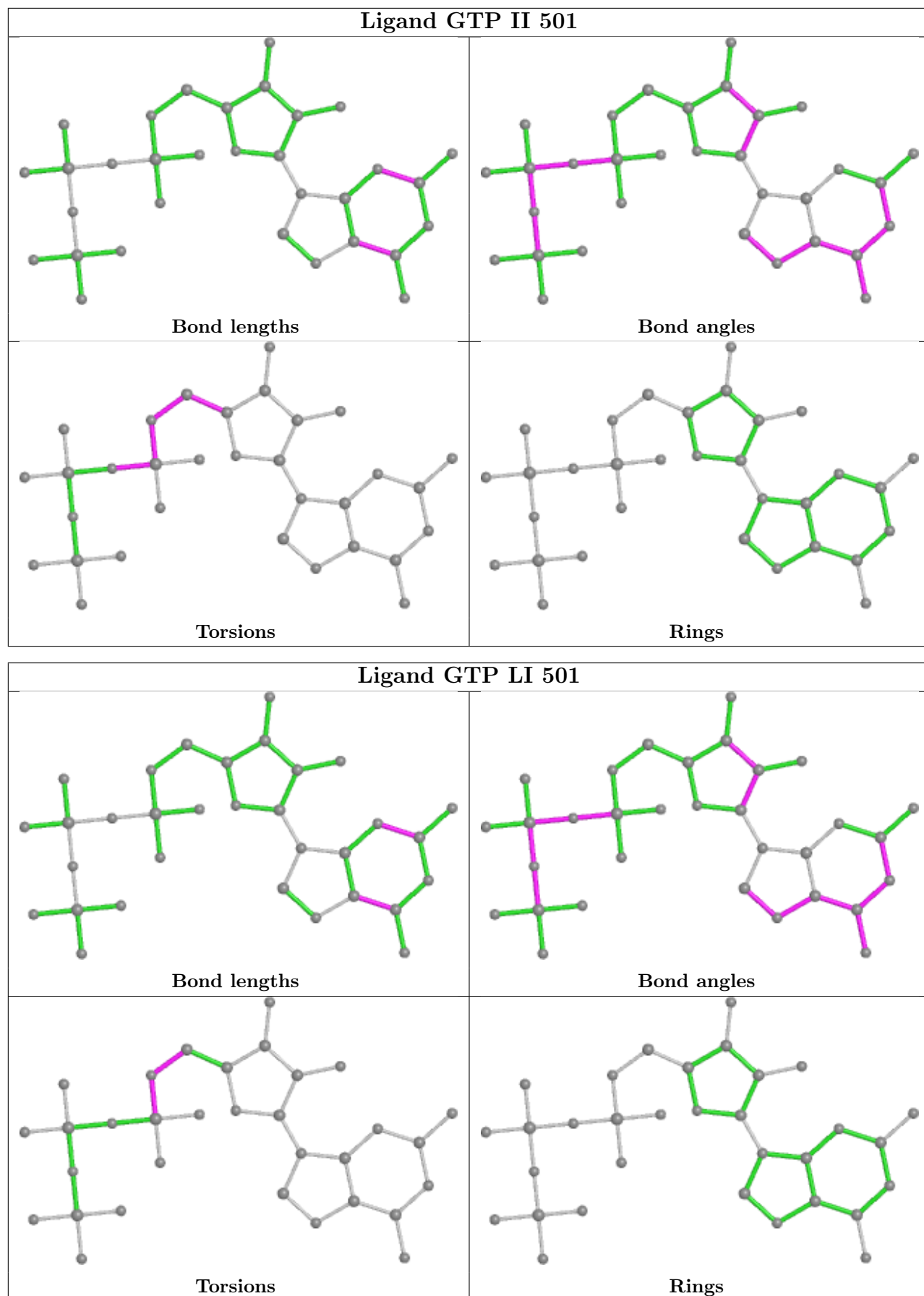
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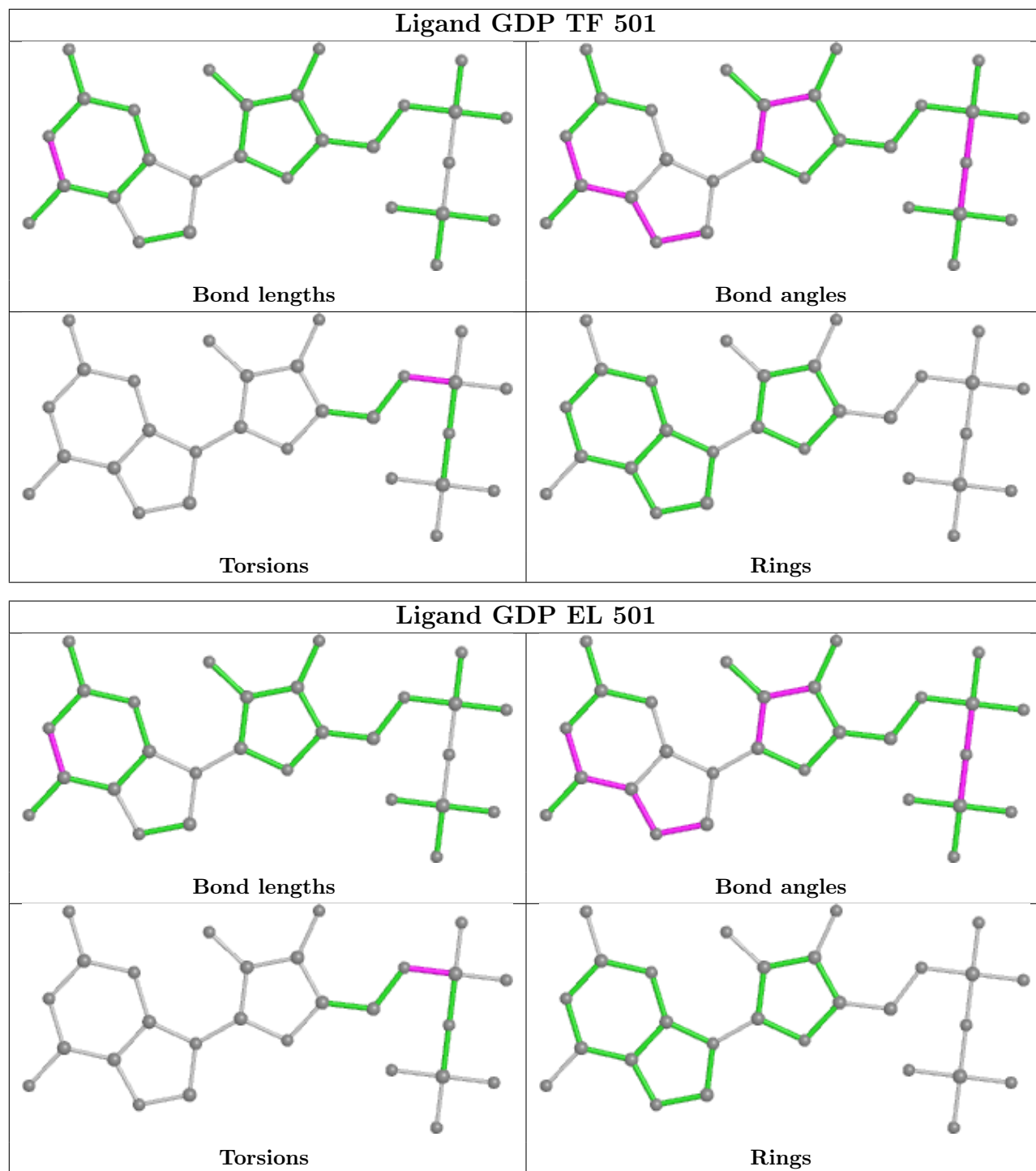
Mol	Chain	Res	Type	Atoms
56	WG	501	GTP	C5'-O5'-PA-O2A
58	EL	501	GDP	C5'-O5'-PA-O1A
58	FD	501	GDP	C5'-O5'-PA-O1A
58	FM	502	GDP	C5'-O5'-PA-O1A
58	GD	501	GDP	C5'-O5'-PA-O1A
58	GL	501	GDP	C5'-O5'-PA-O1A
58	JH	501	GDP	C5'-O5'-PA-O1A
58	LM	501	GDP	C5'-O5'-PA-O1A
58	PD	501	GDP	C5'-O5'-PA-O1A
58	PF	501	GDP	C5'-O5'-PA-O1A
58	RH	501	GDP	C5'-O5'-PA-O1A
58	SD	501	GDP	C5'-O5'-PA-O1A
58	UM	501	GDP	C5'-O5'-PA-O1A
56	LA	501	GTP	C3'-C4'-C5'-O5'
56	RG	501	GTP	C3'-C4'-C5'-O5'
56	VG	501	GTP	C3'-C4'-C5'-O5'
58	UM	501	GDP	C3'-C4'-C5'-O5'

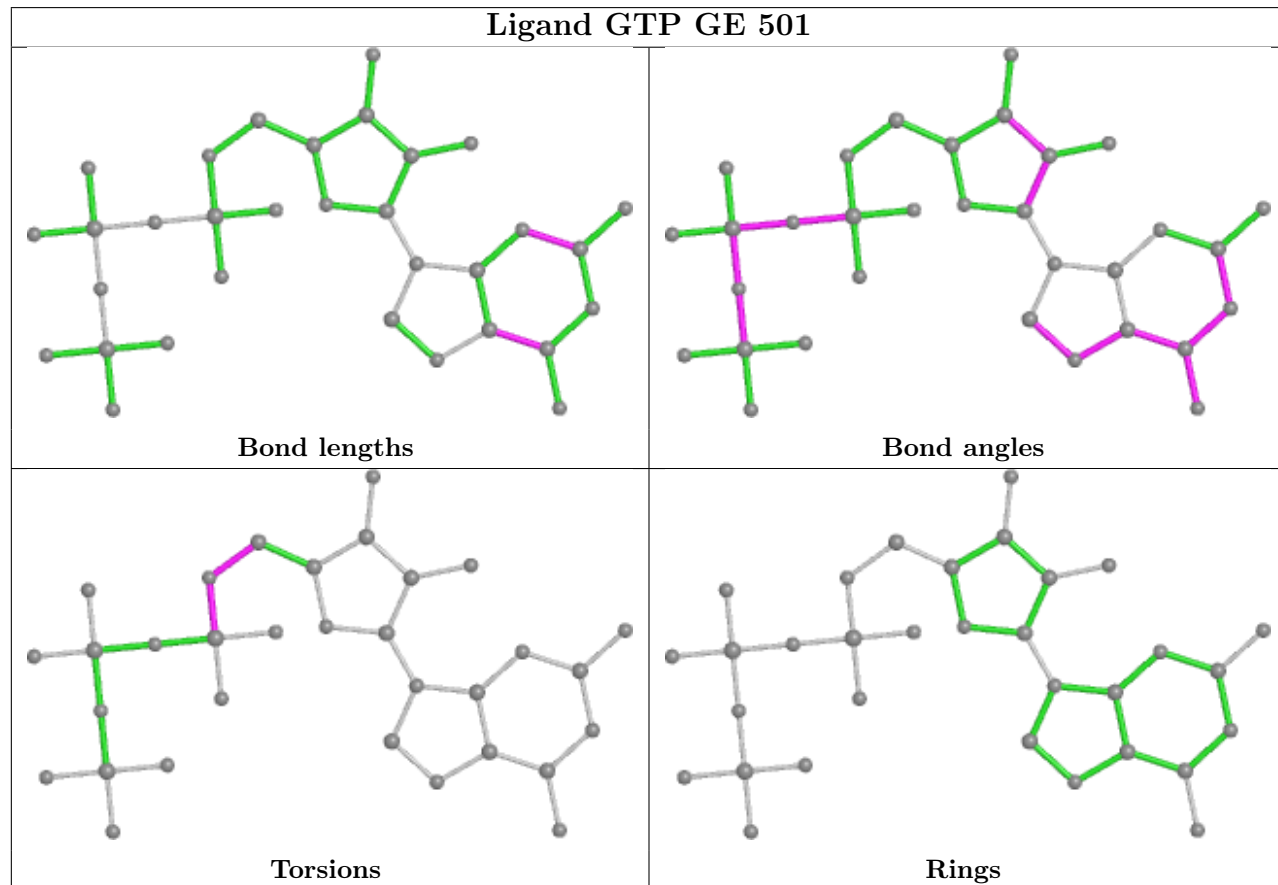
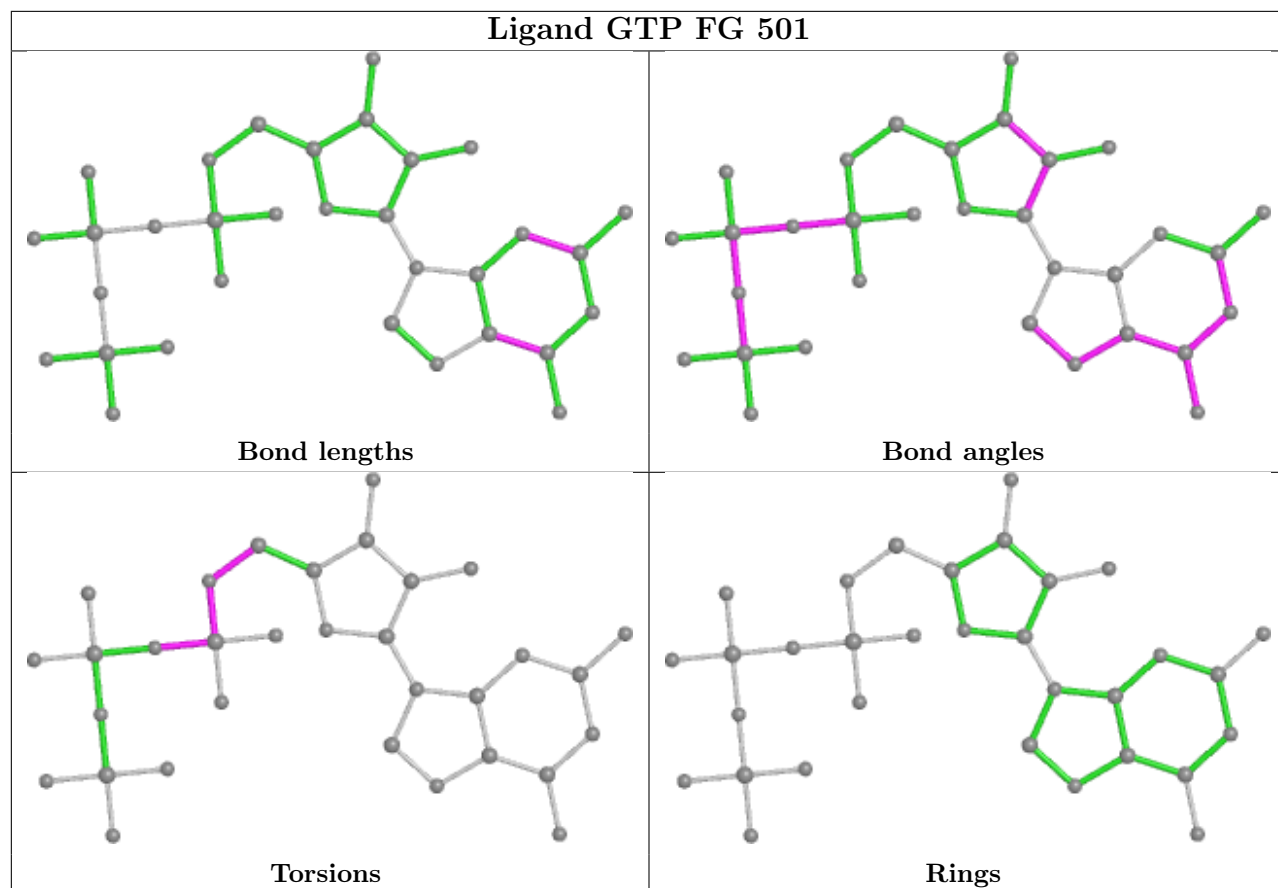
There are no ring outliers.

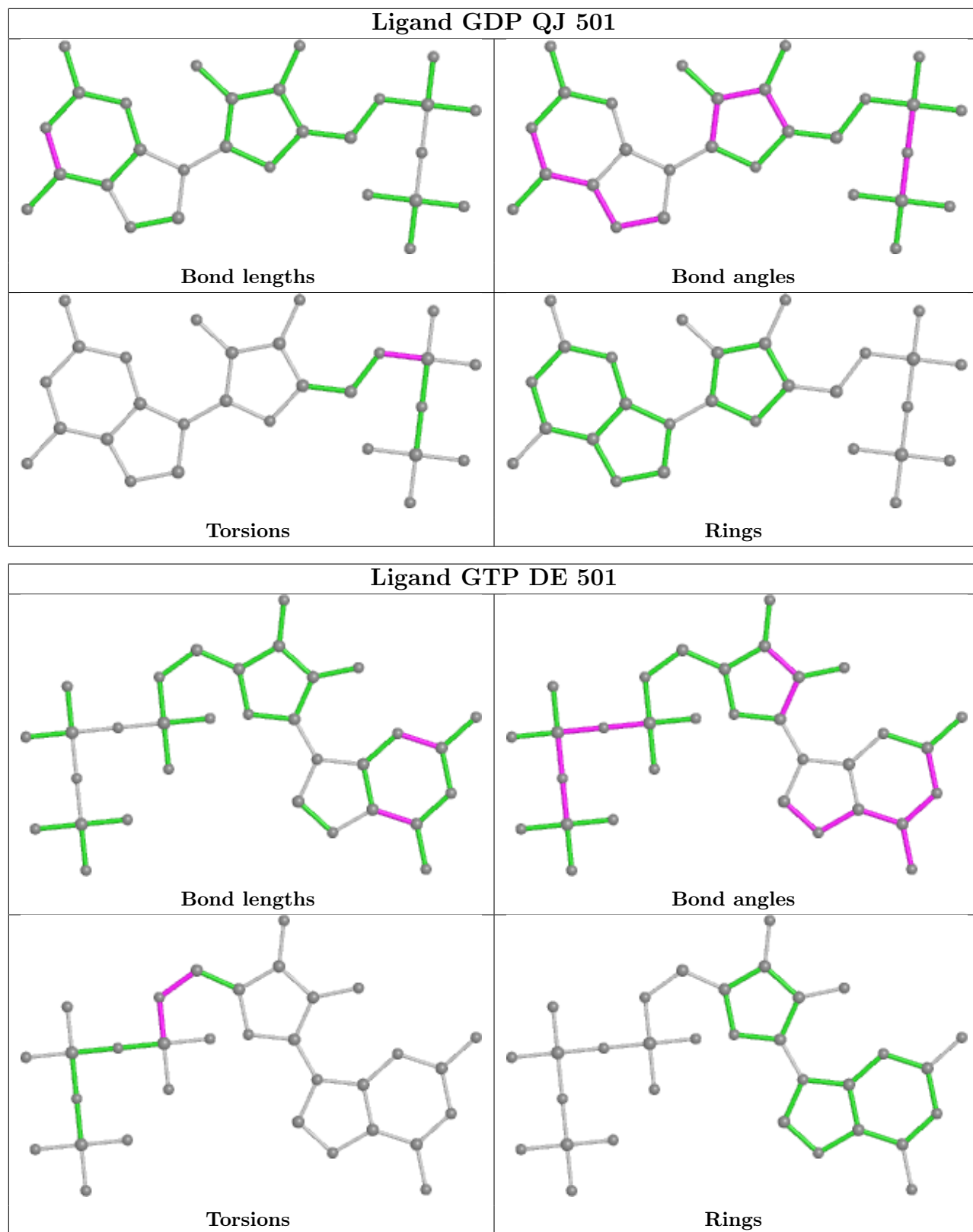
No monomer is involved in short contacts.

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.

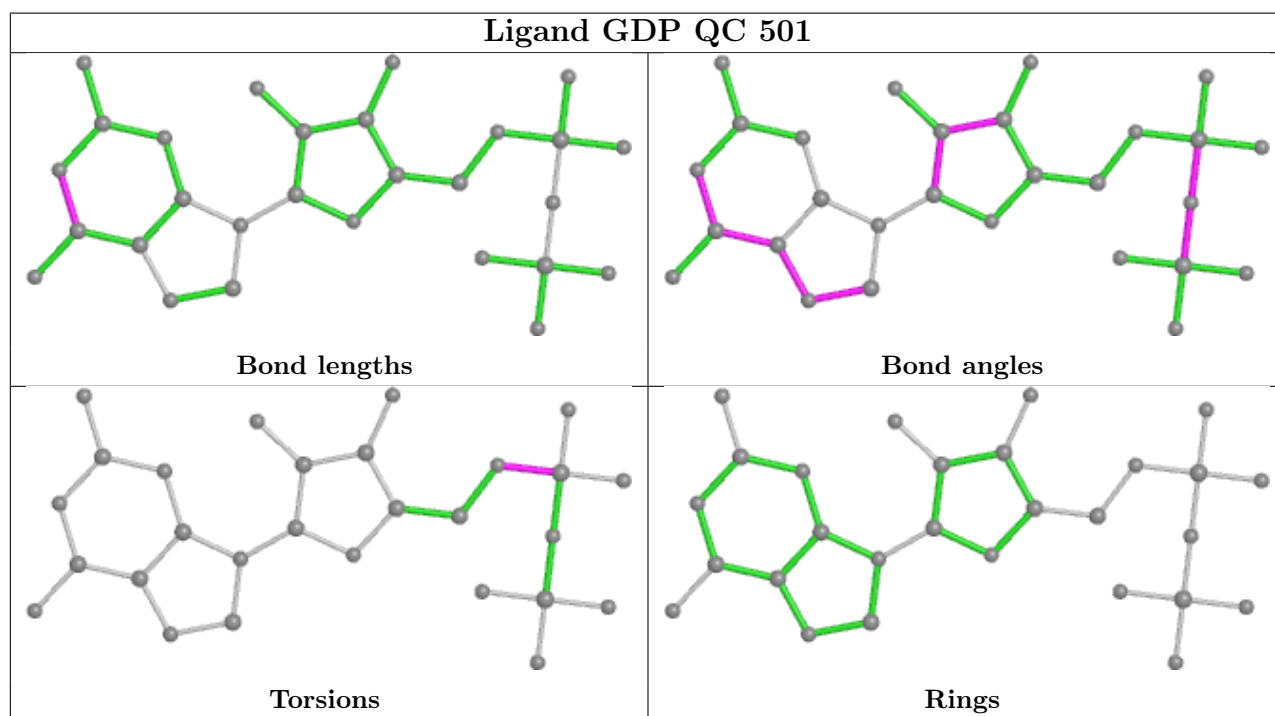
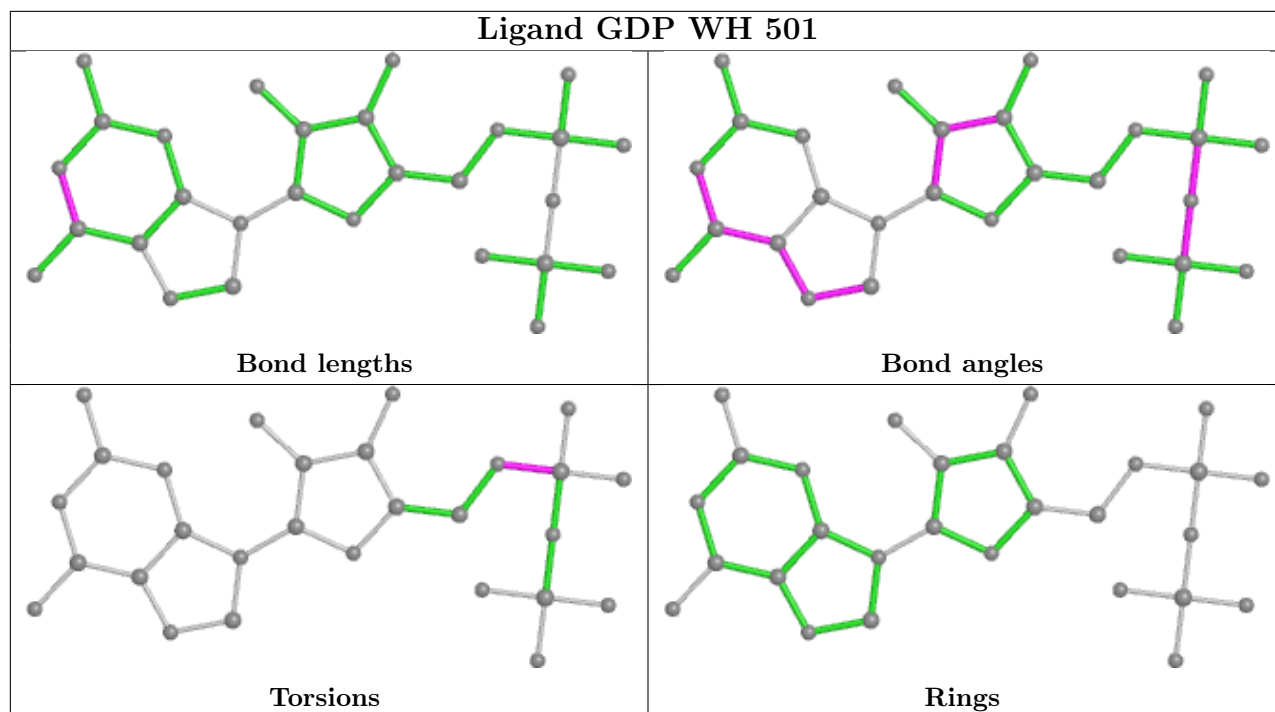


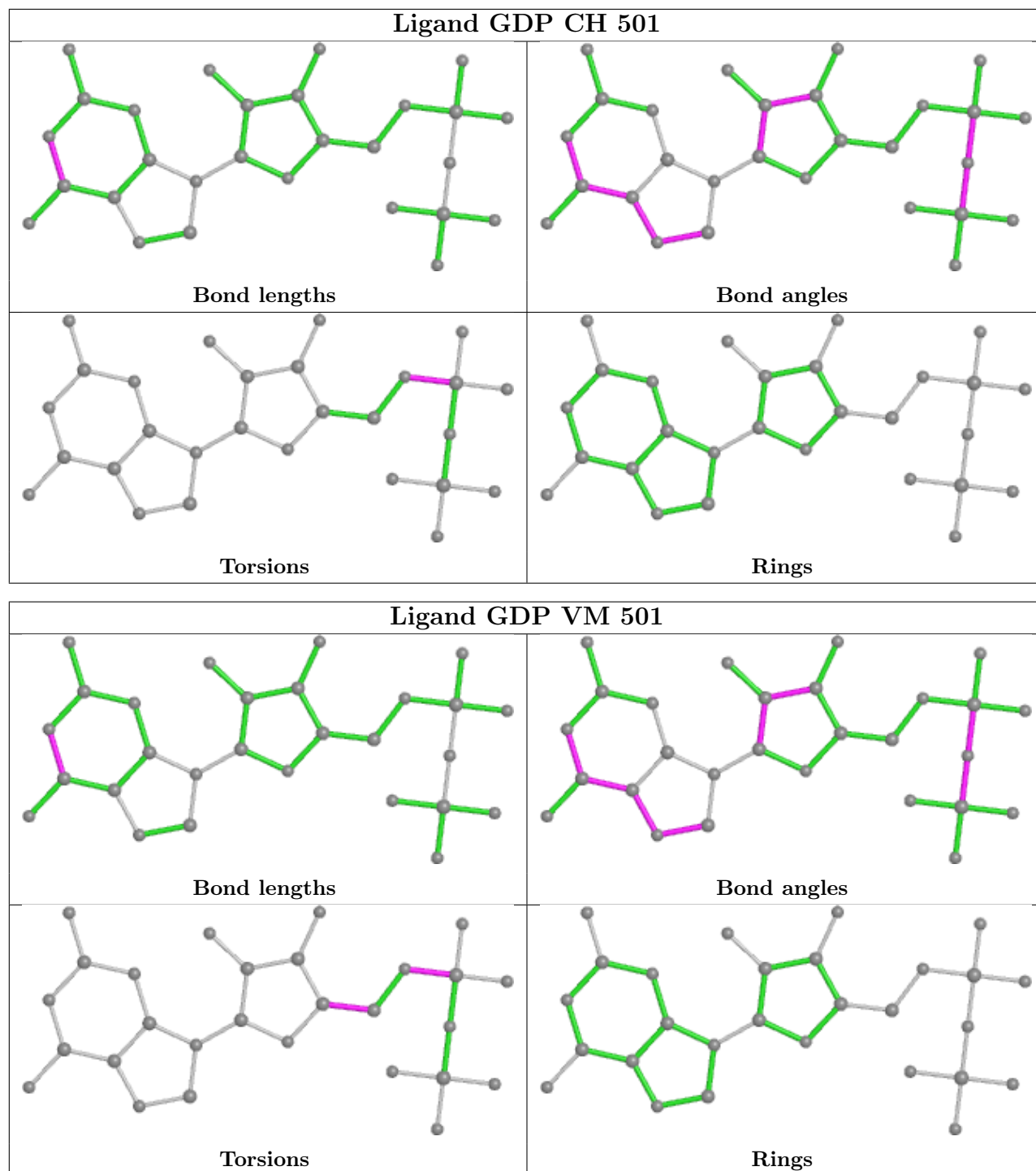


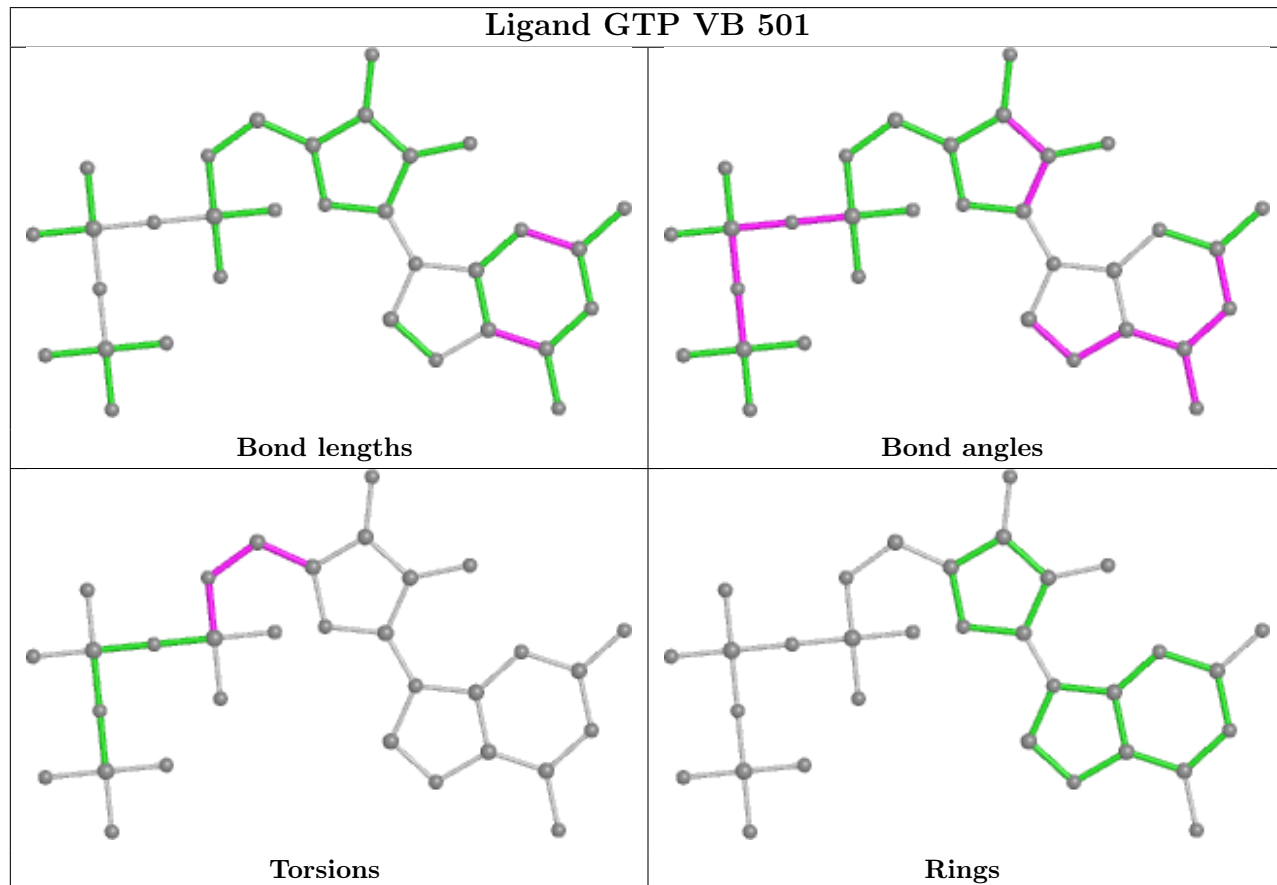
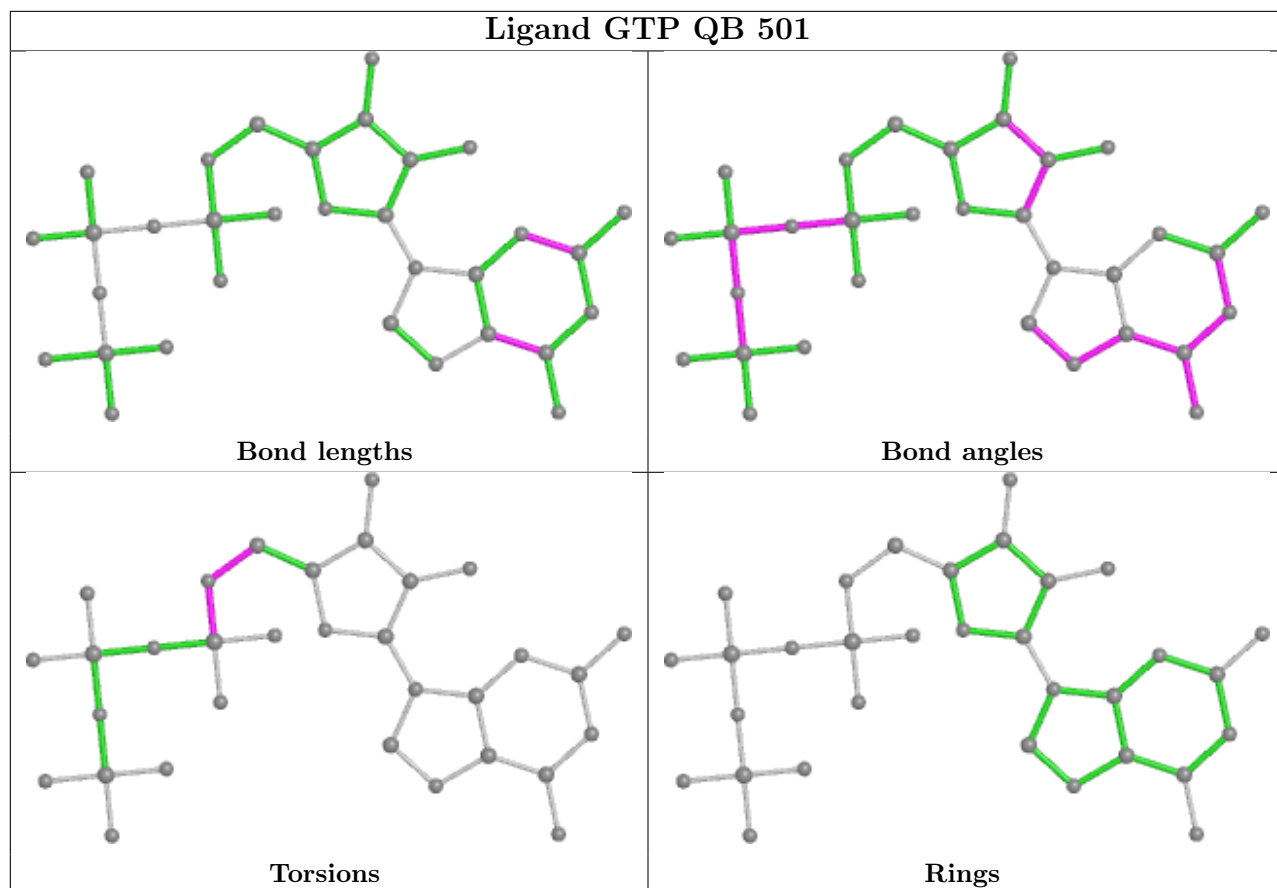


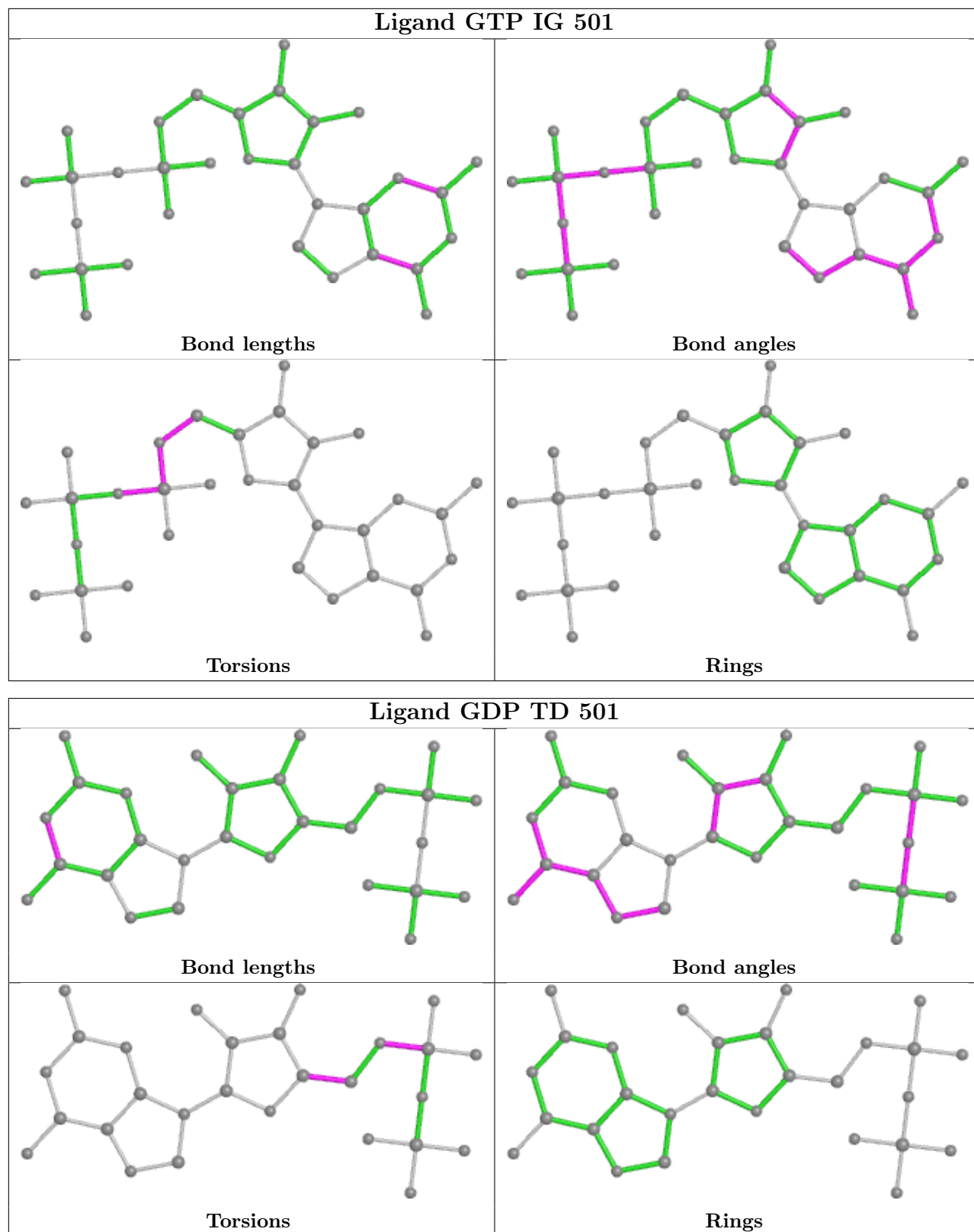


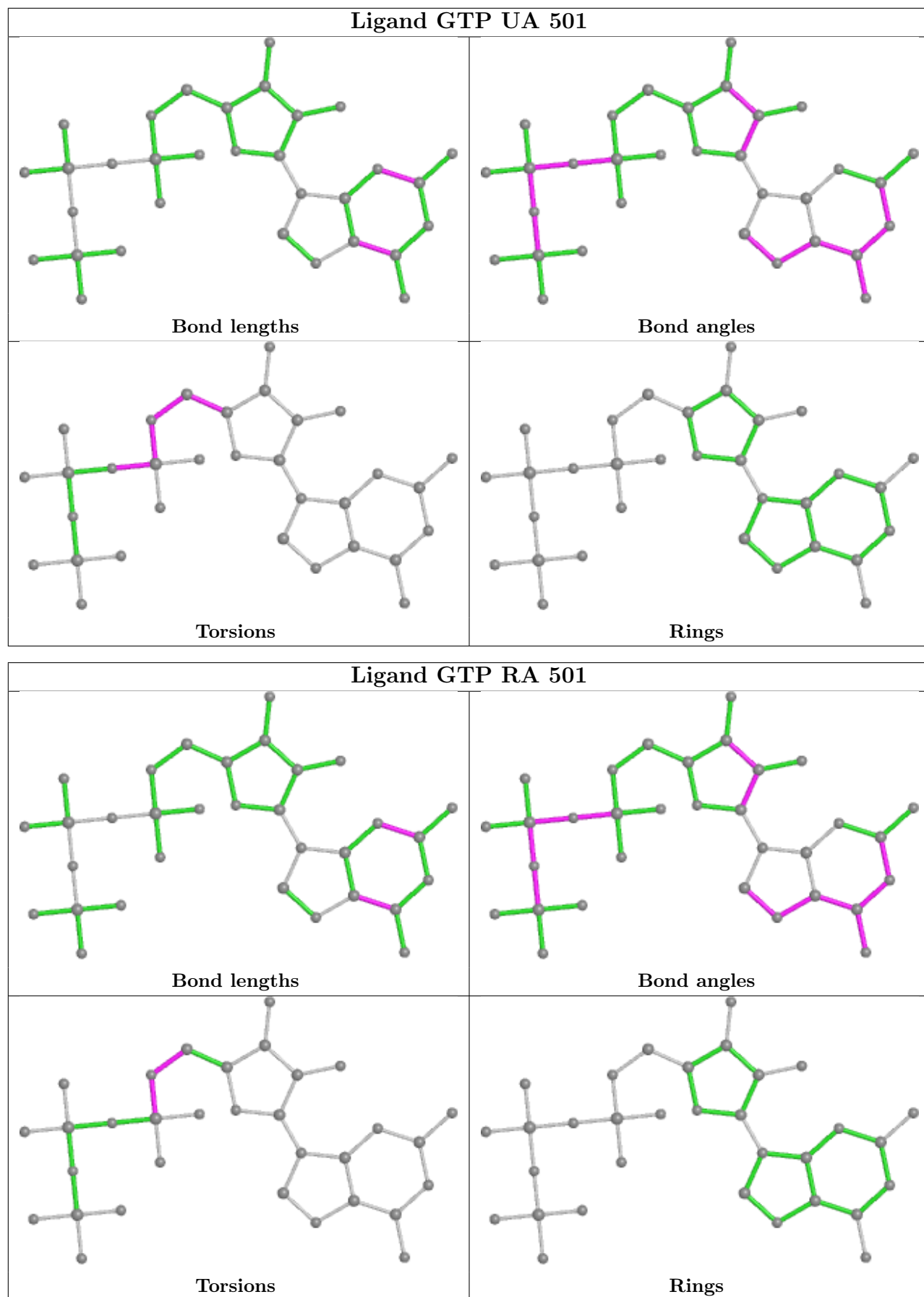


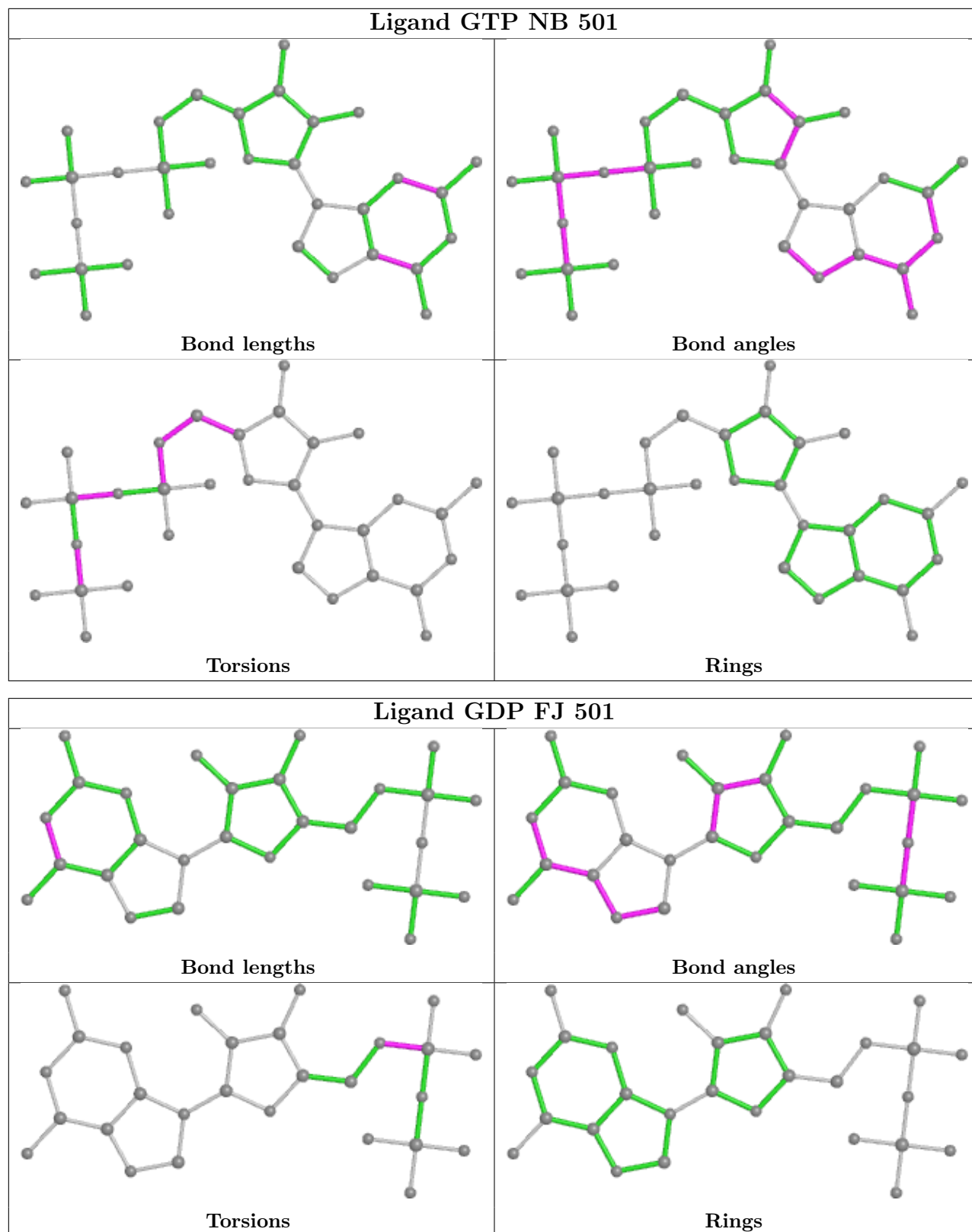


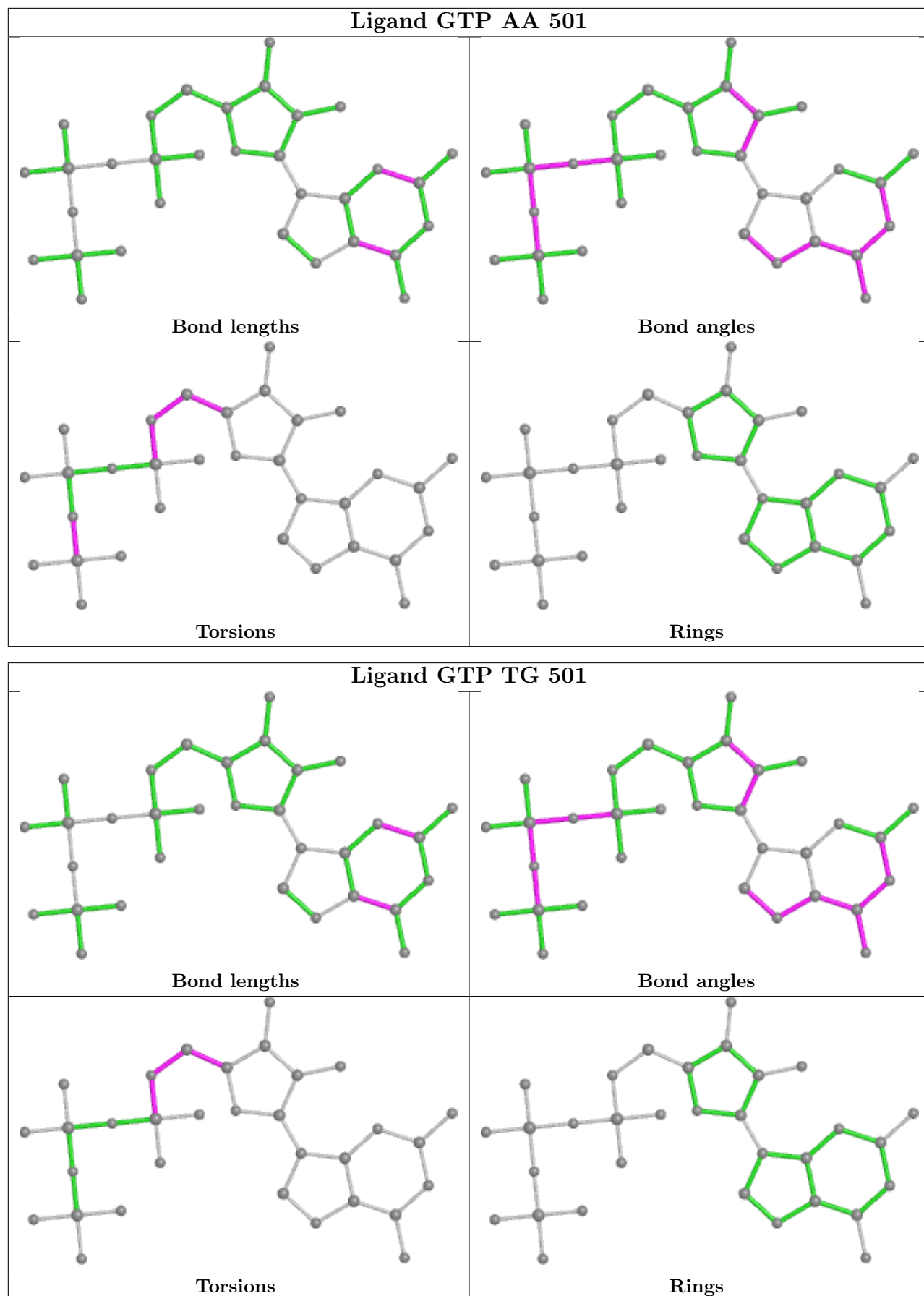


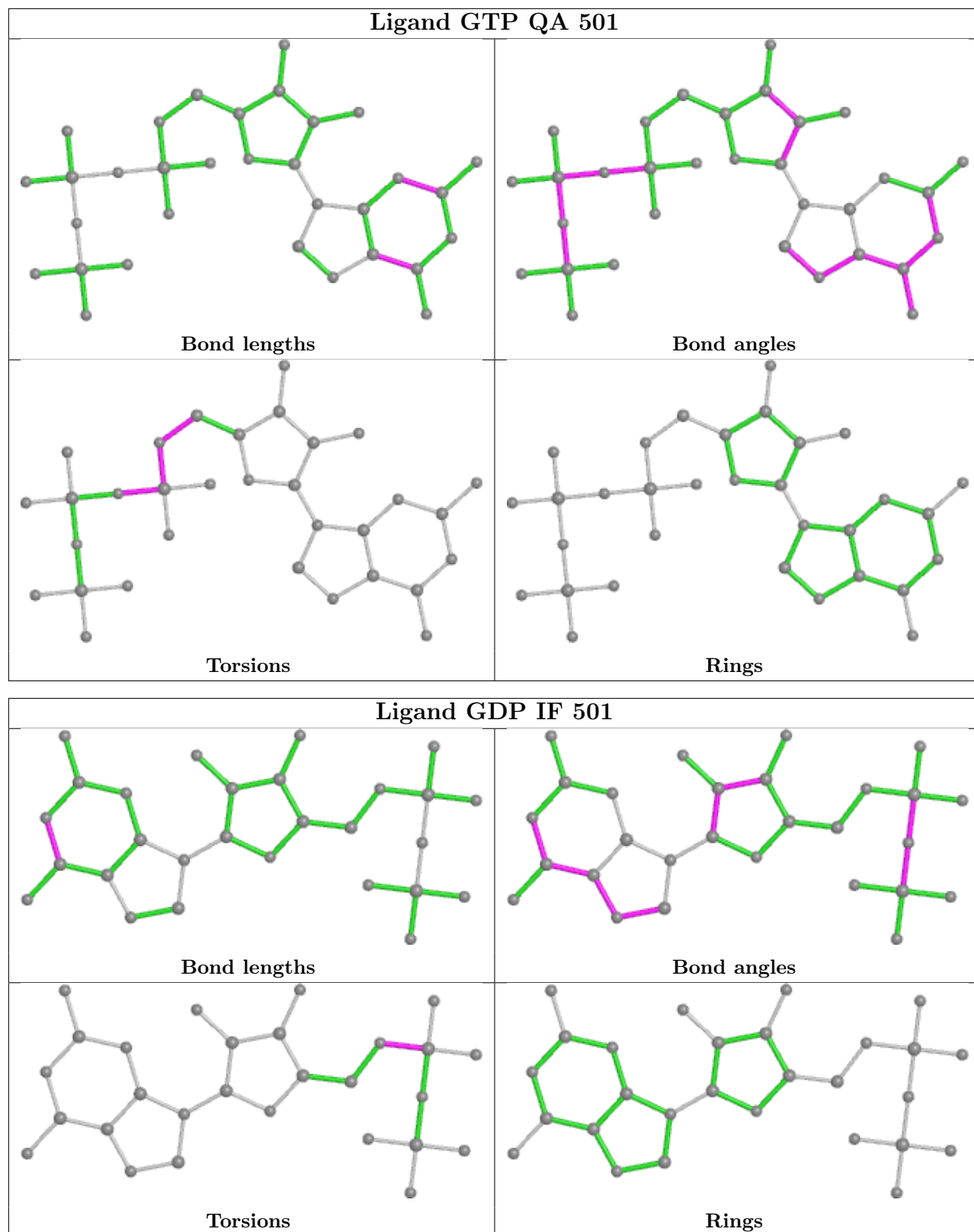




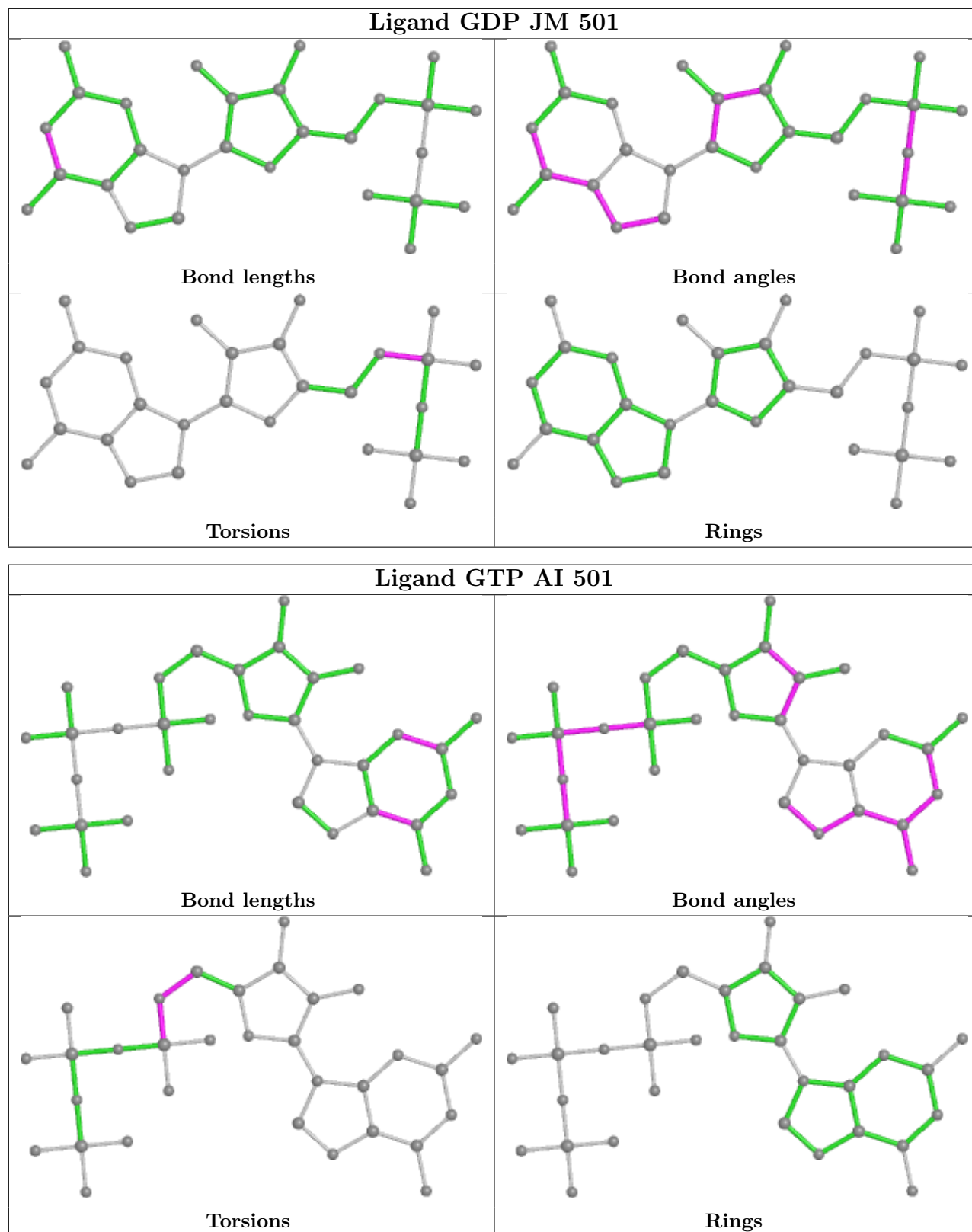


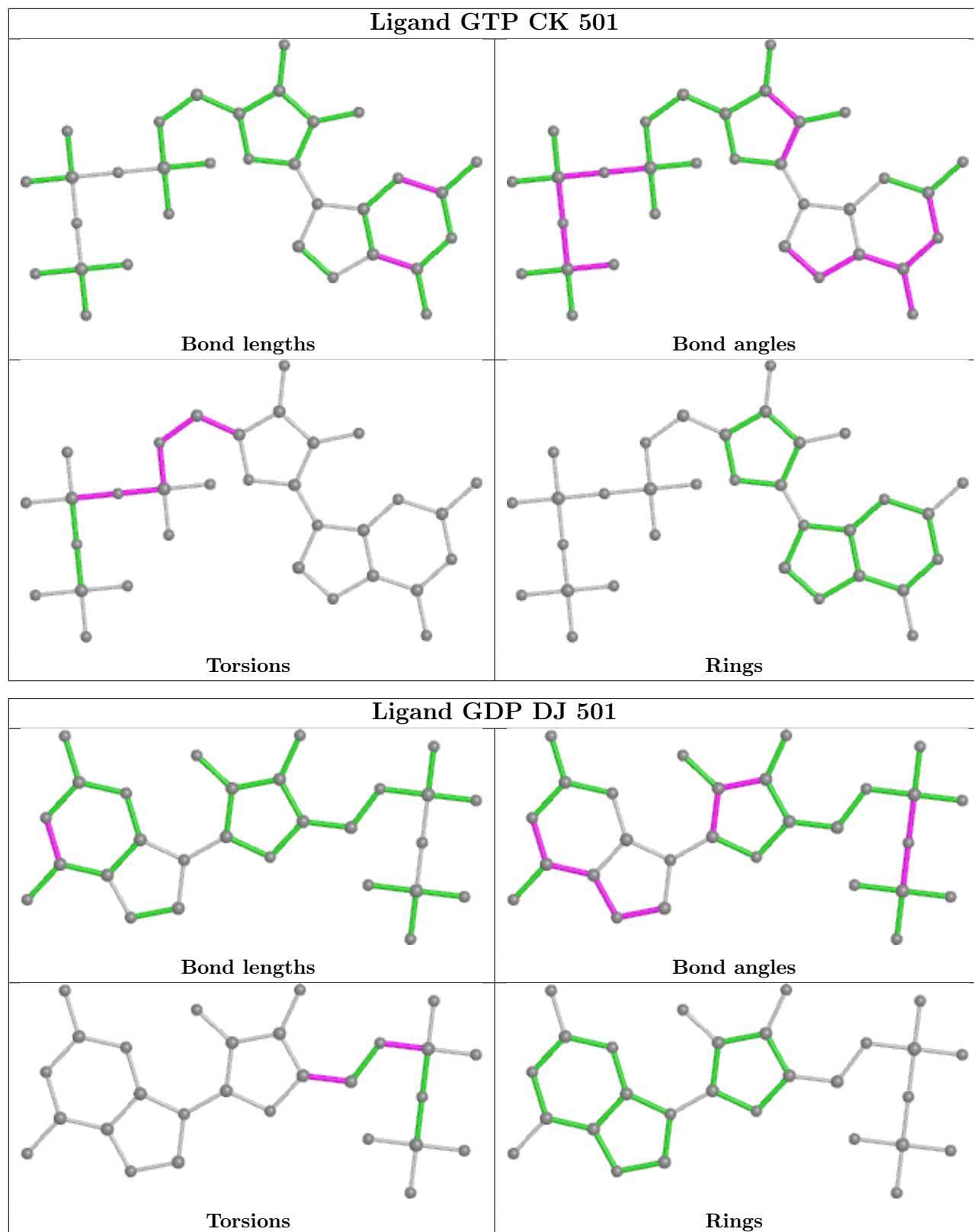


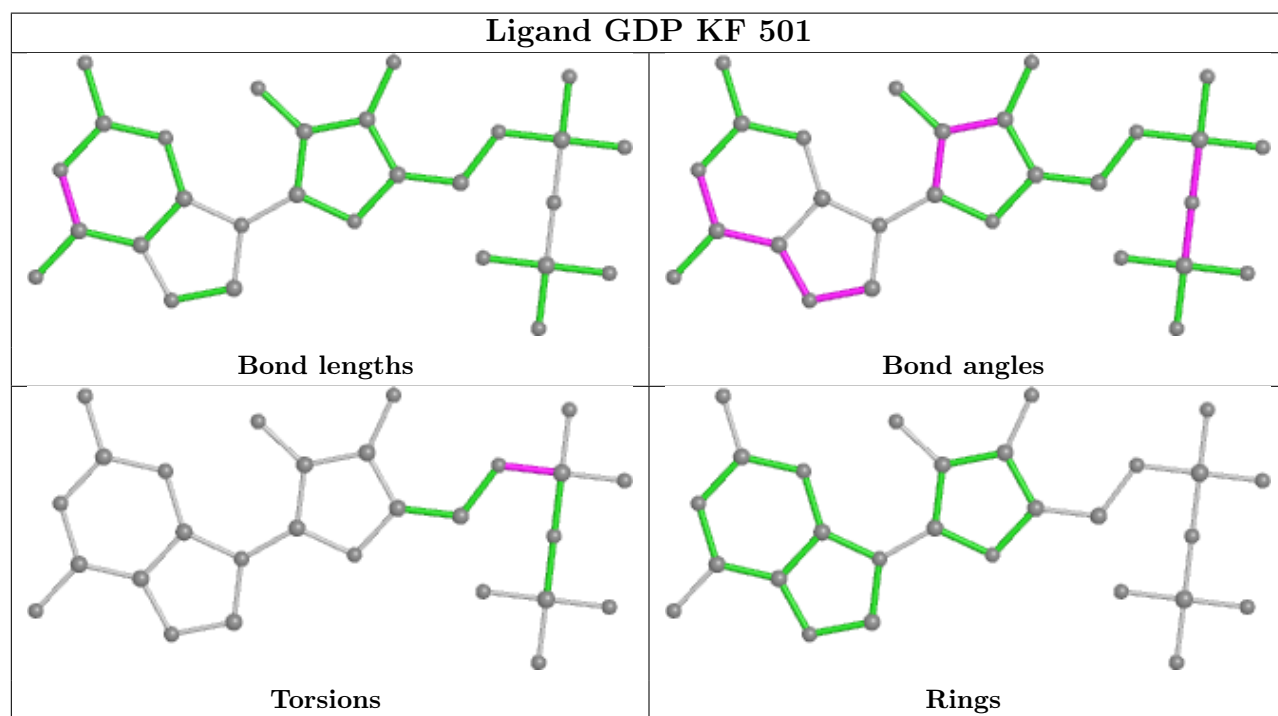
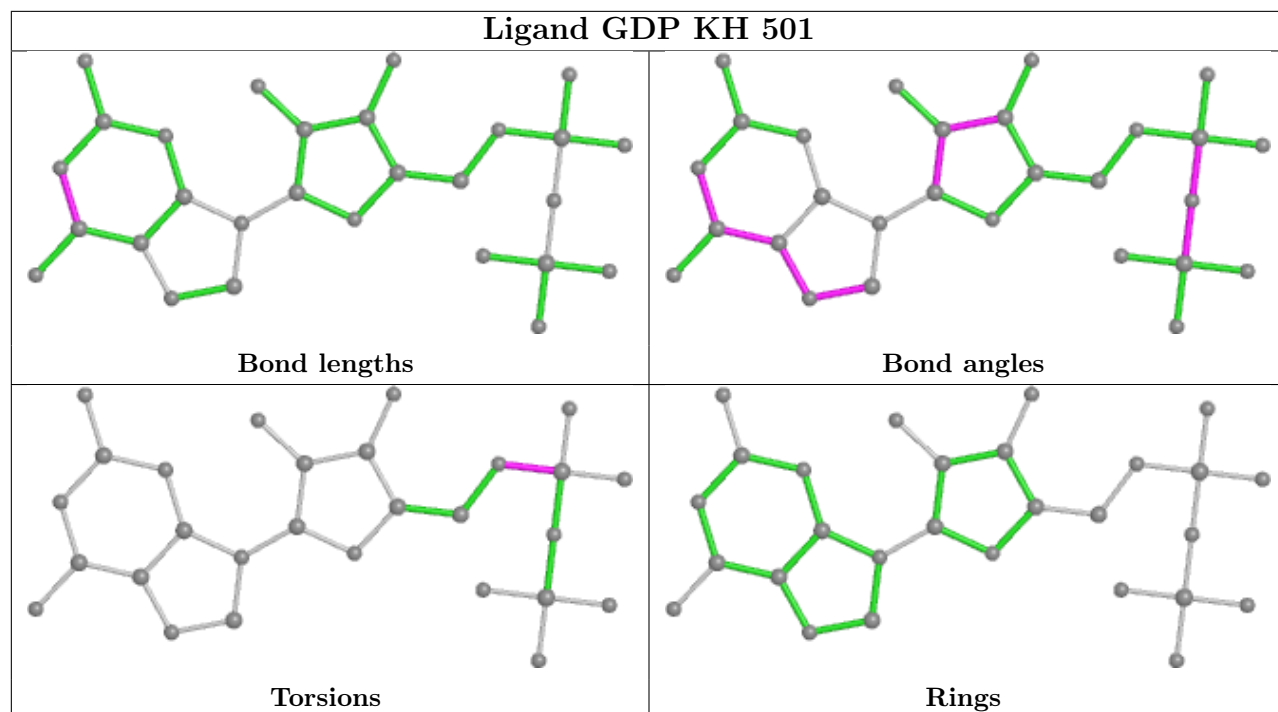


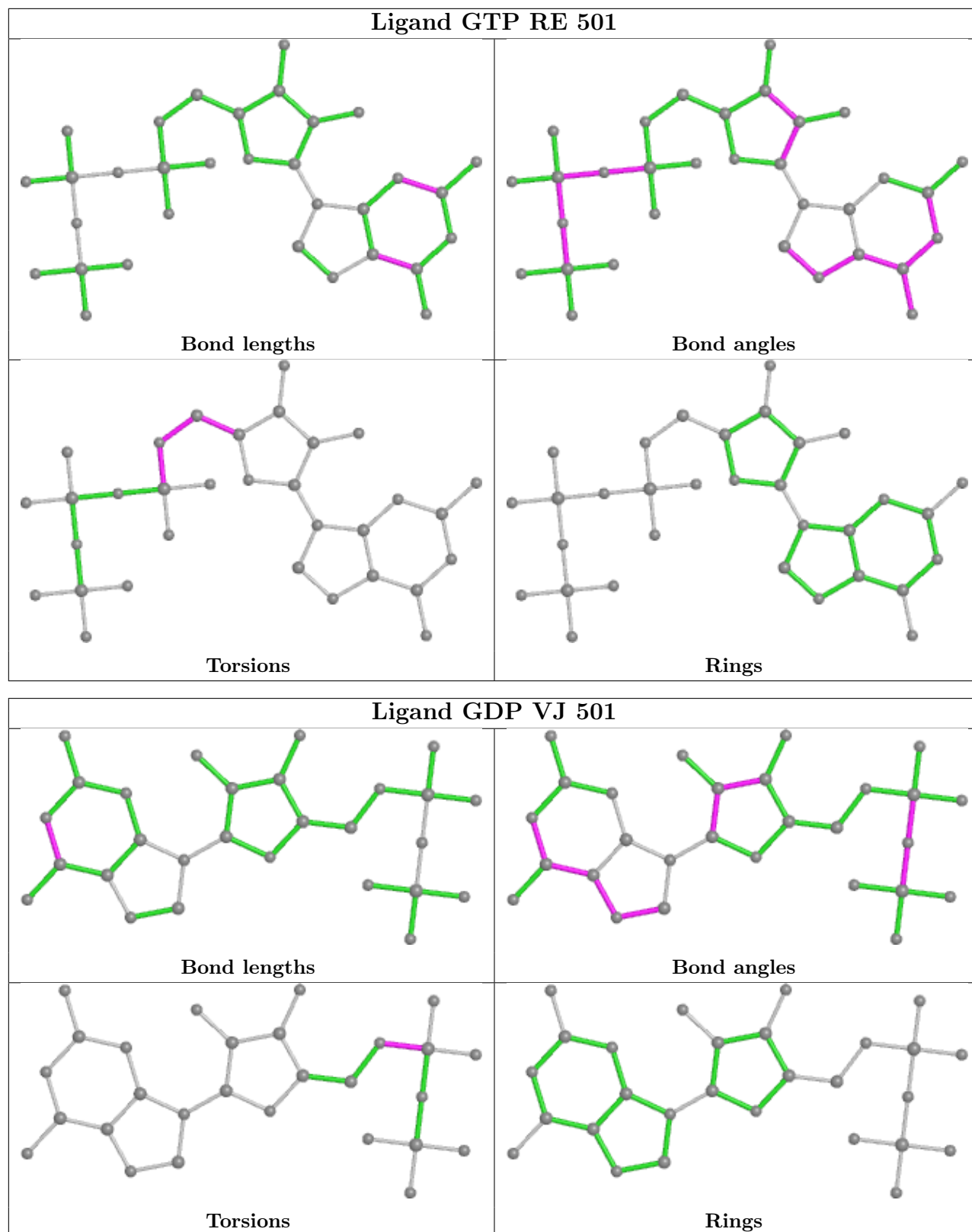


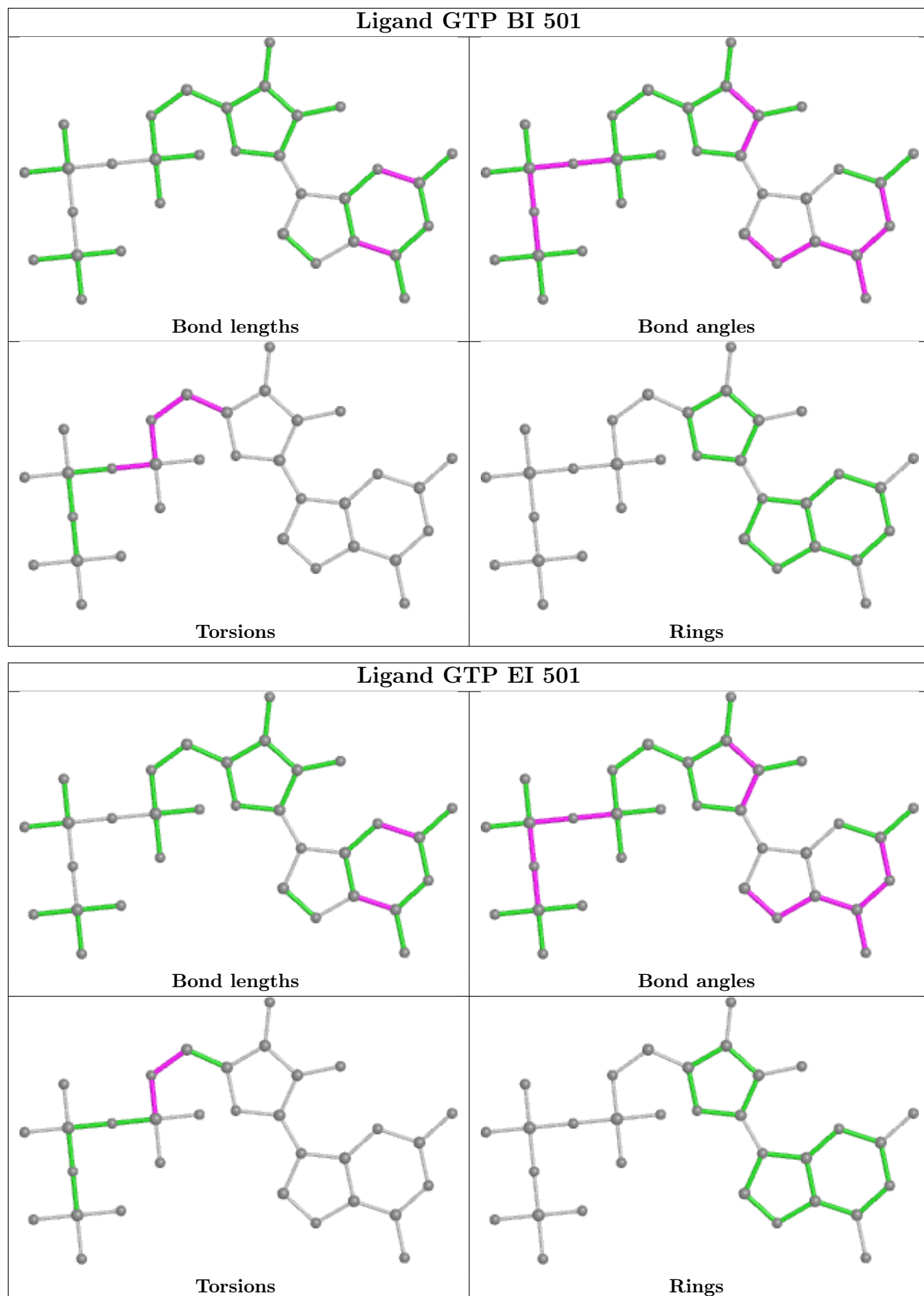


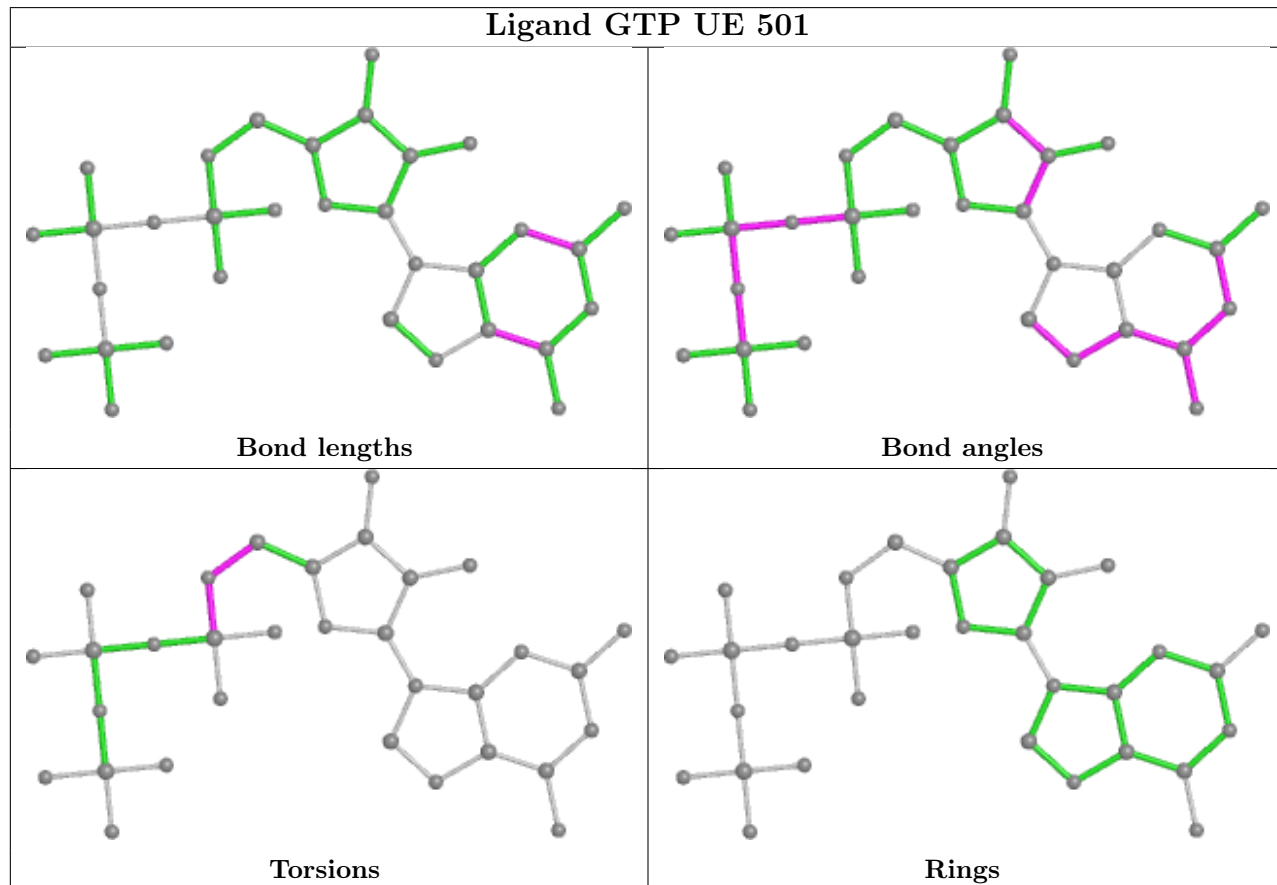
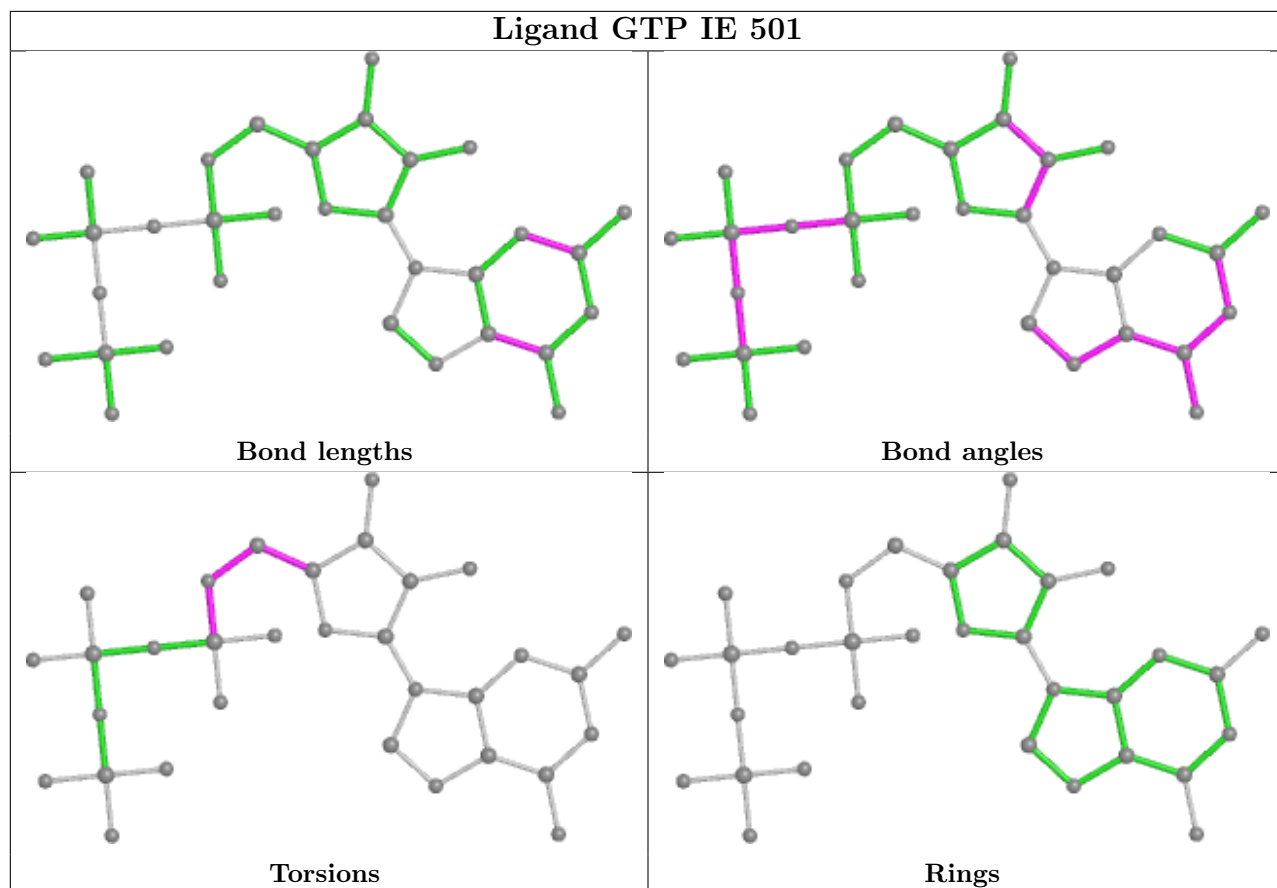


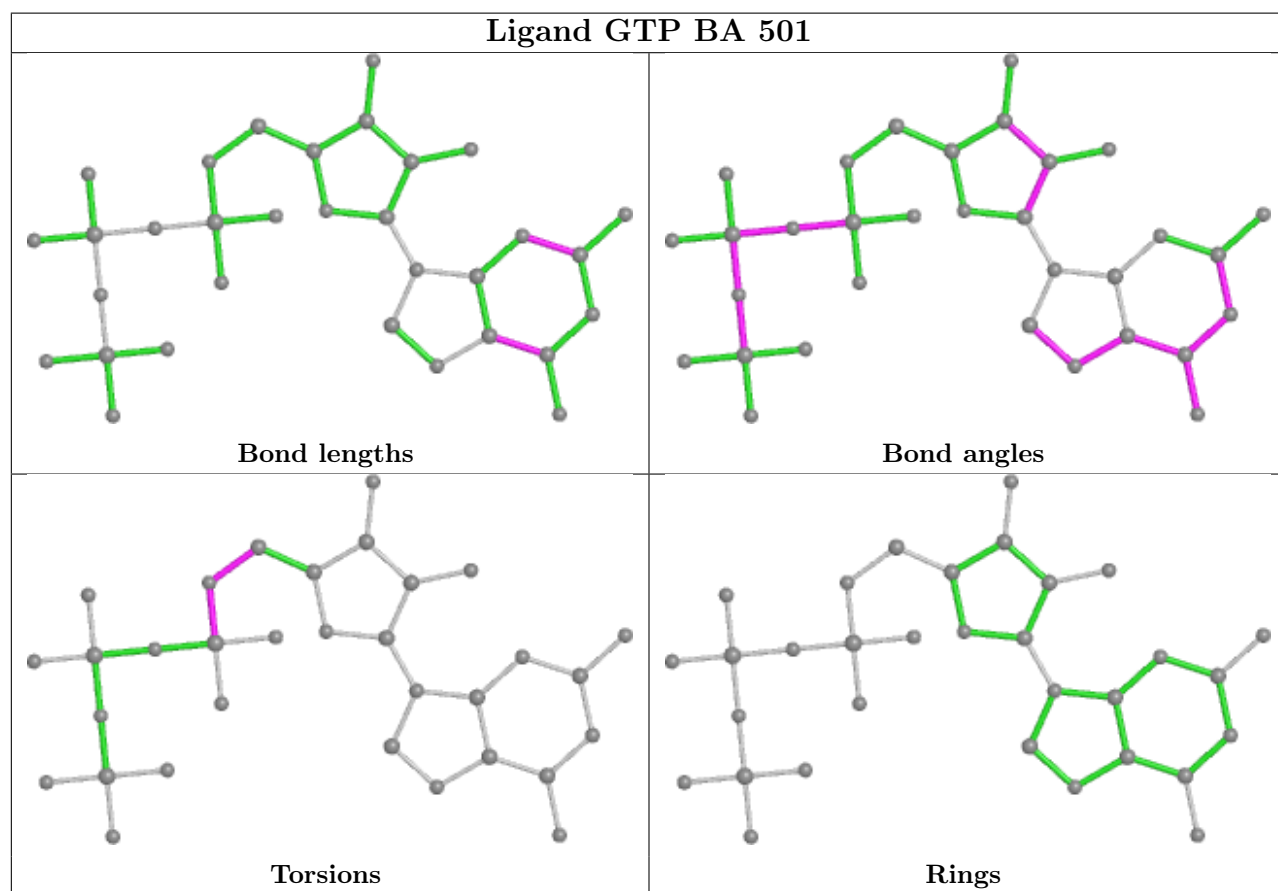
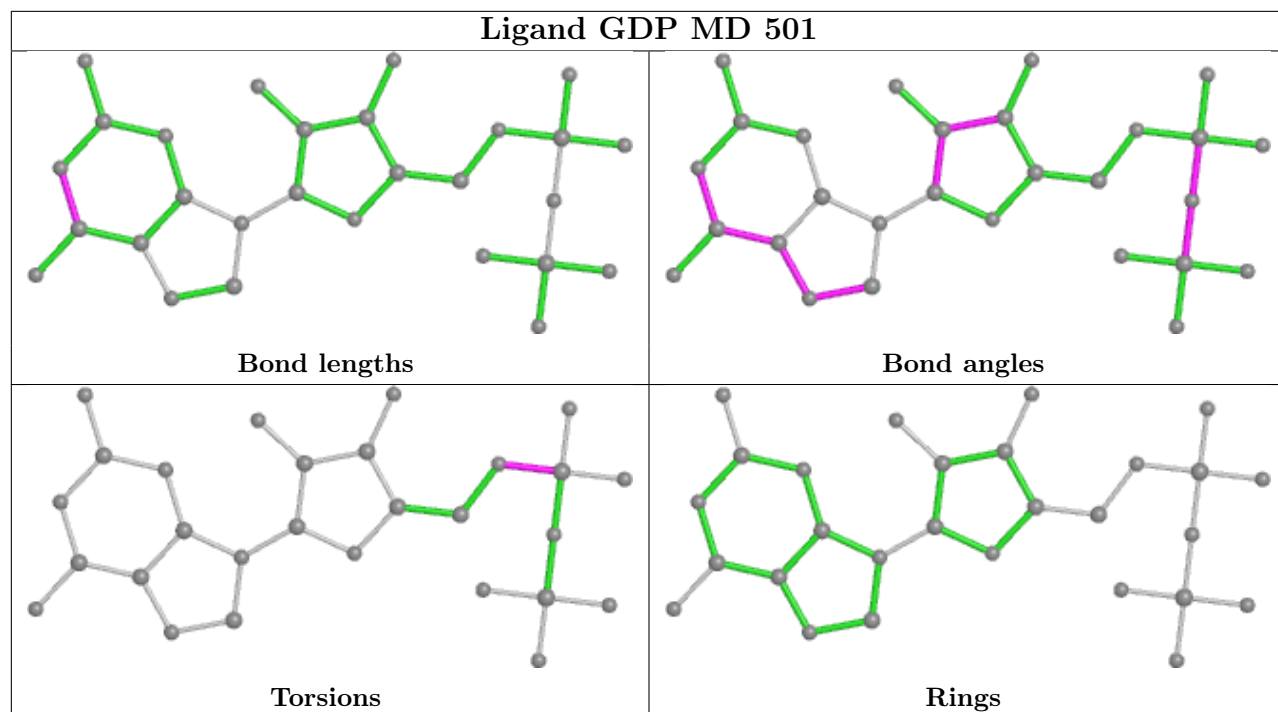


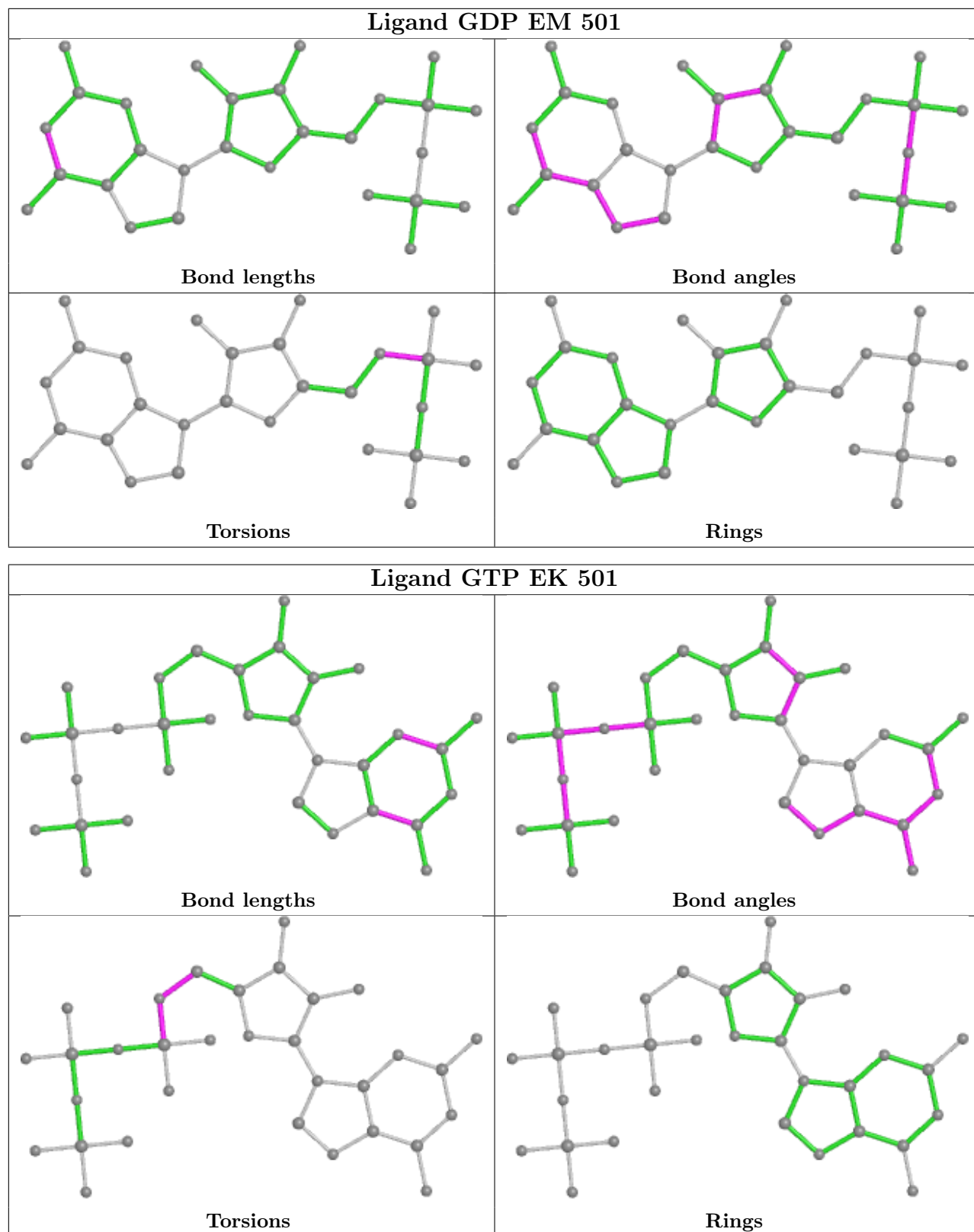




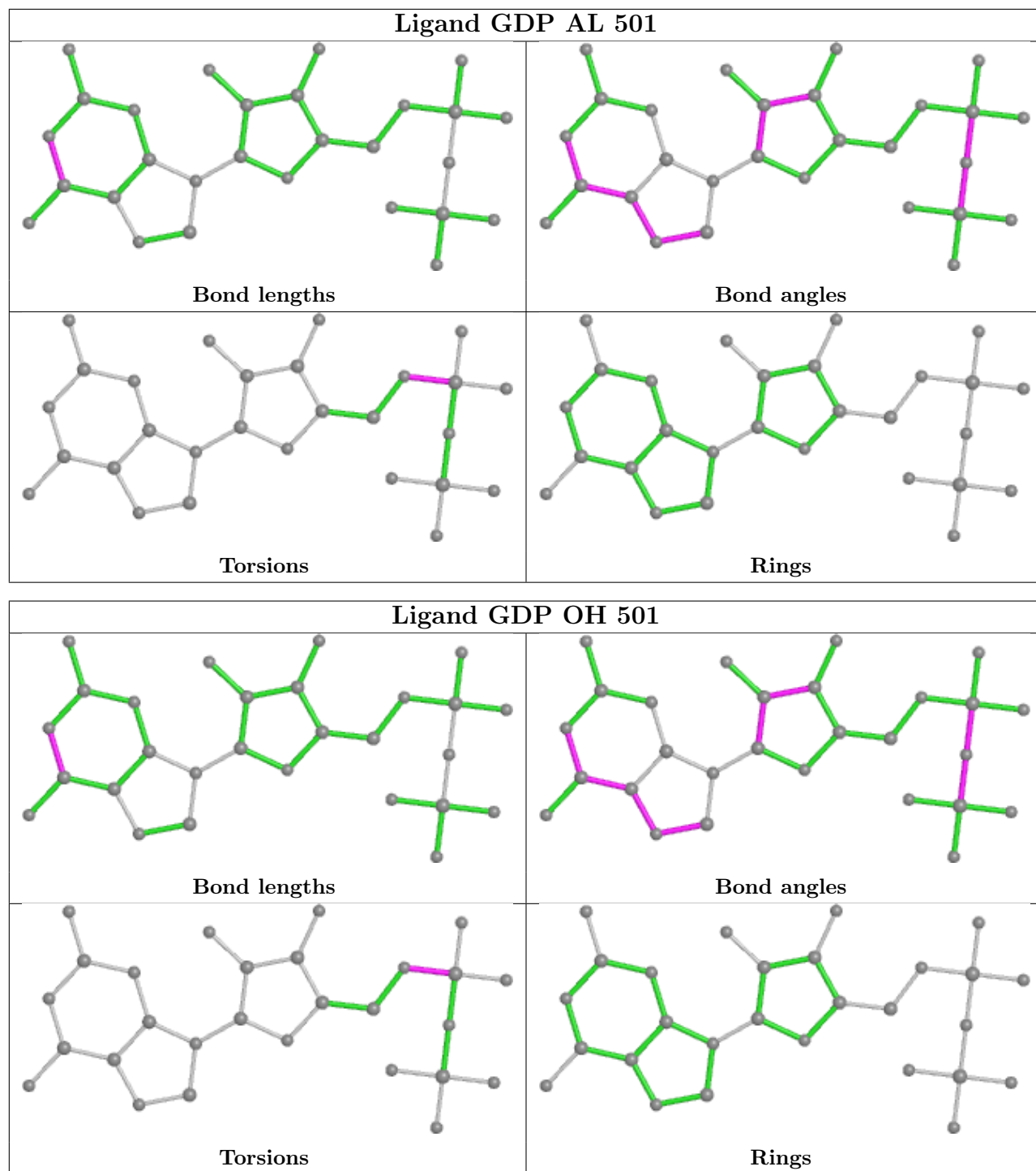


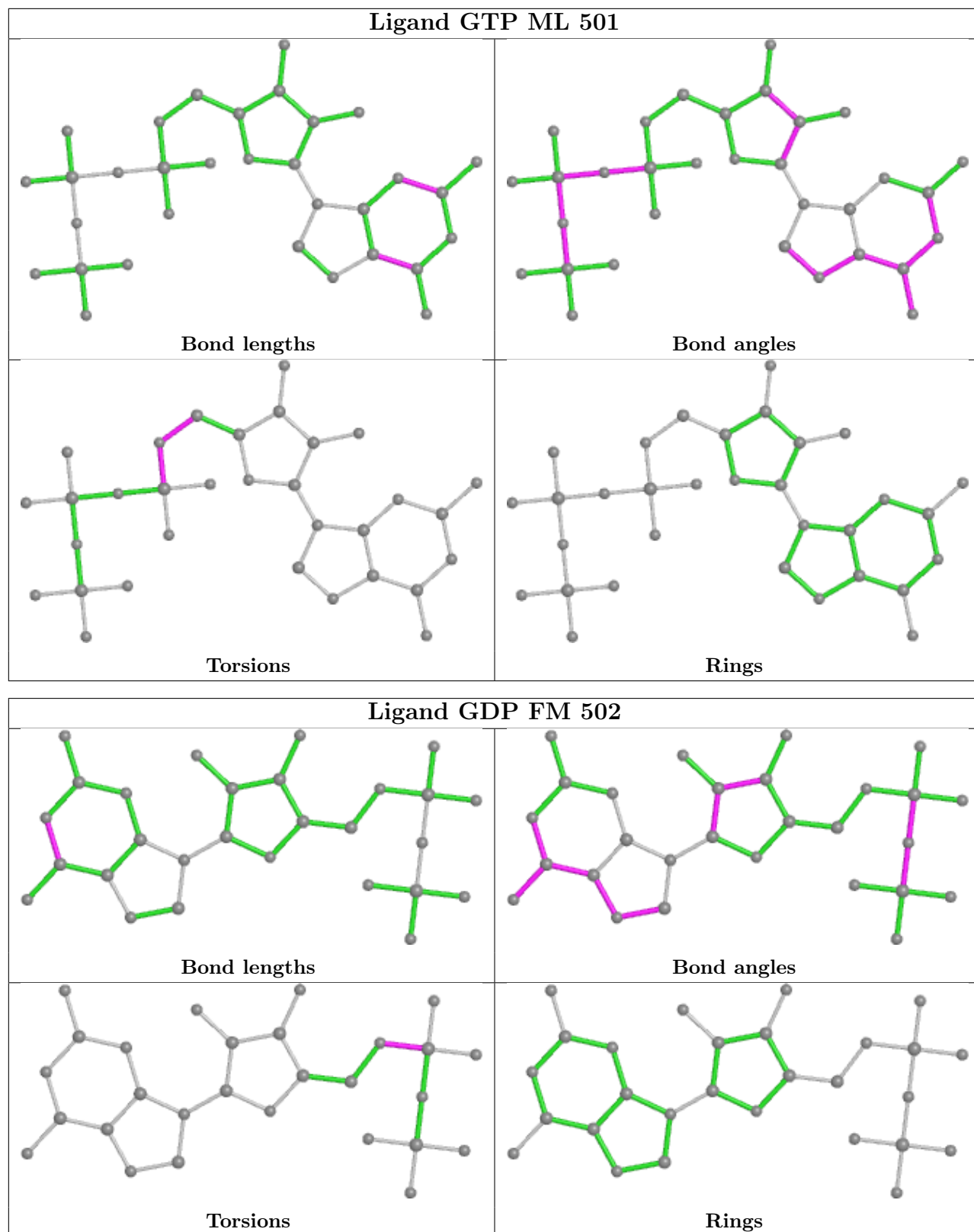


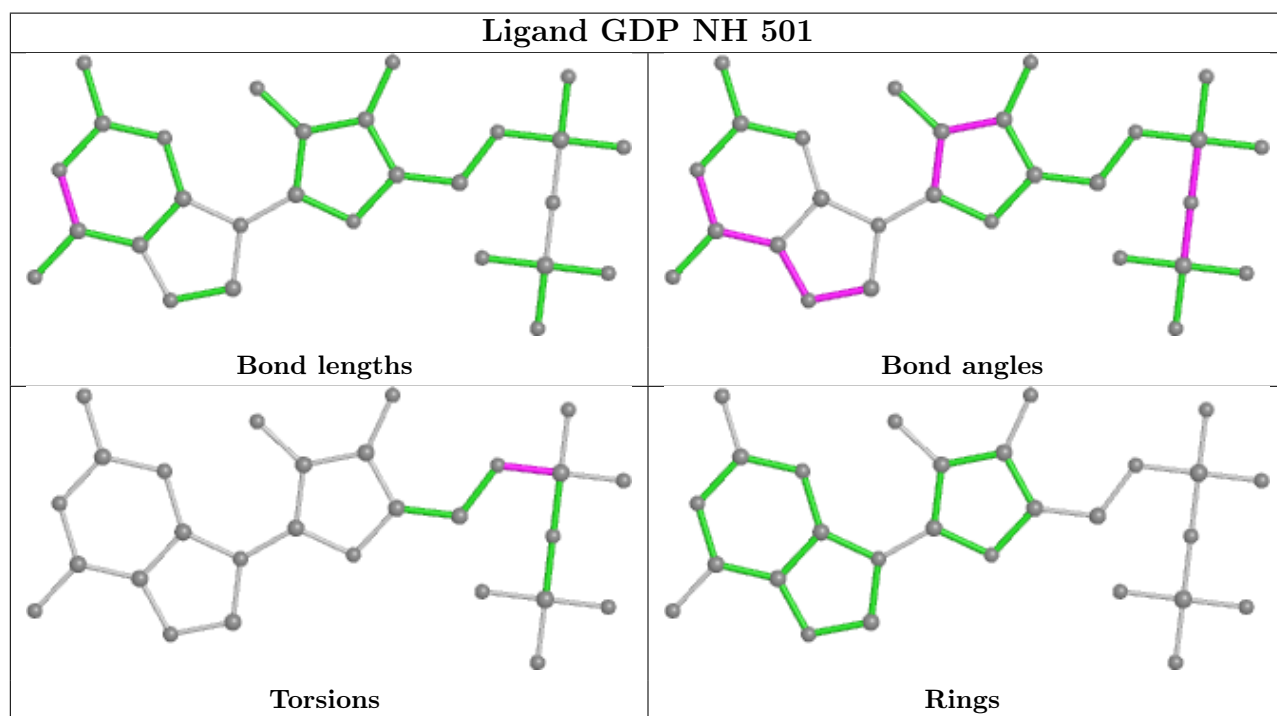
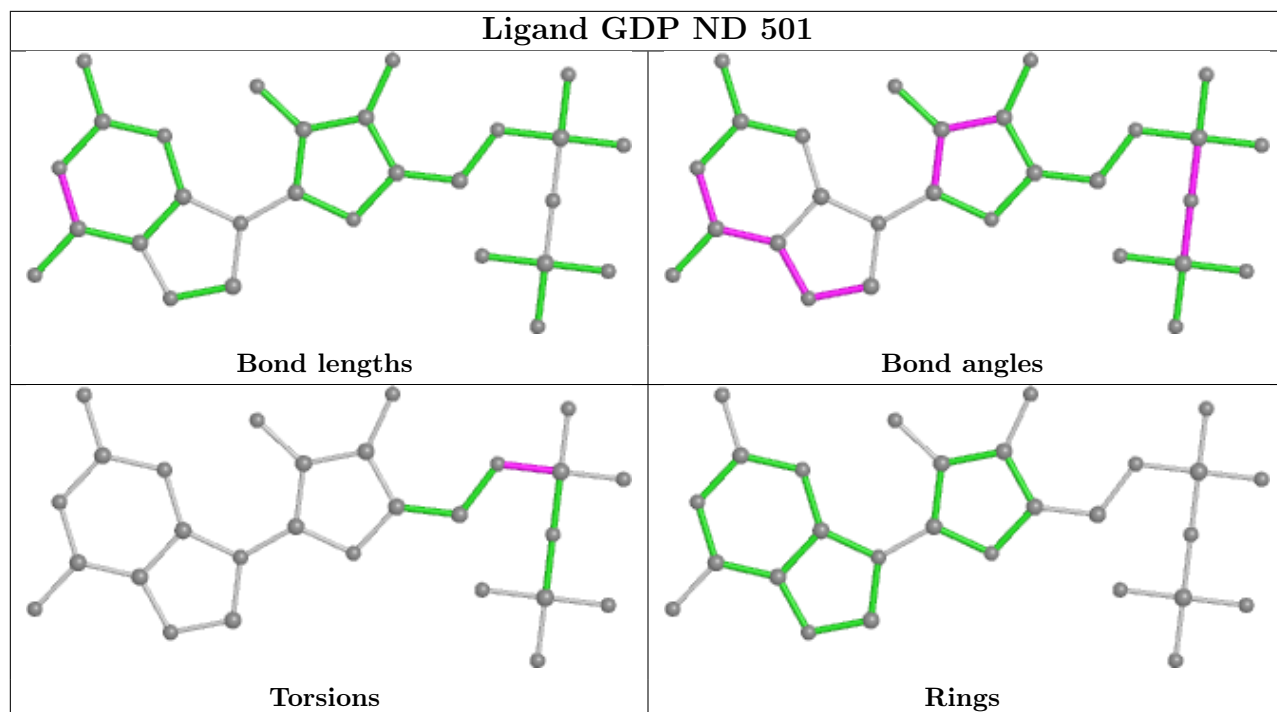


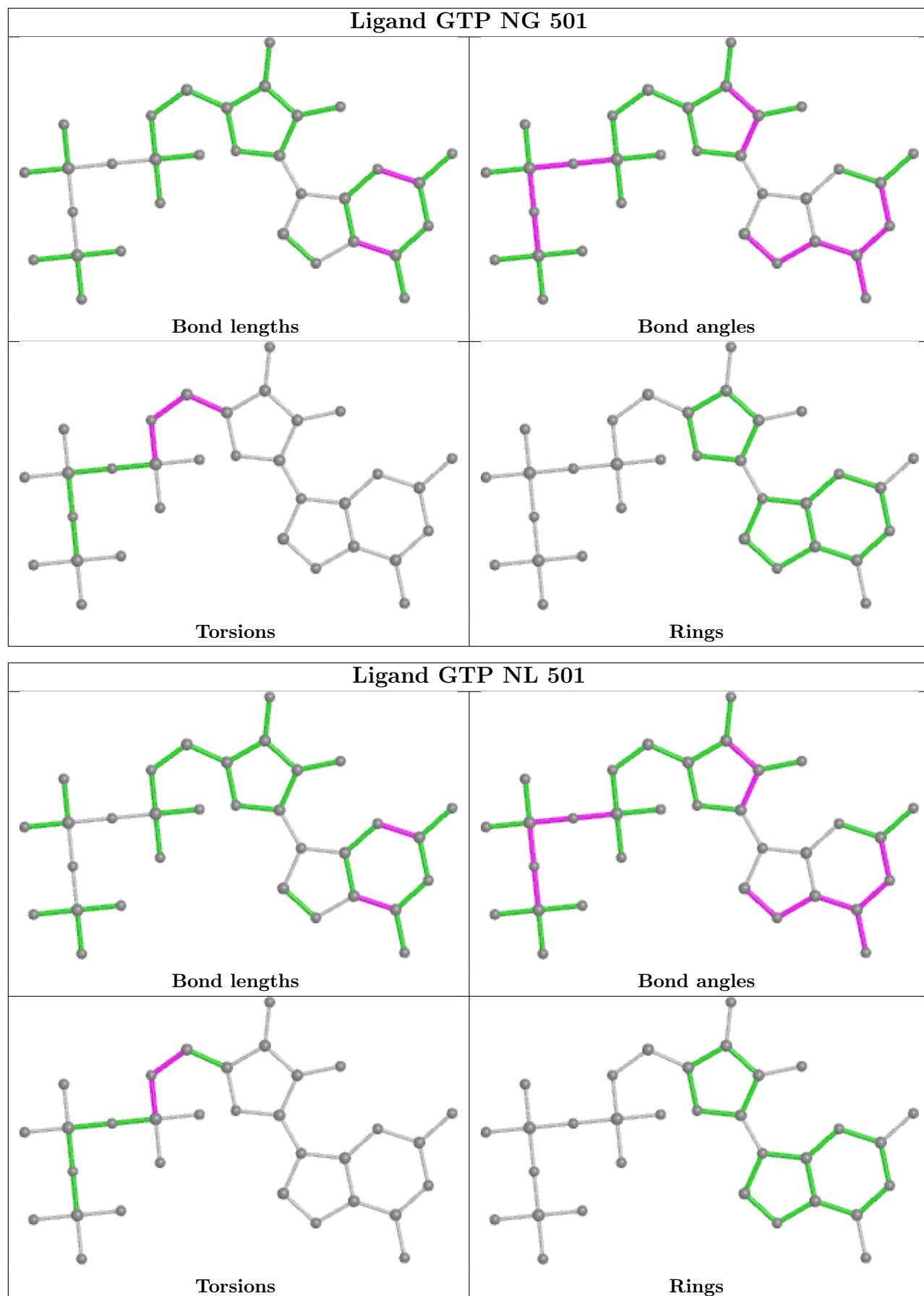


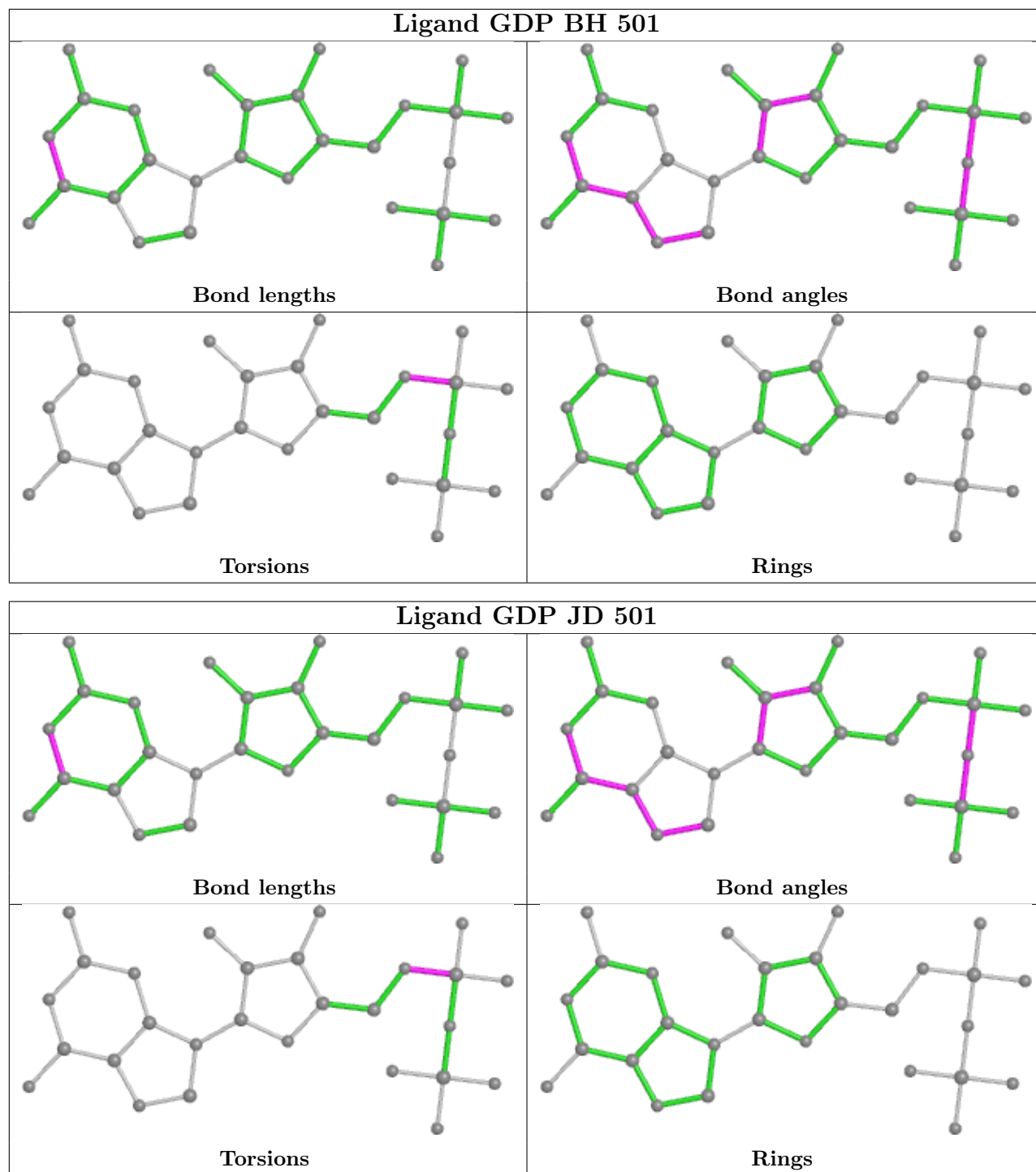


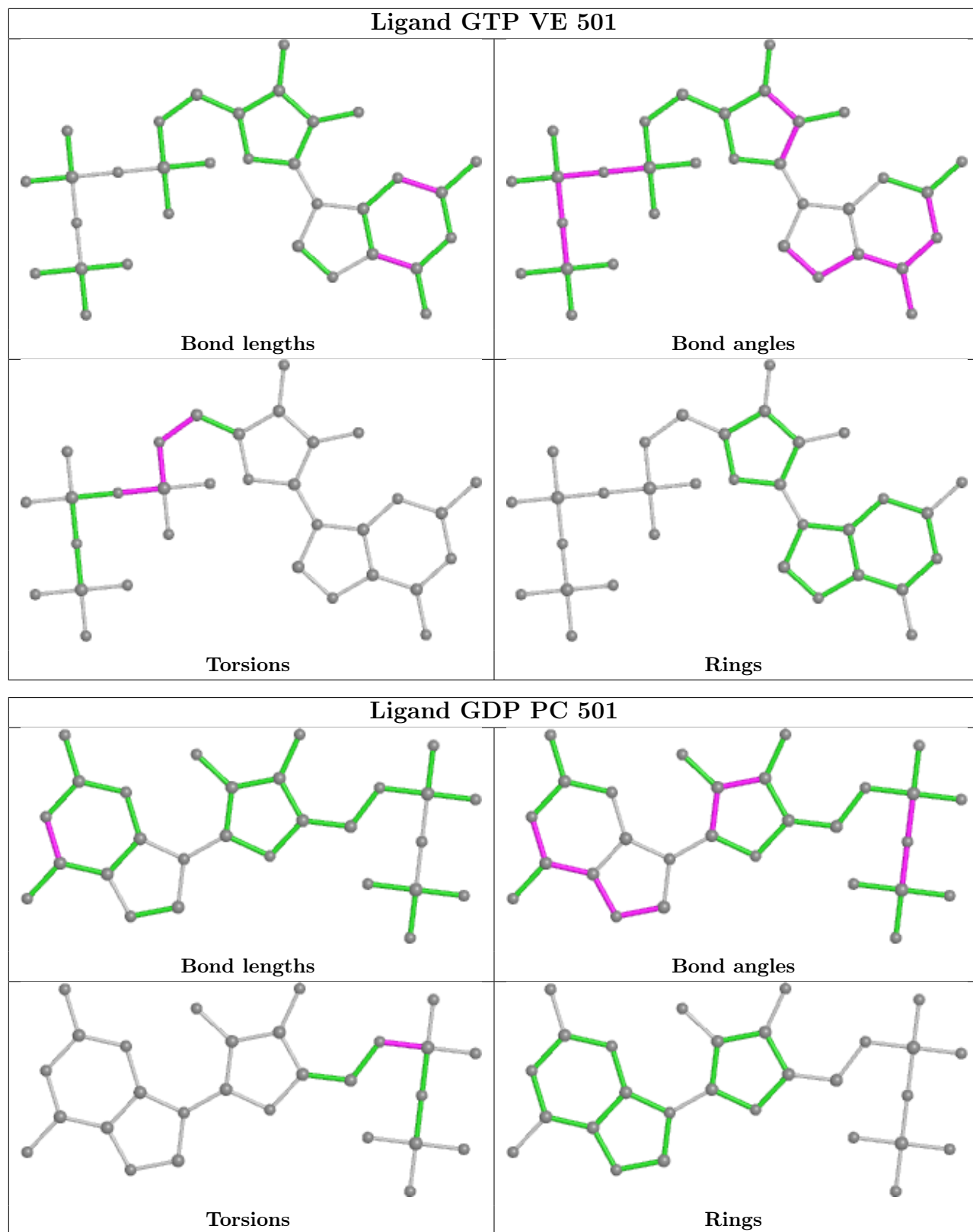


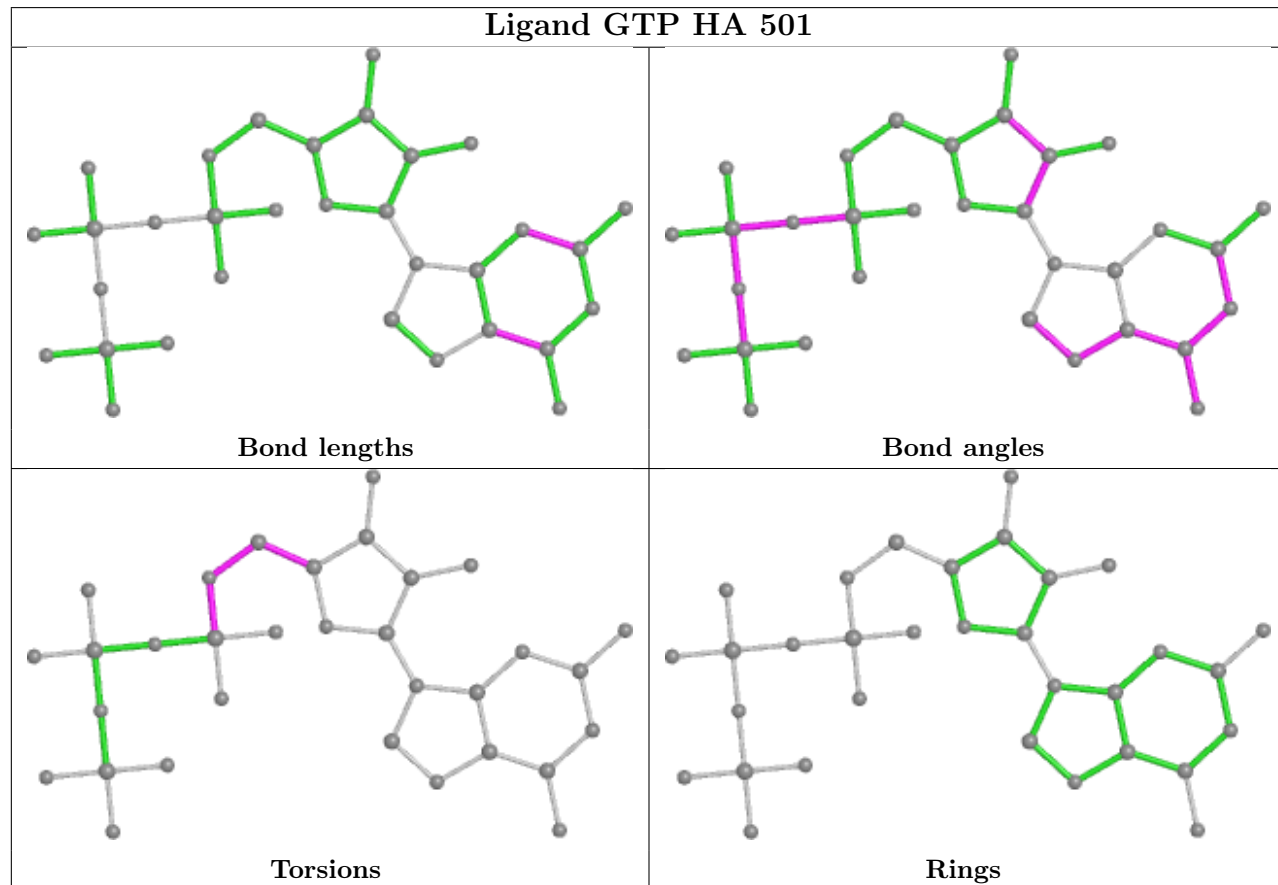
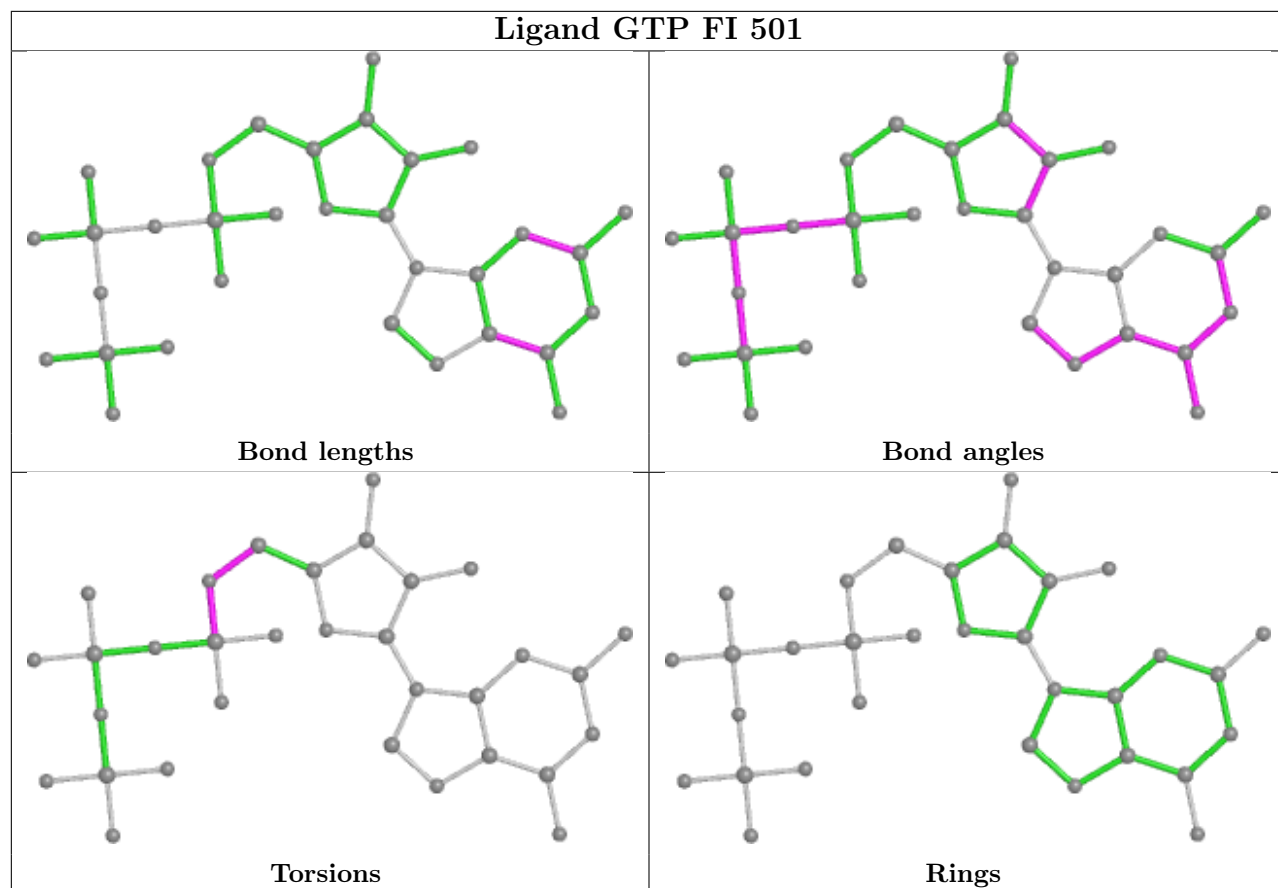


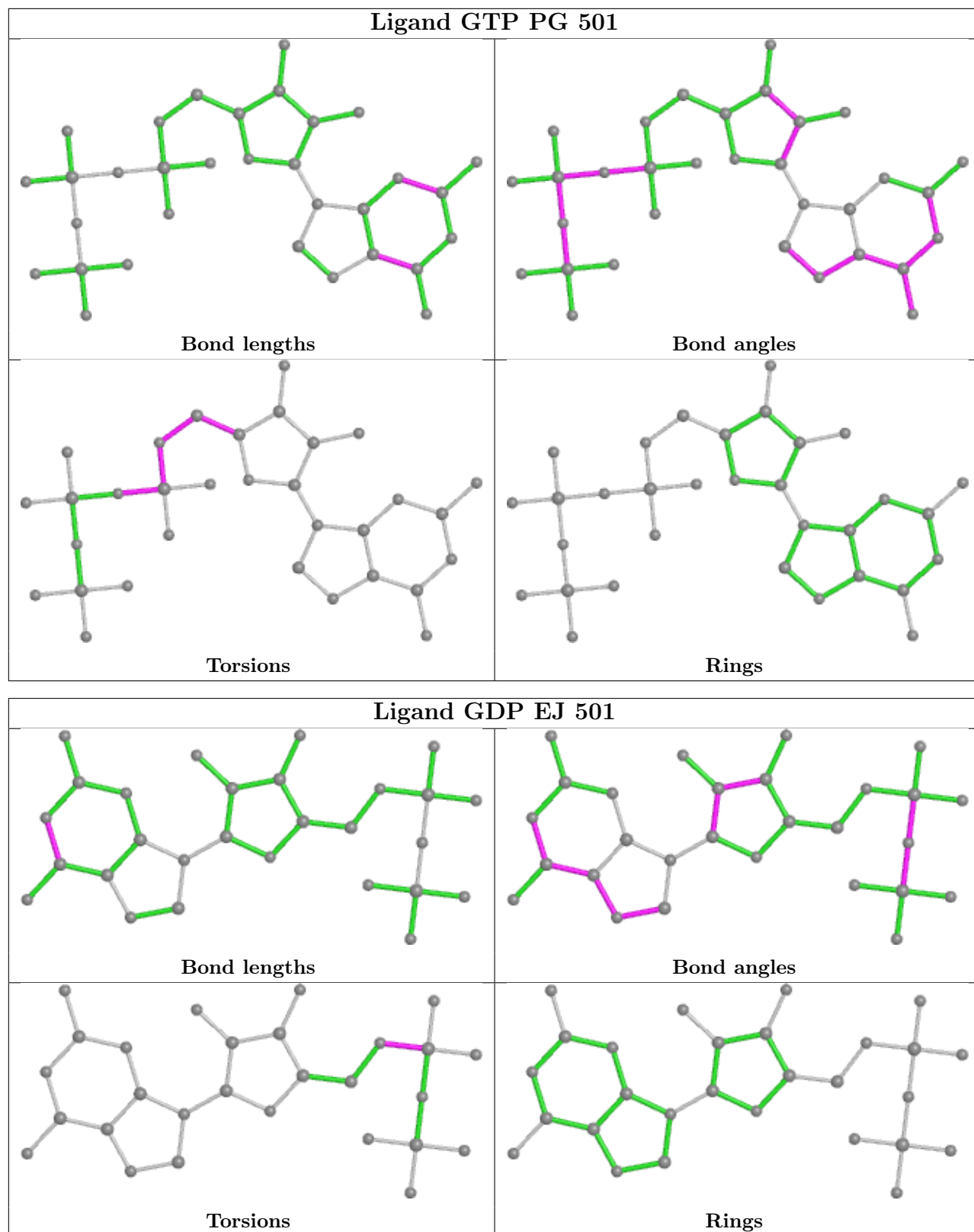




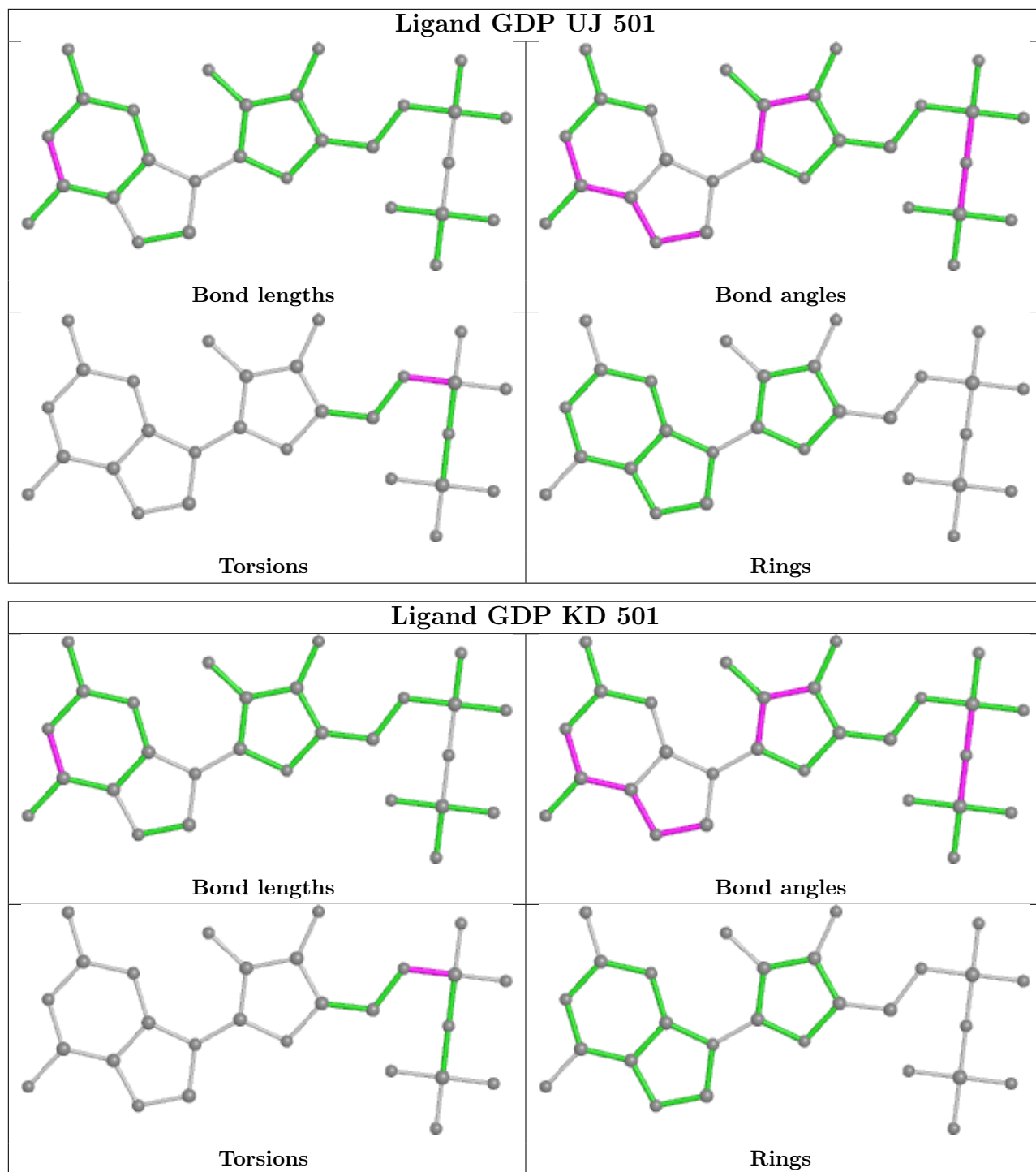


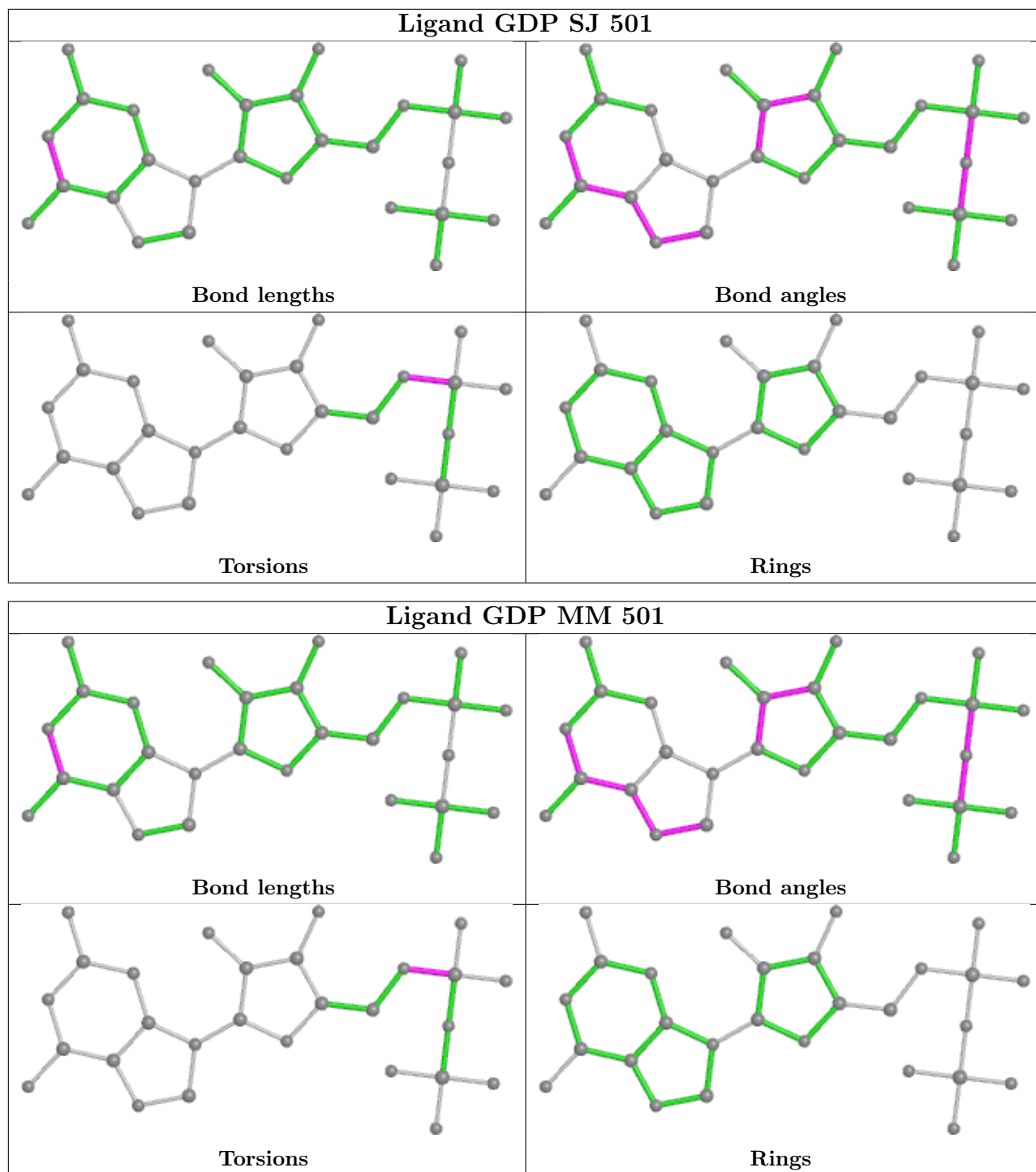


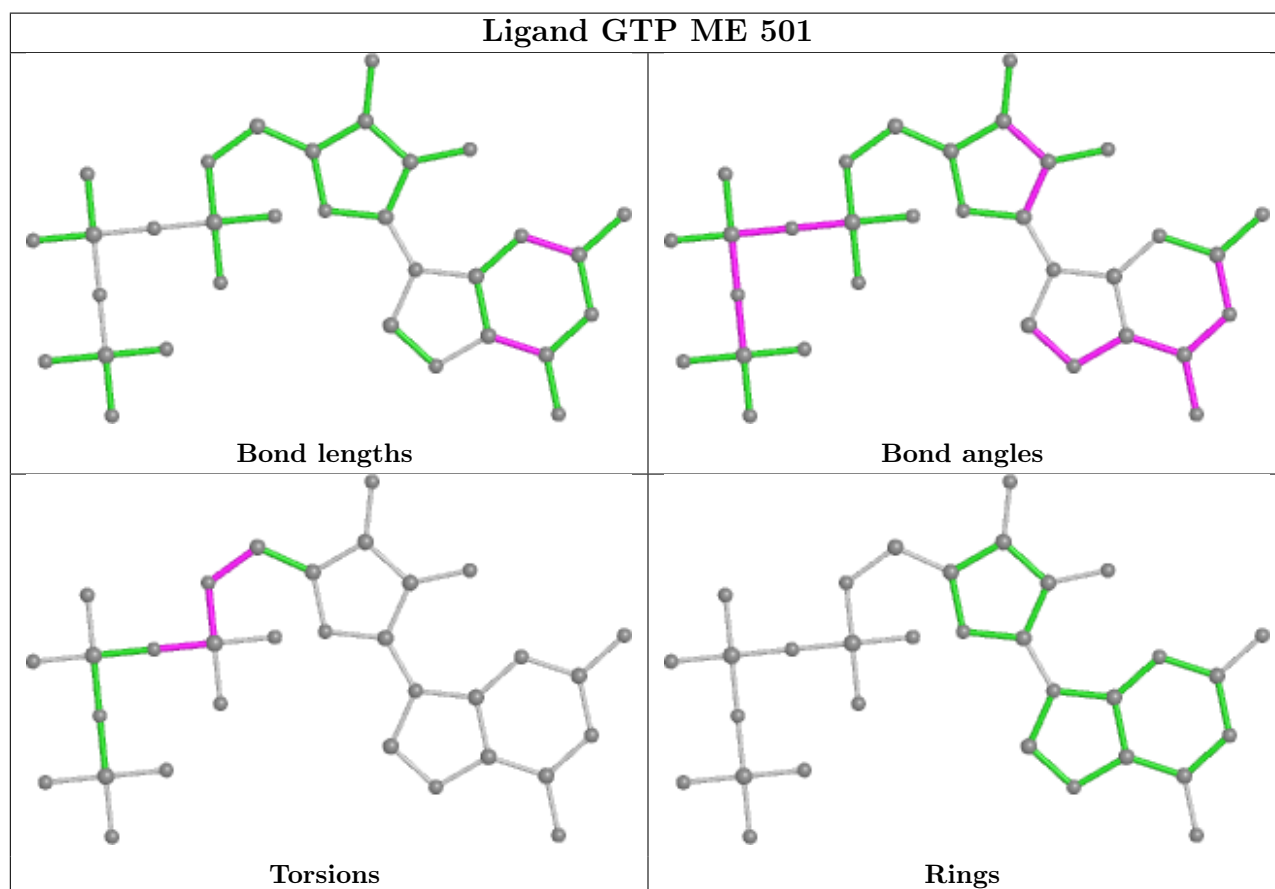
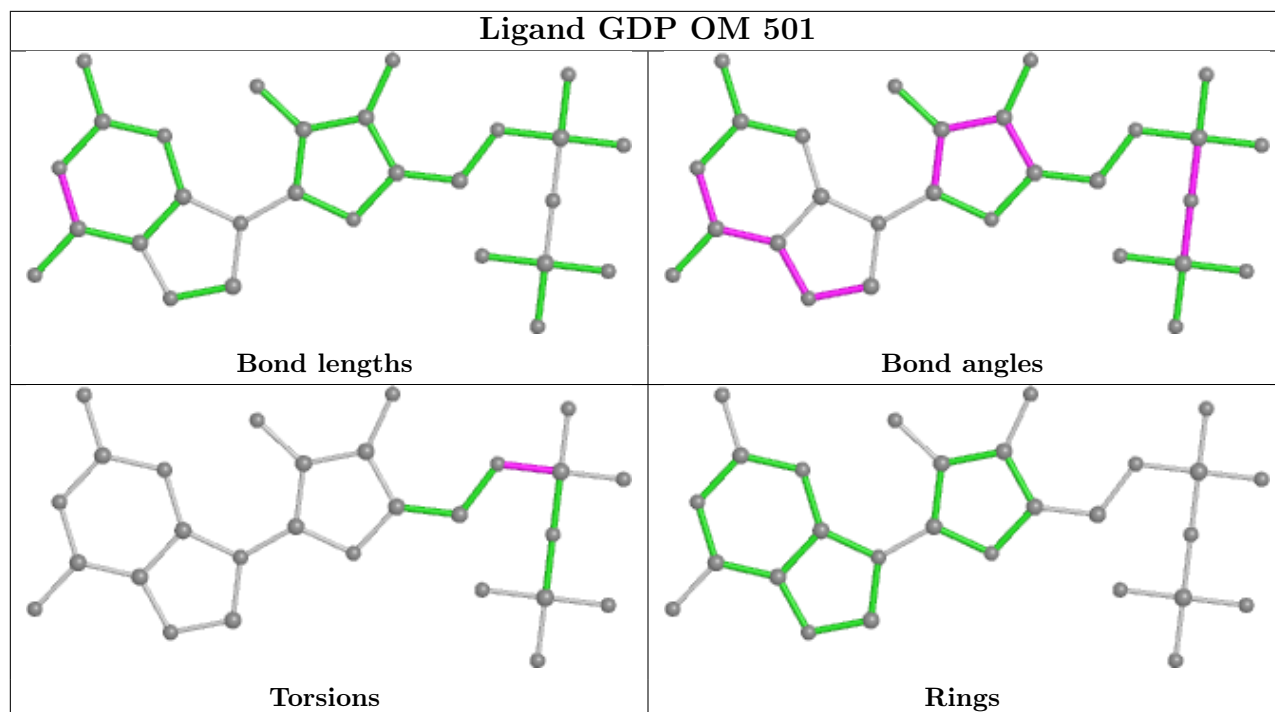


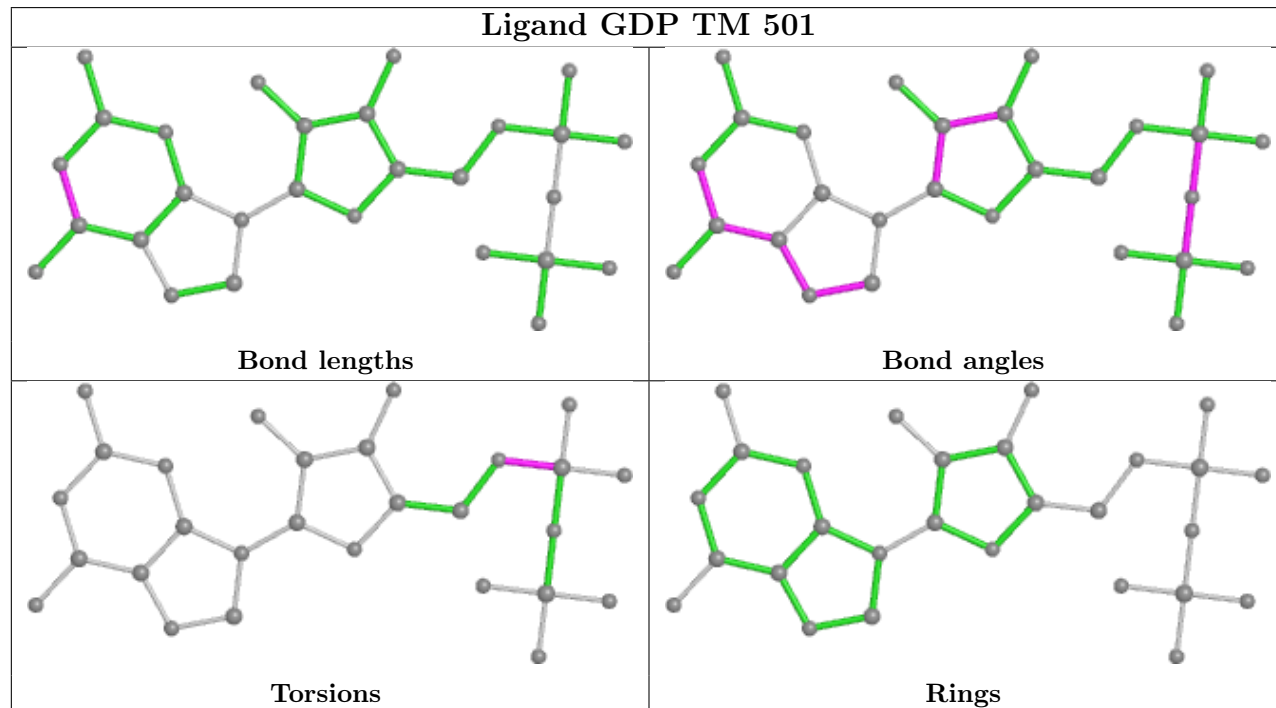
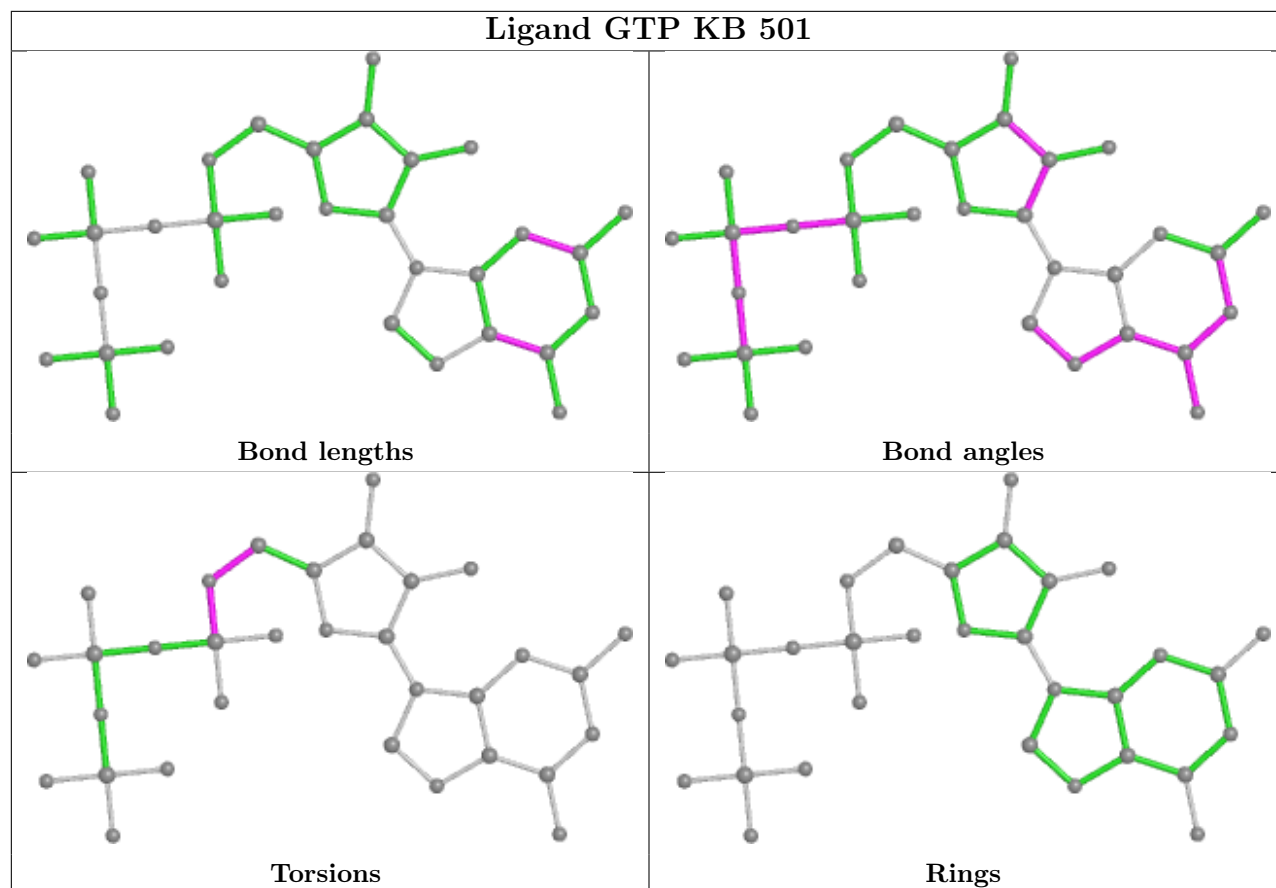


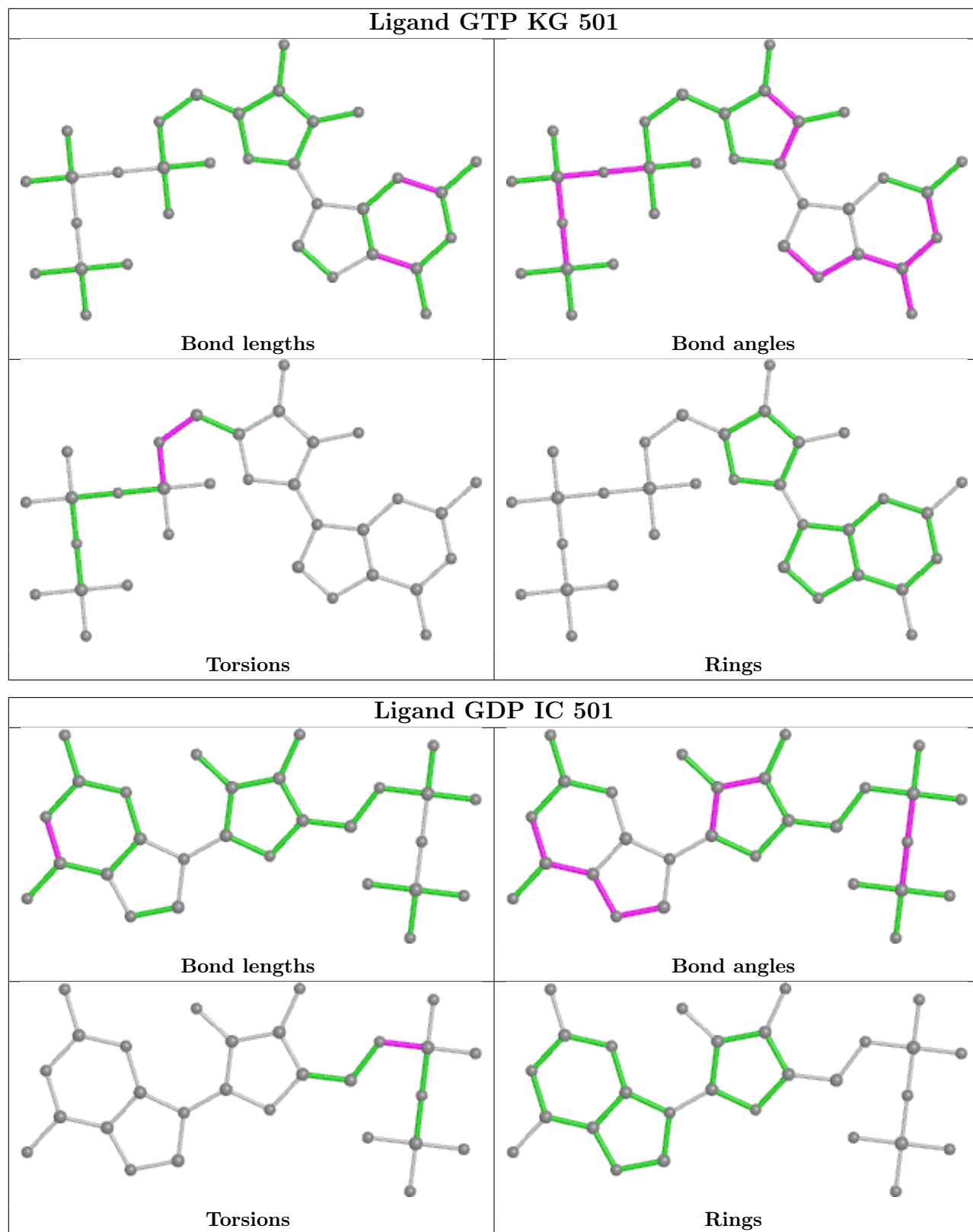


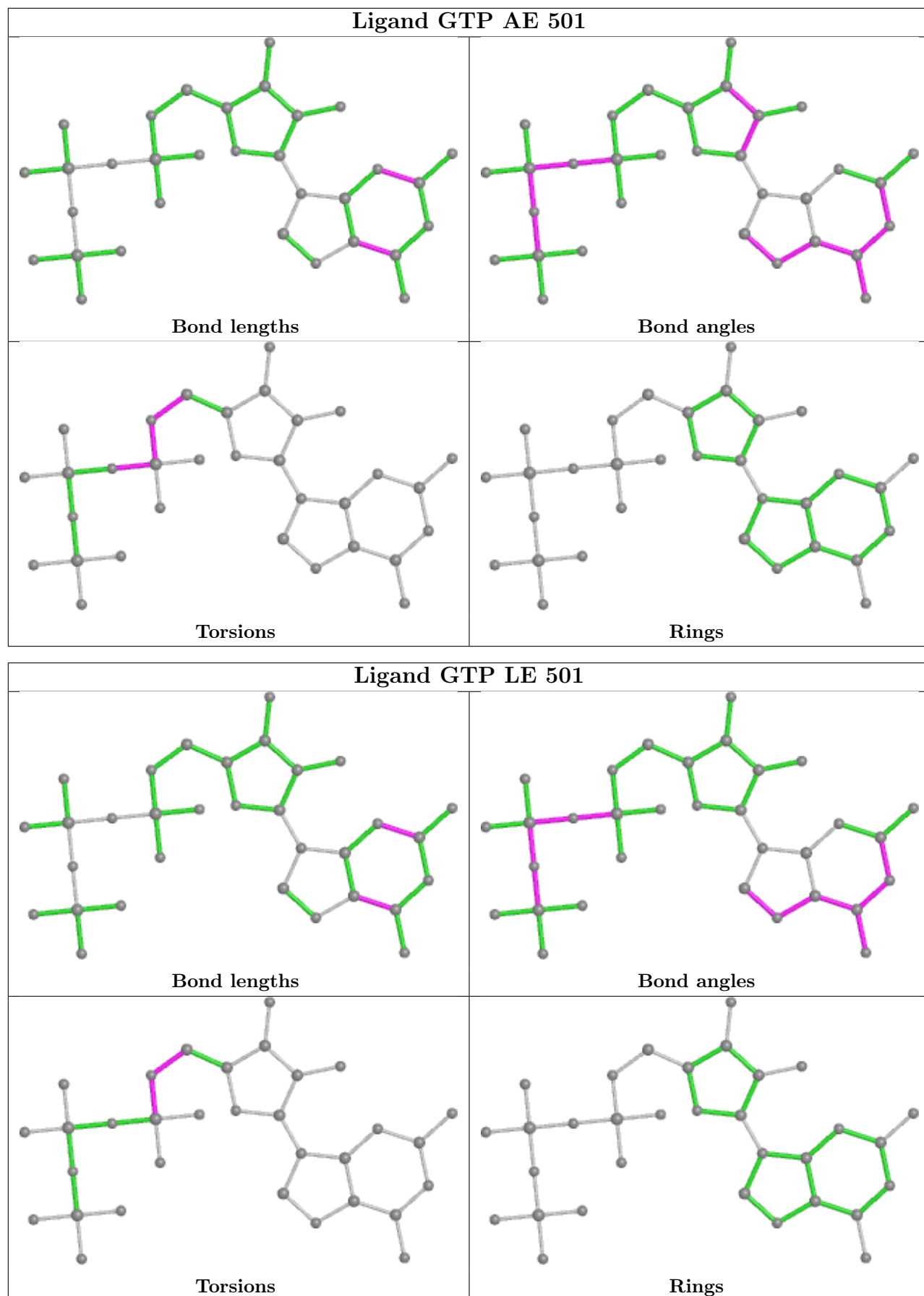


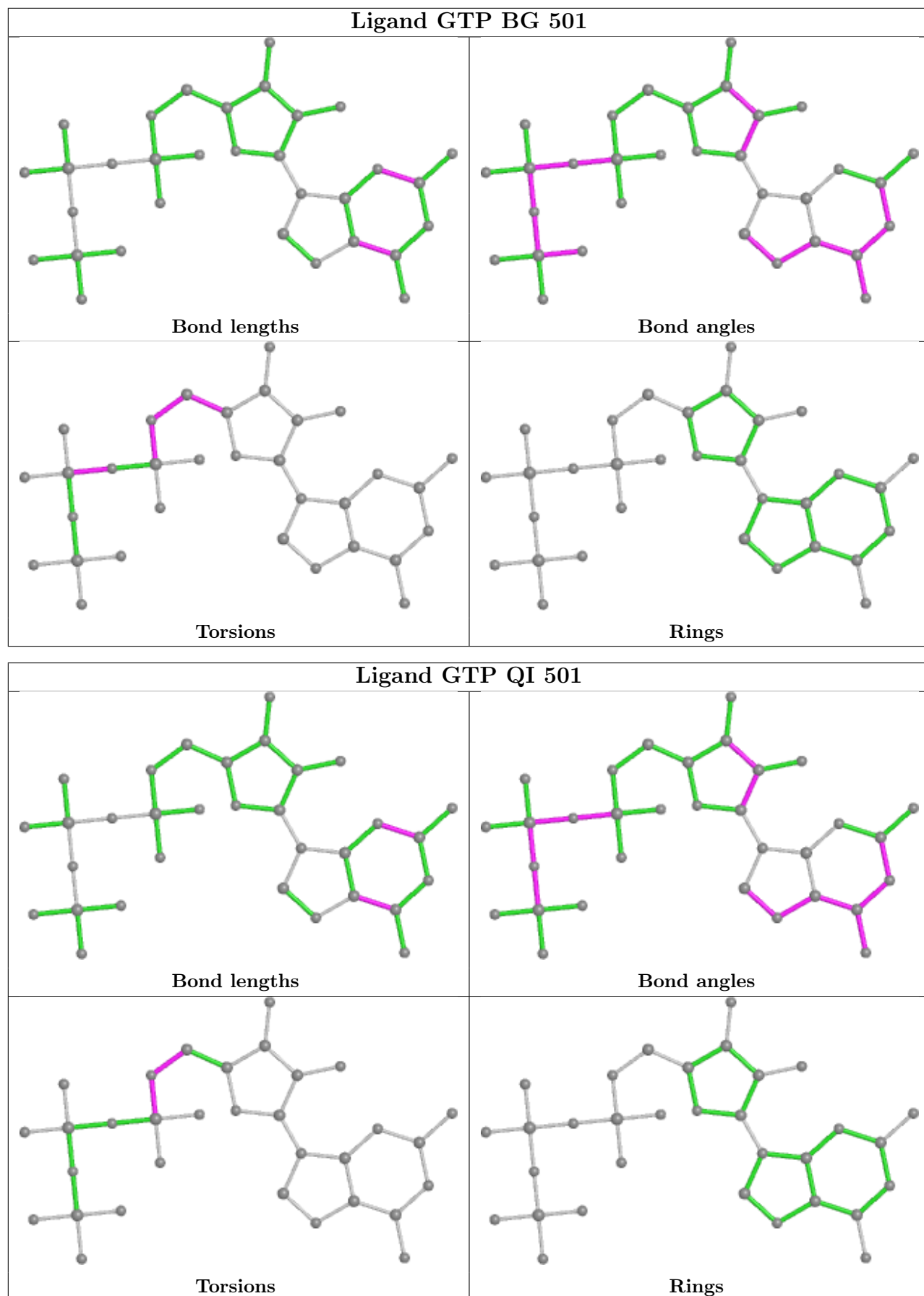


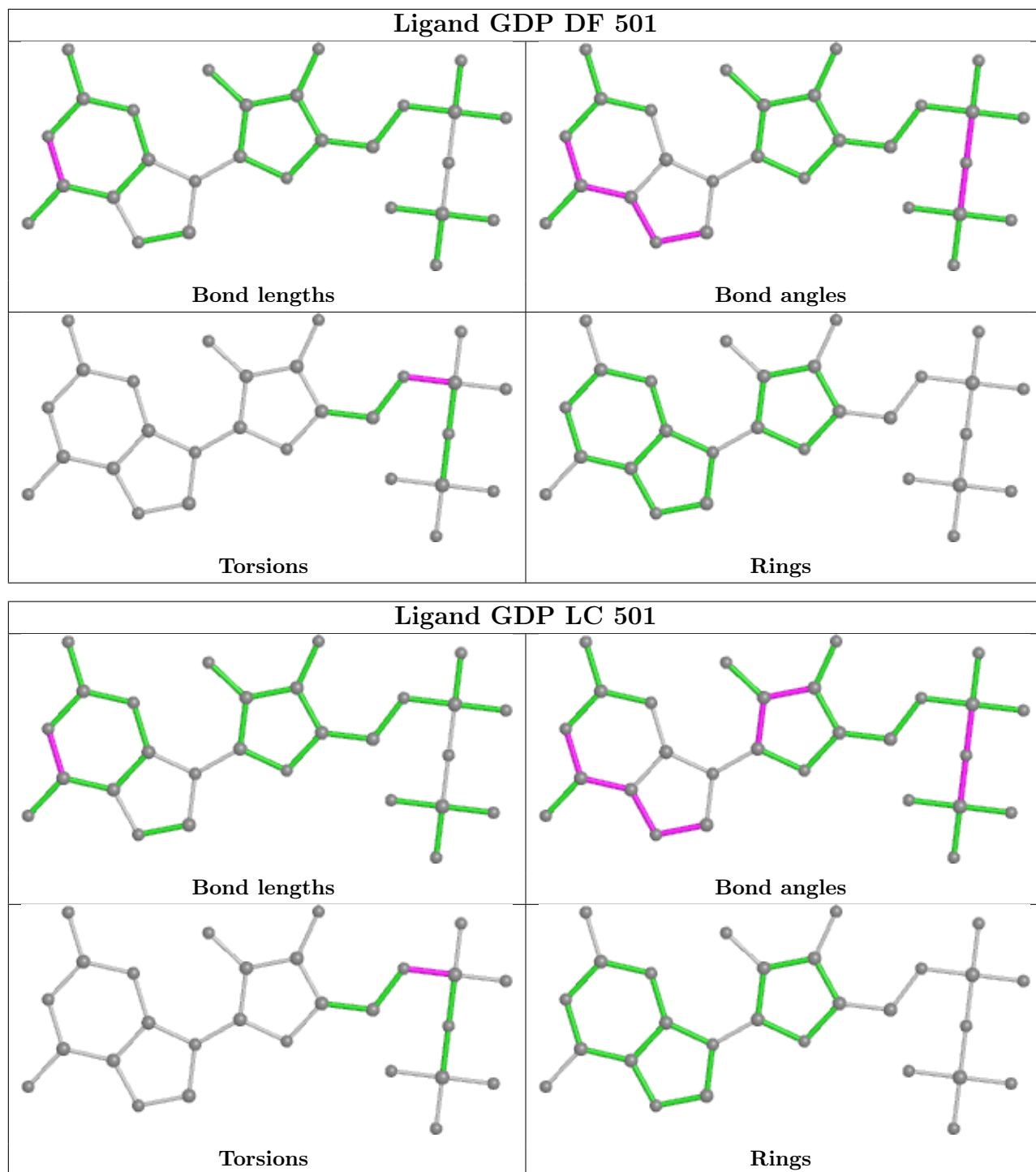




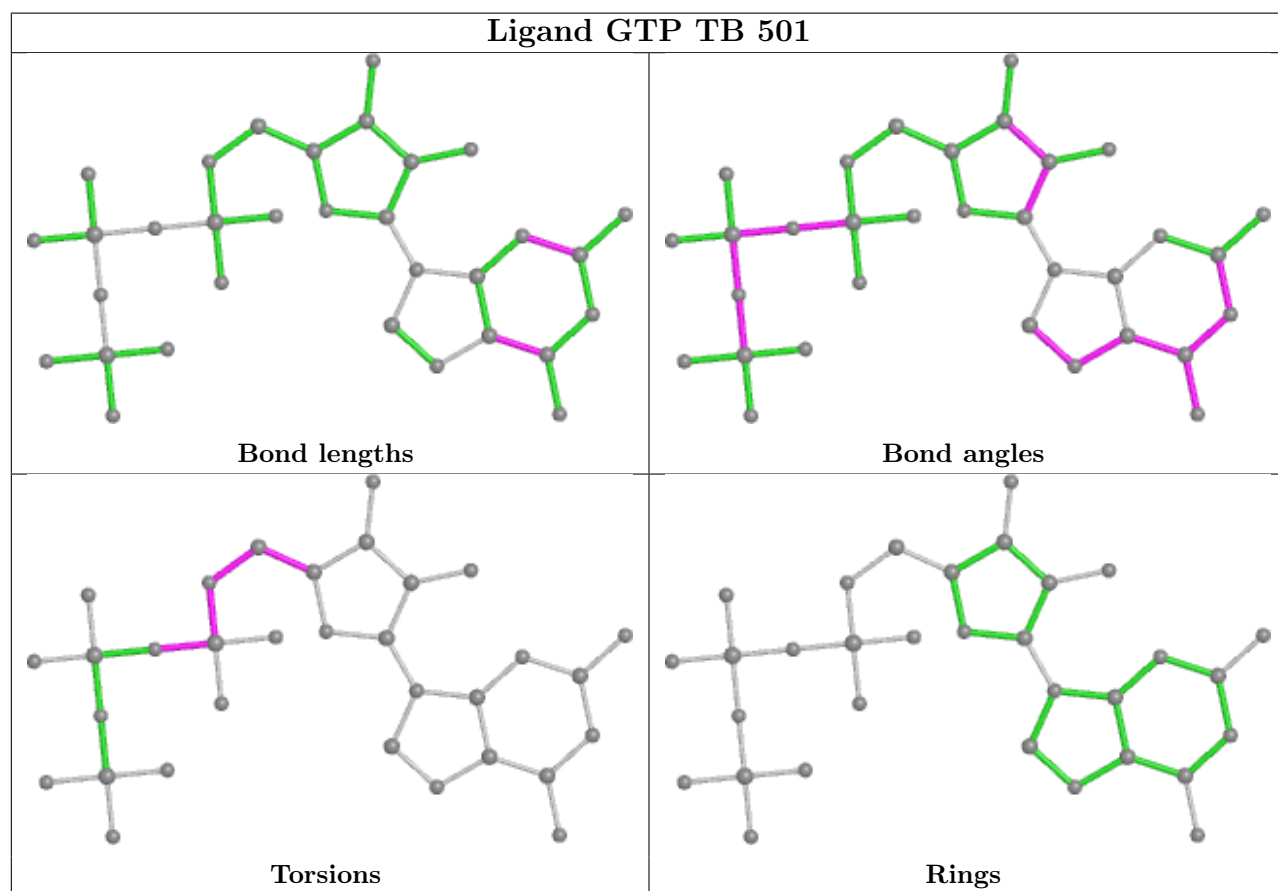
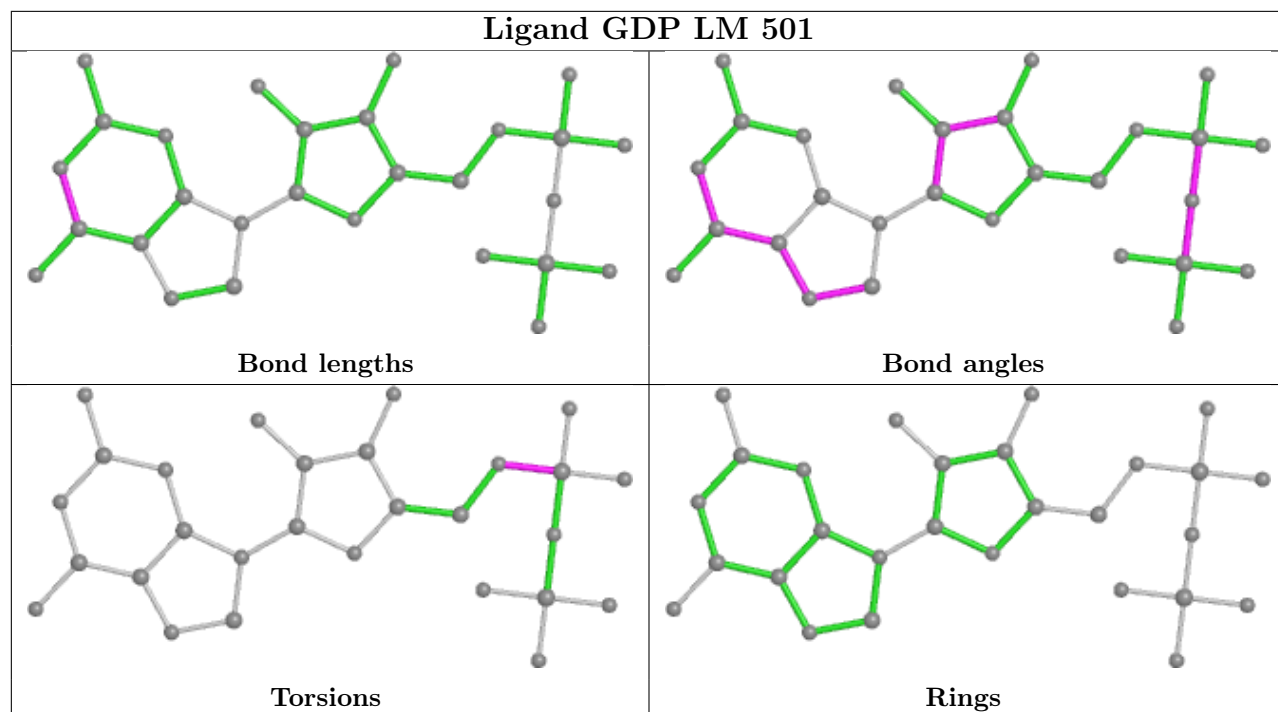


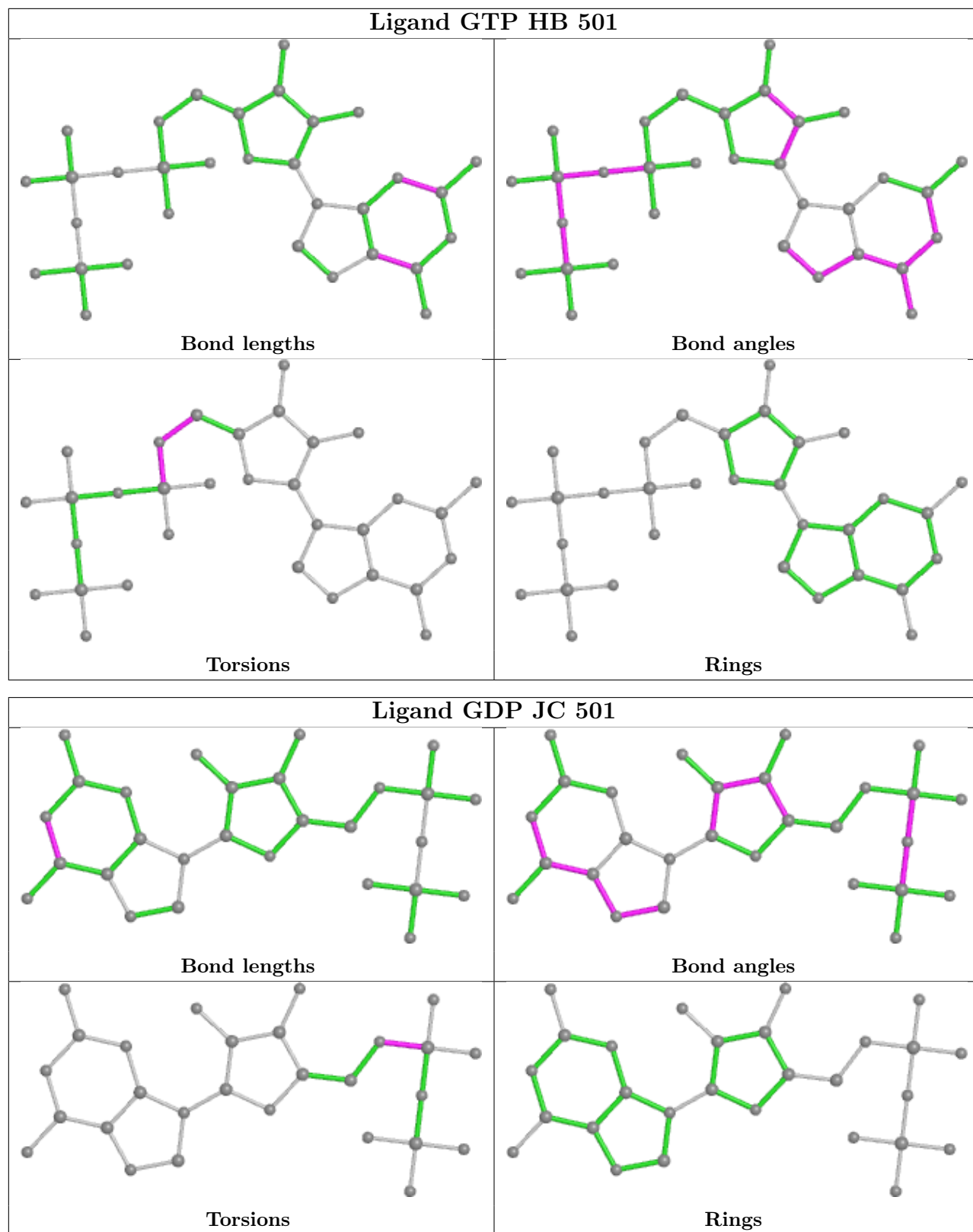


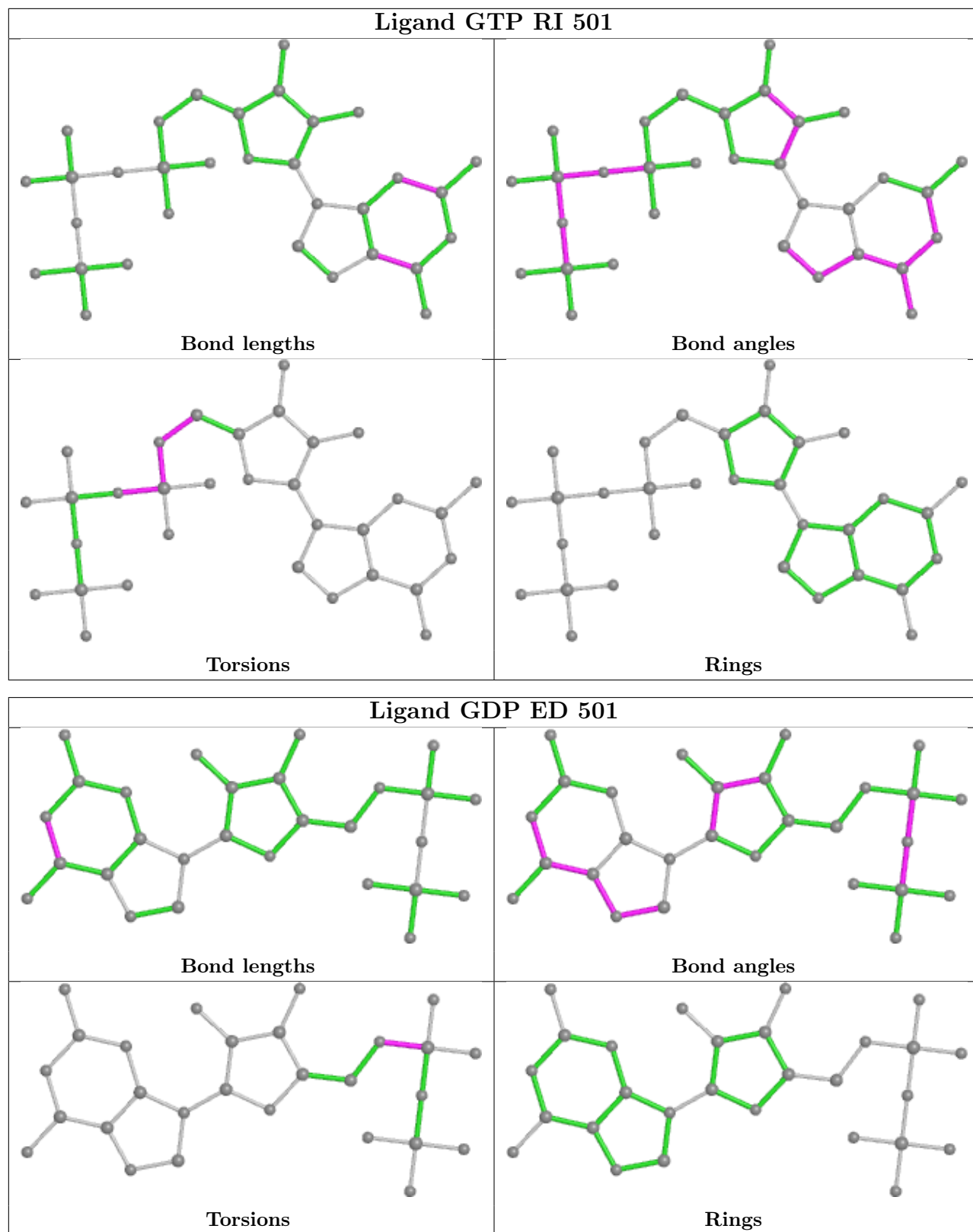


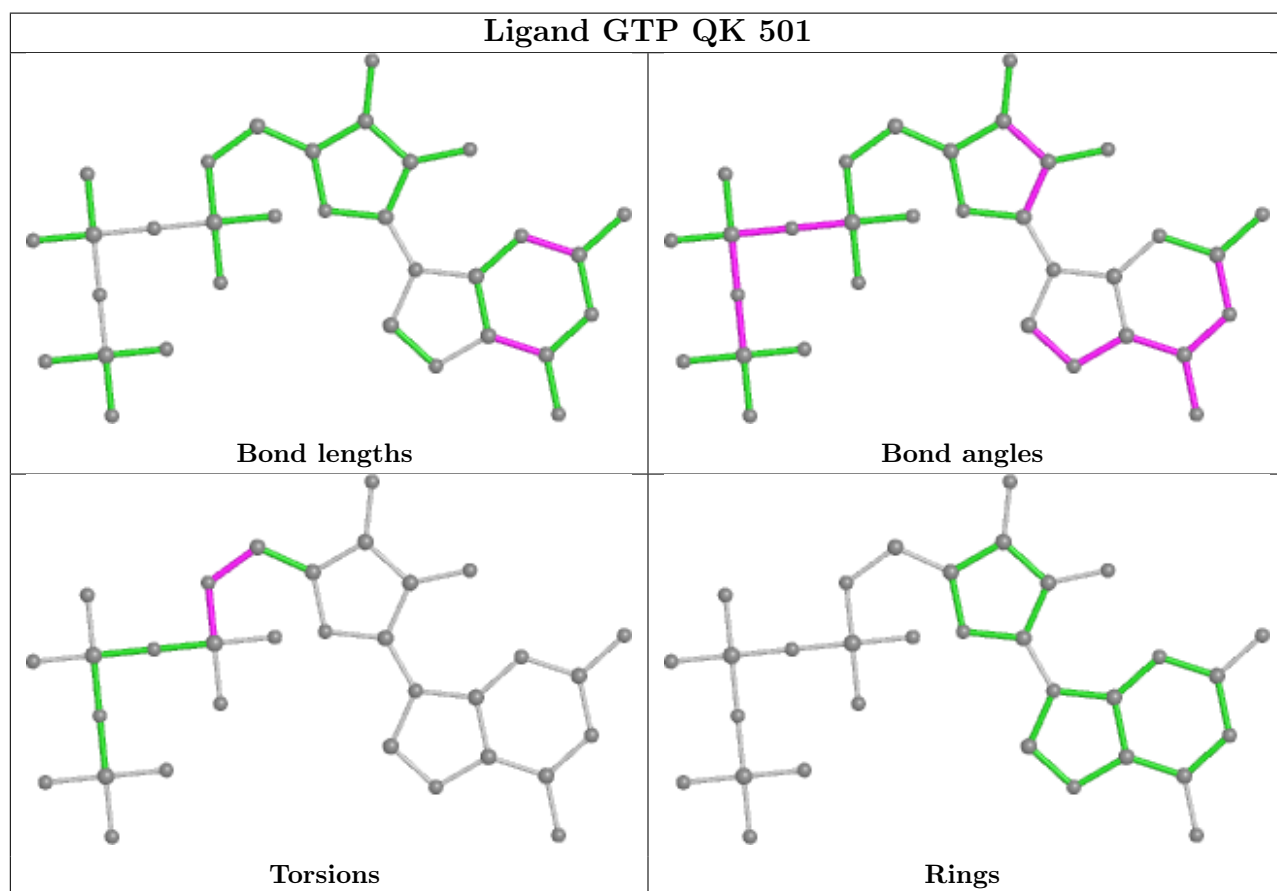
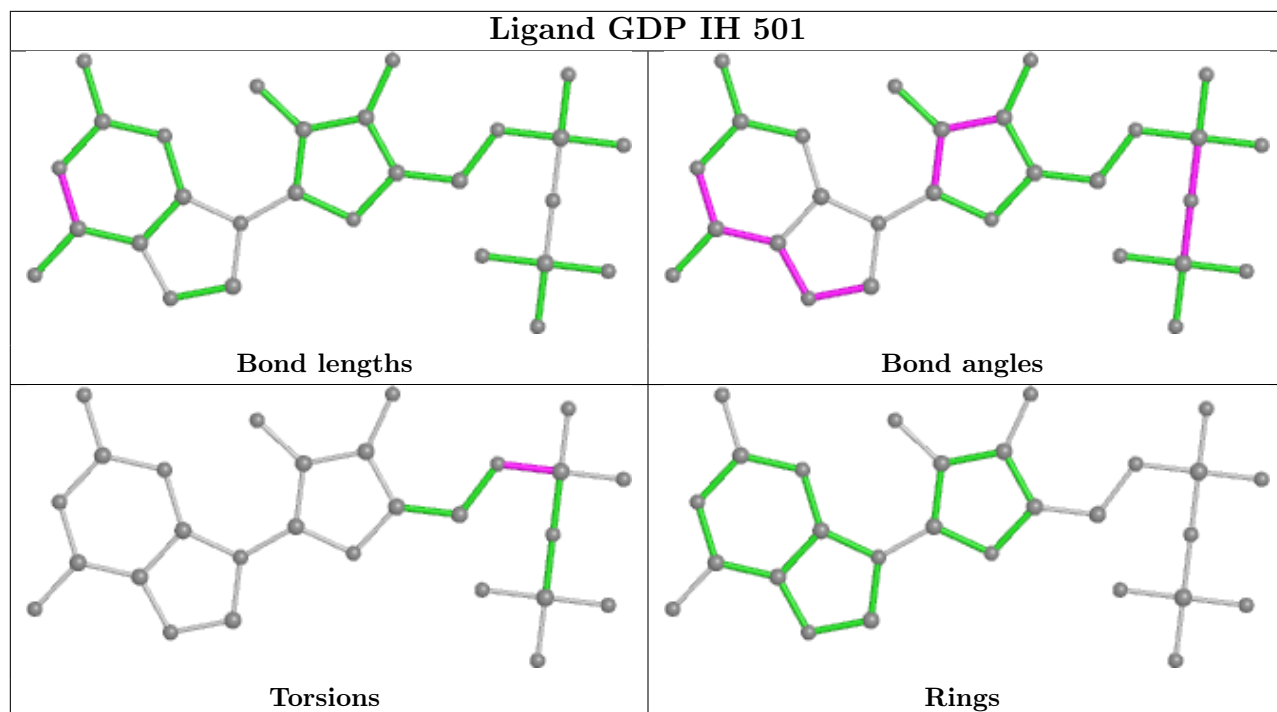


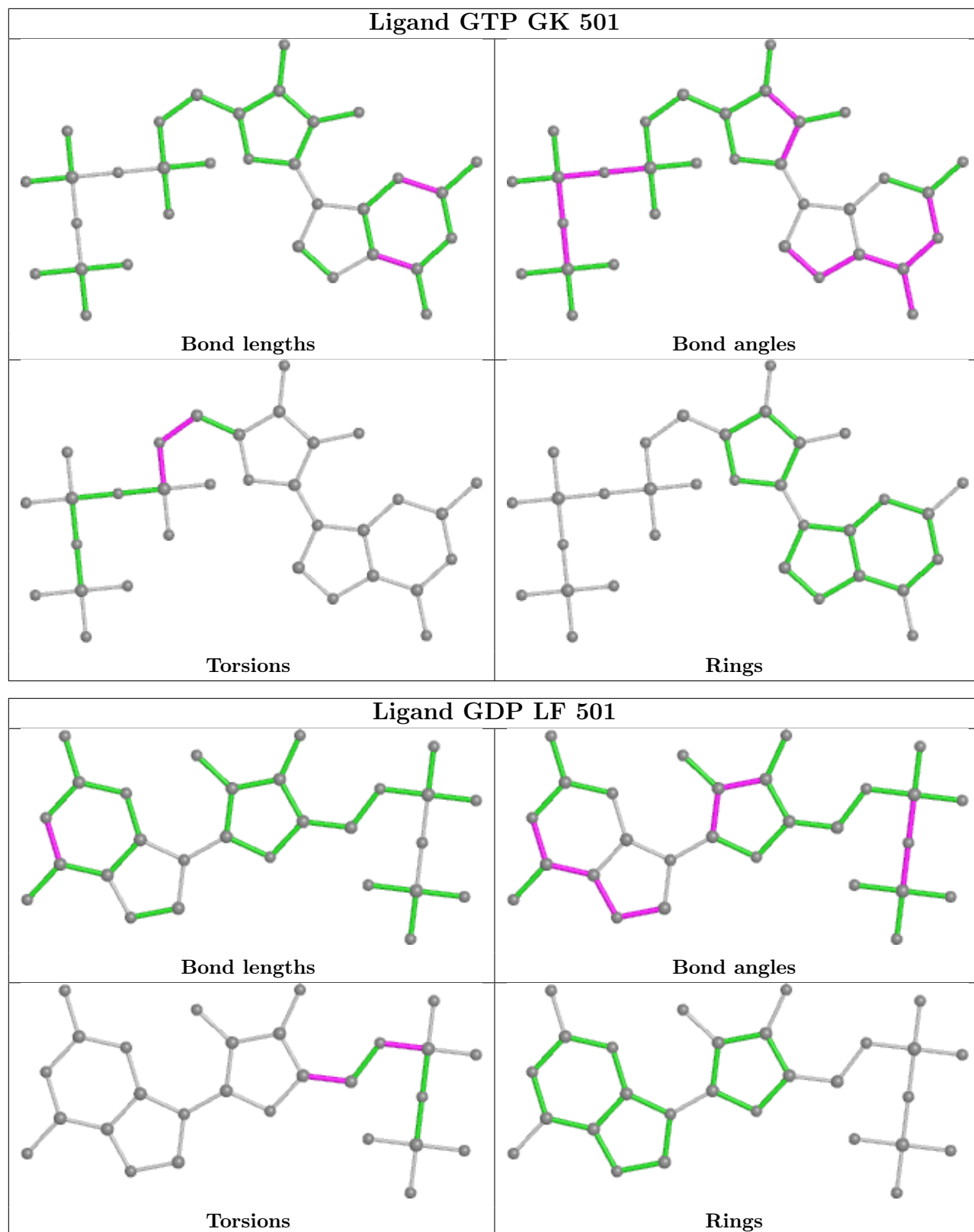


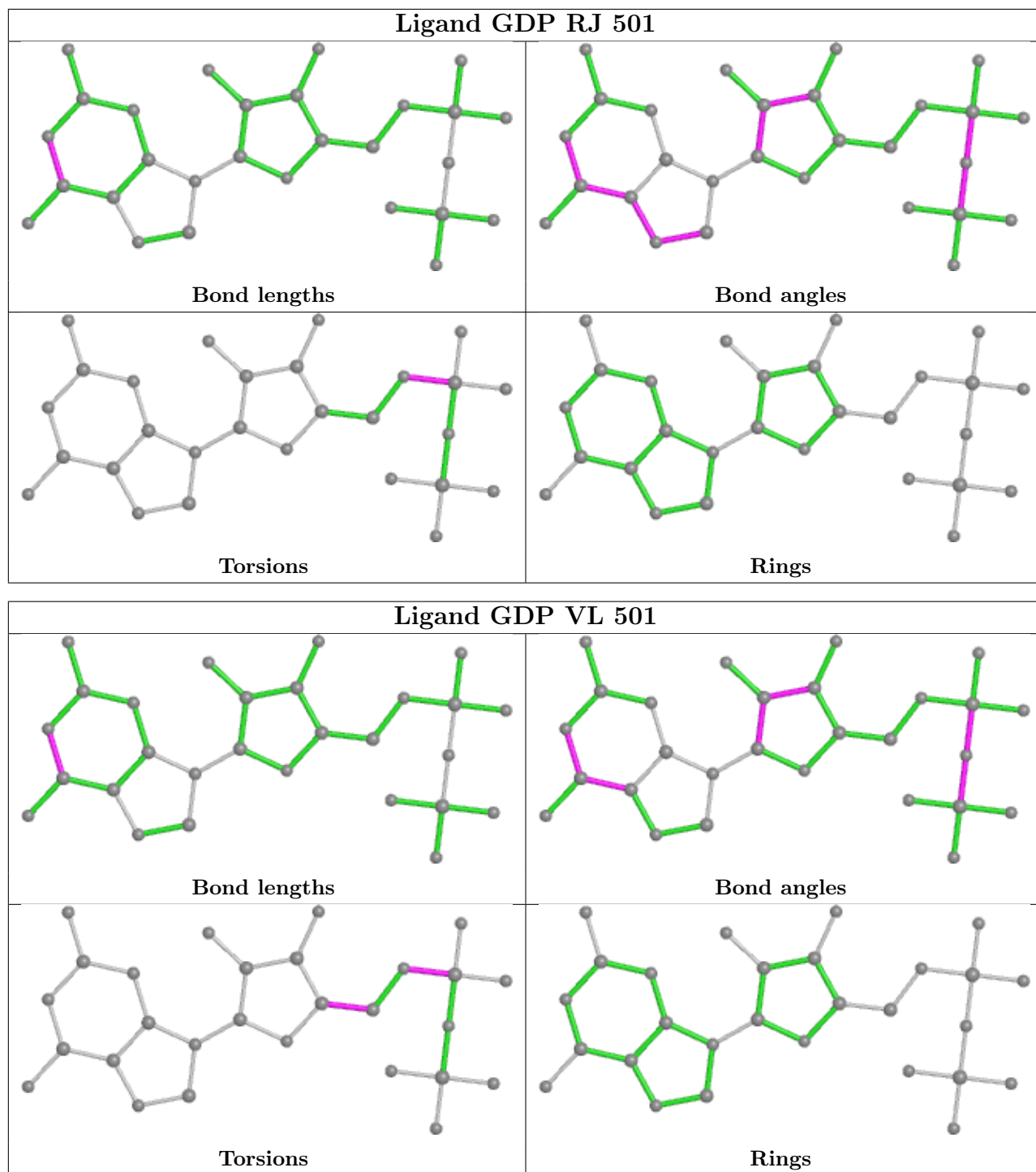


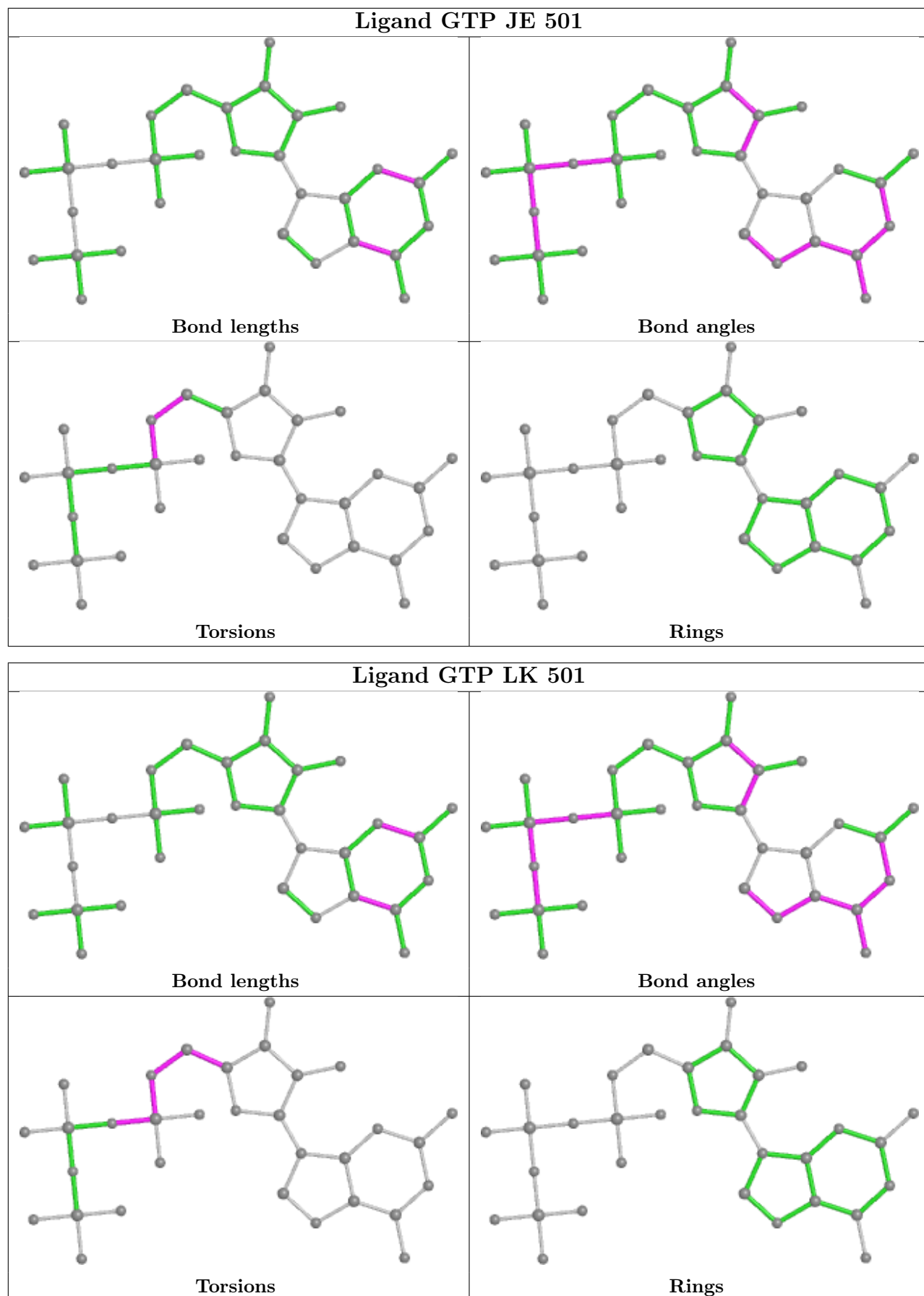


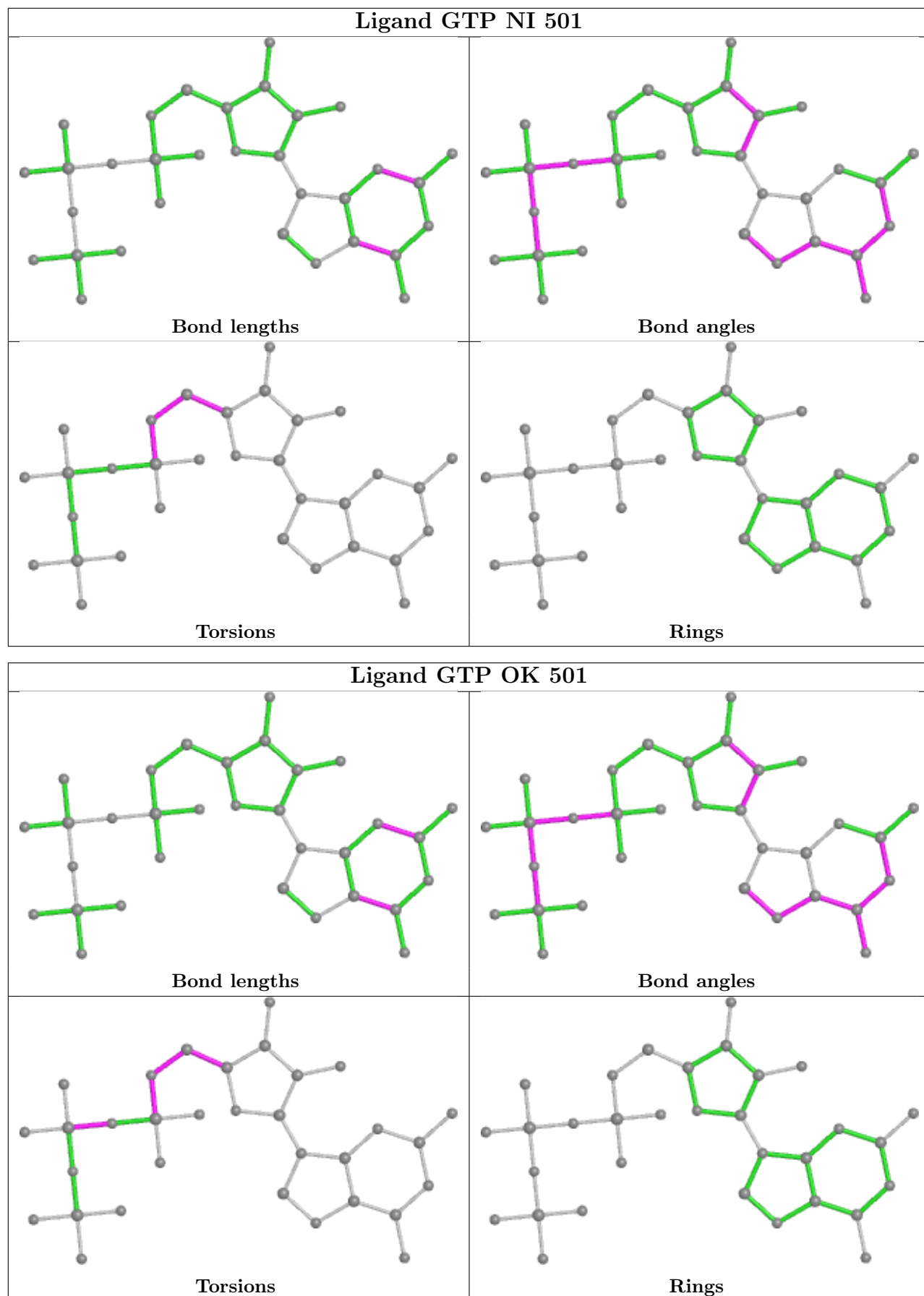




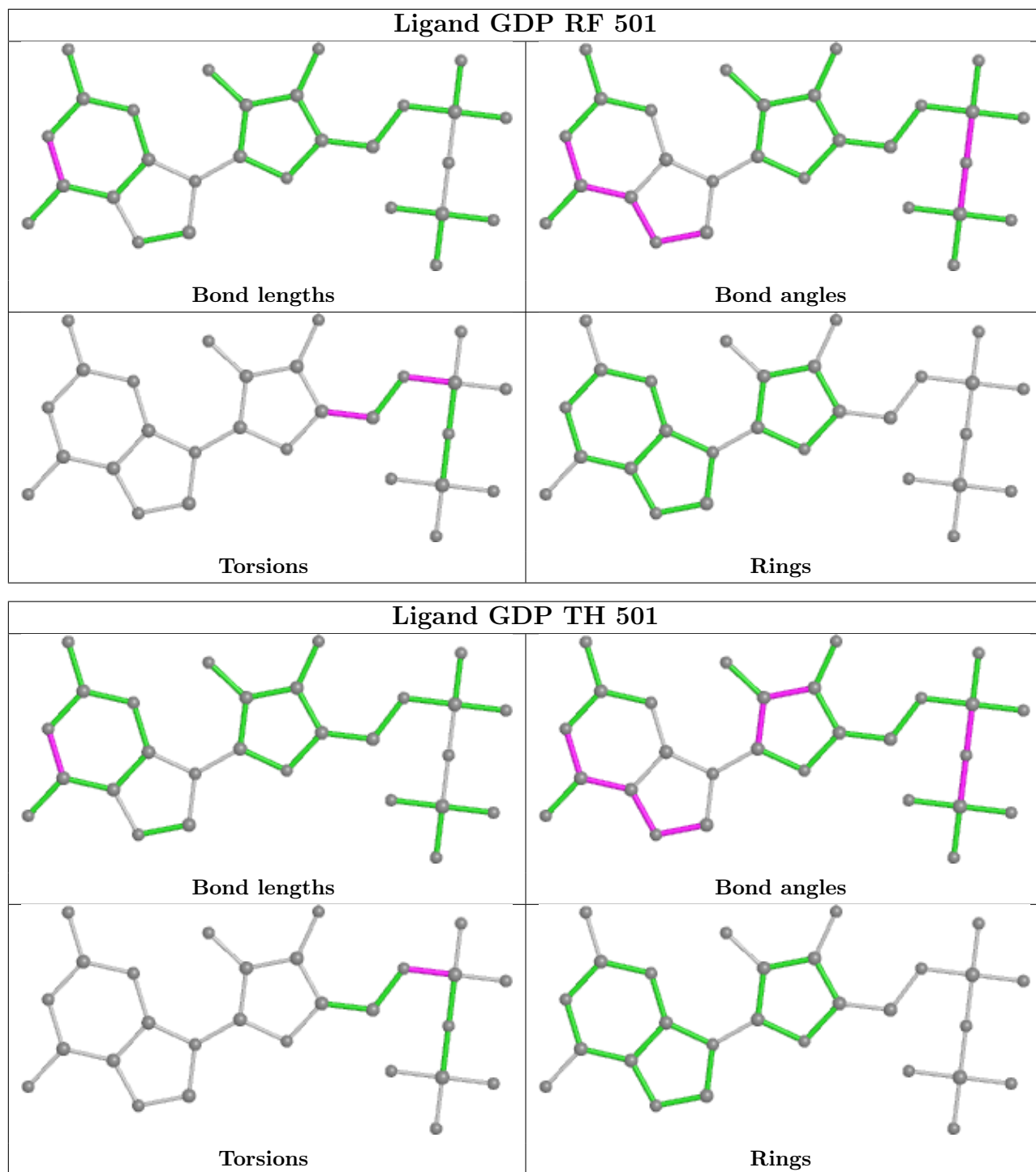


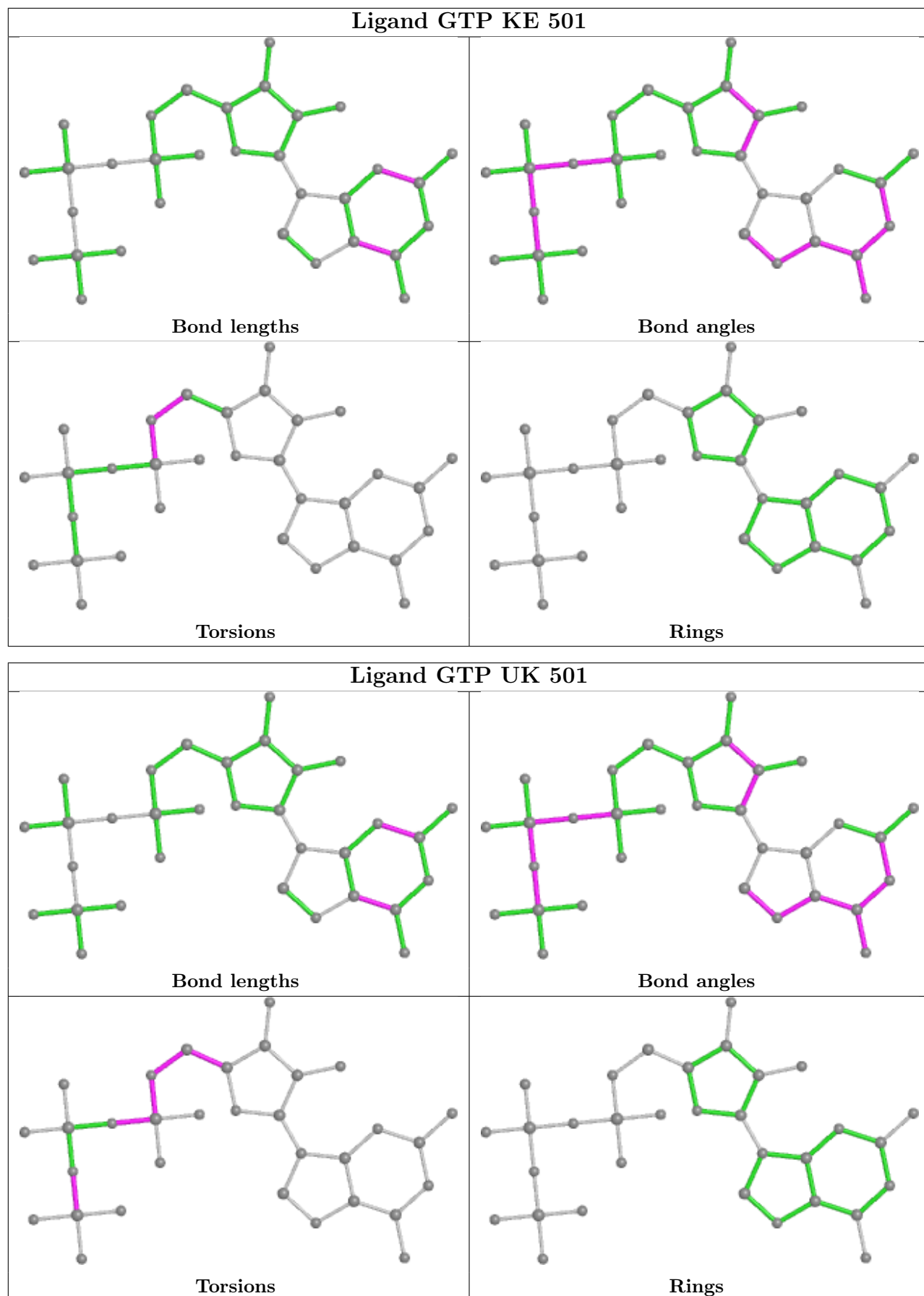


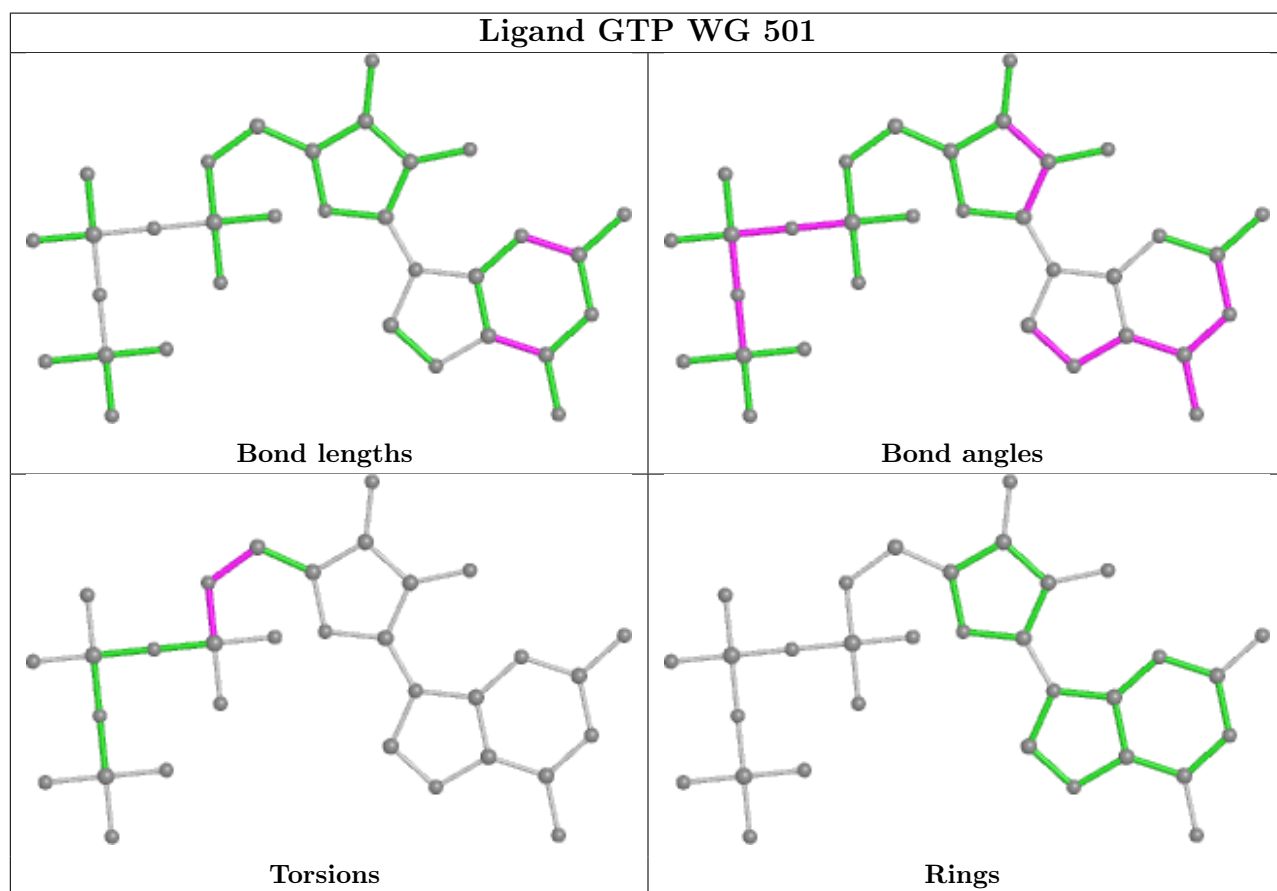
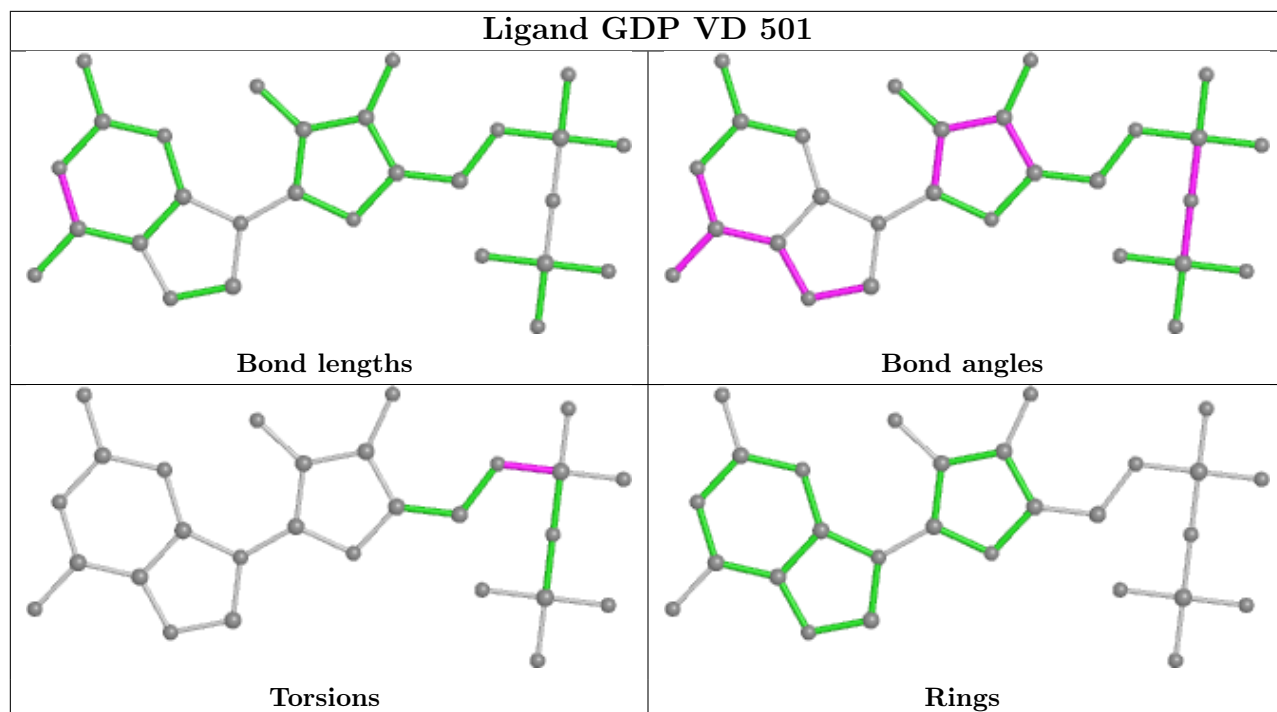


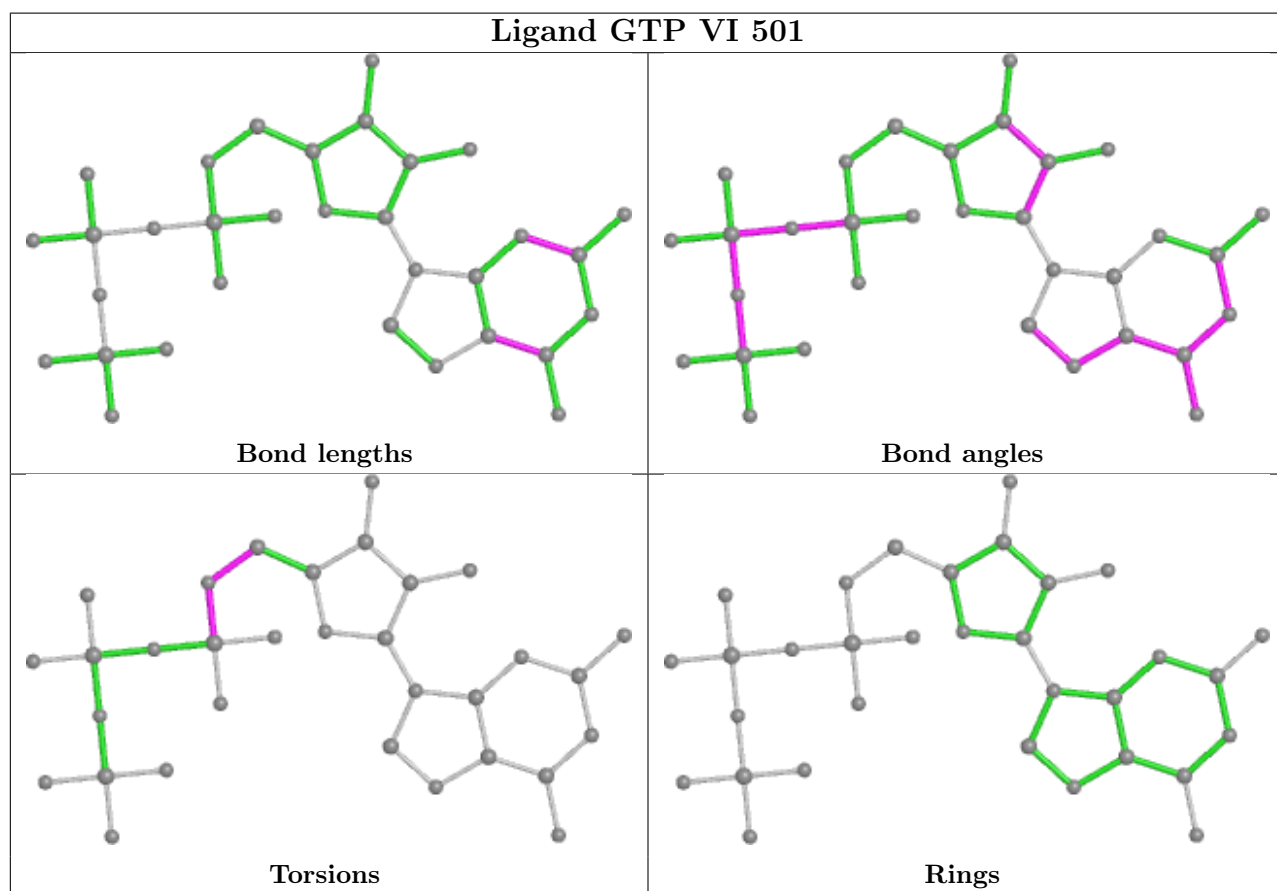
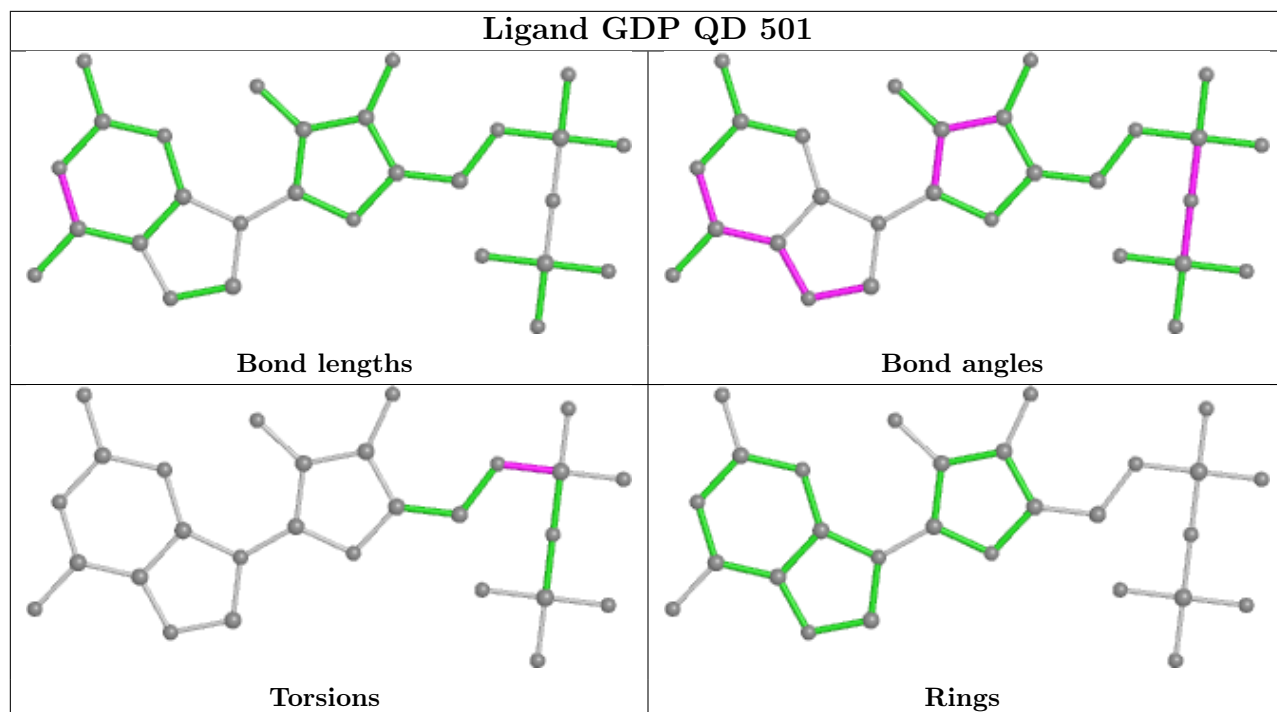


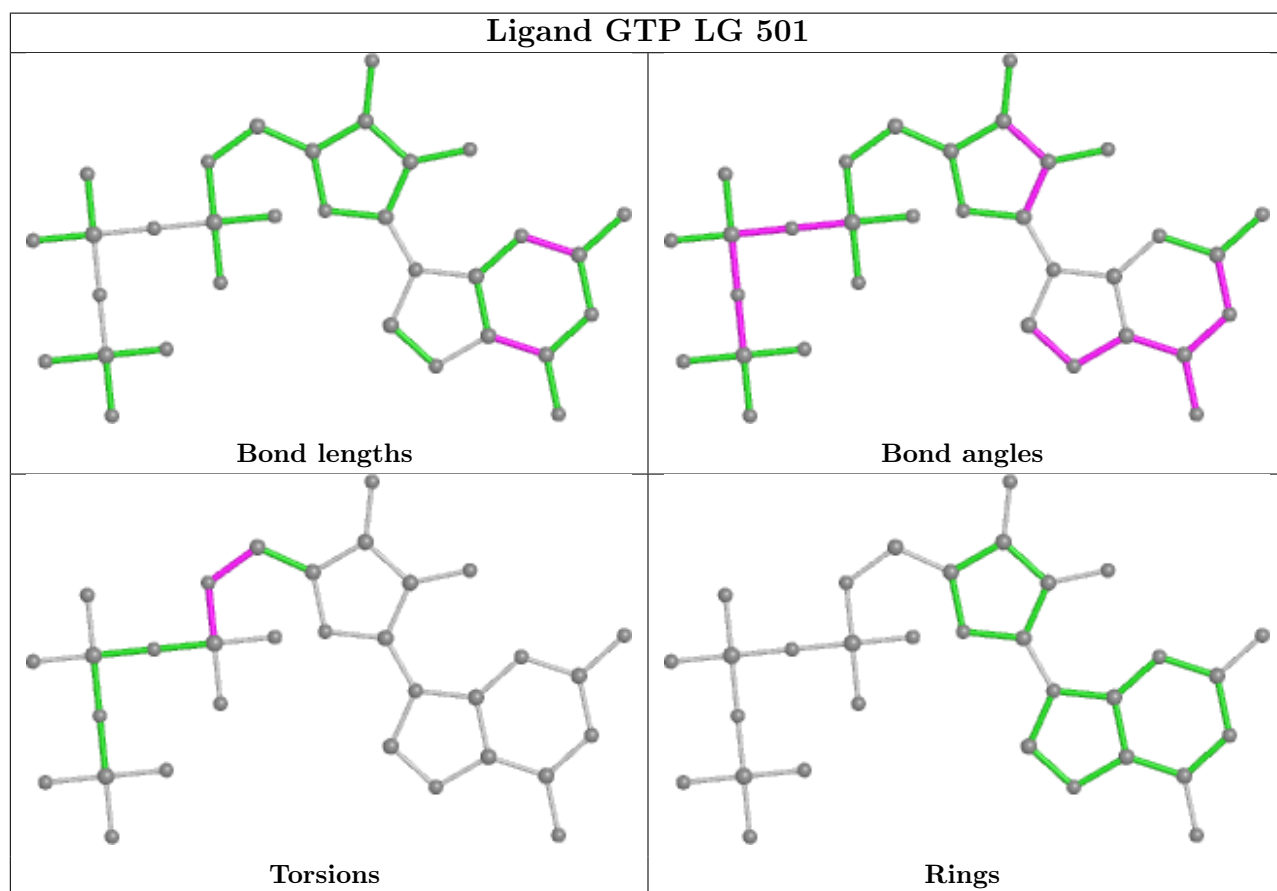
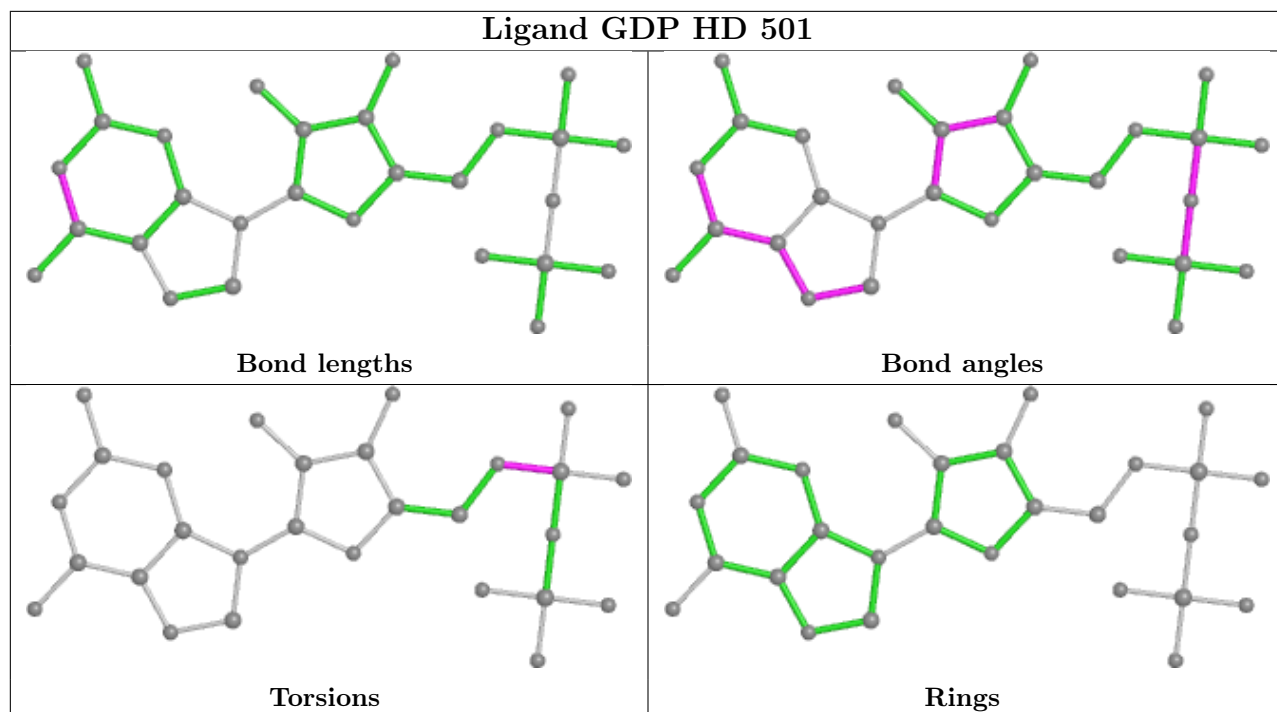


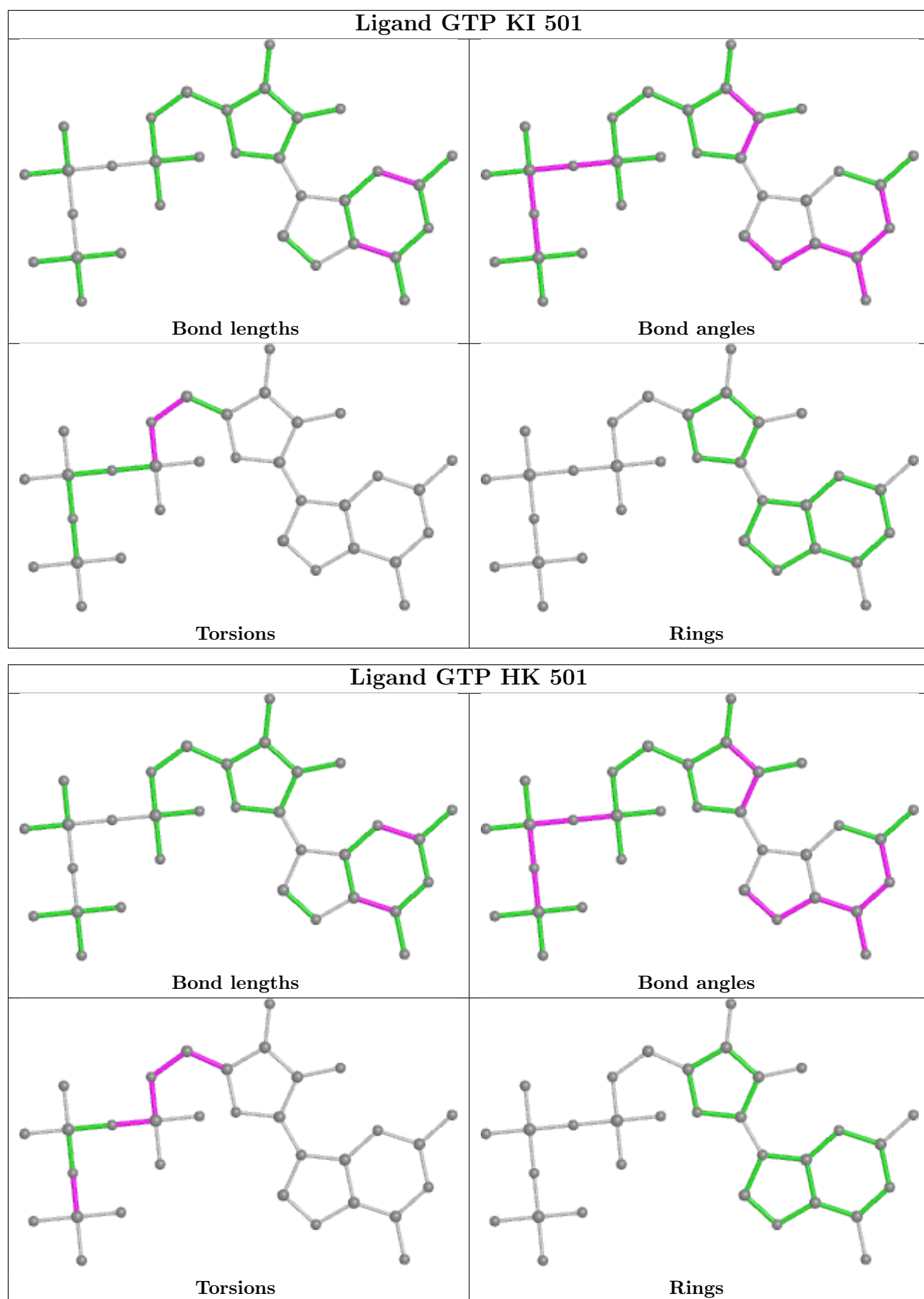


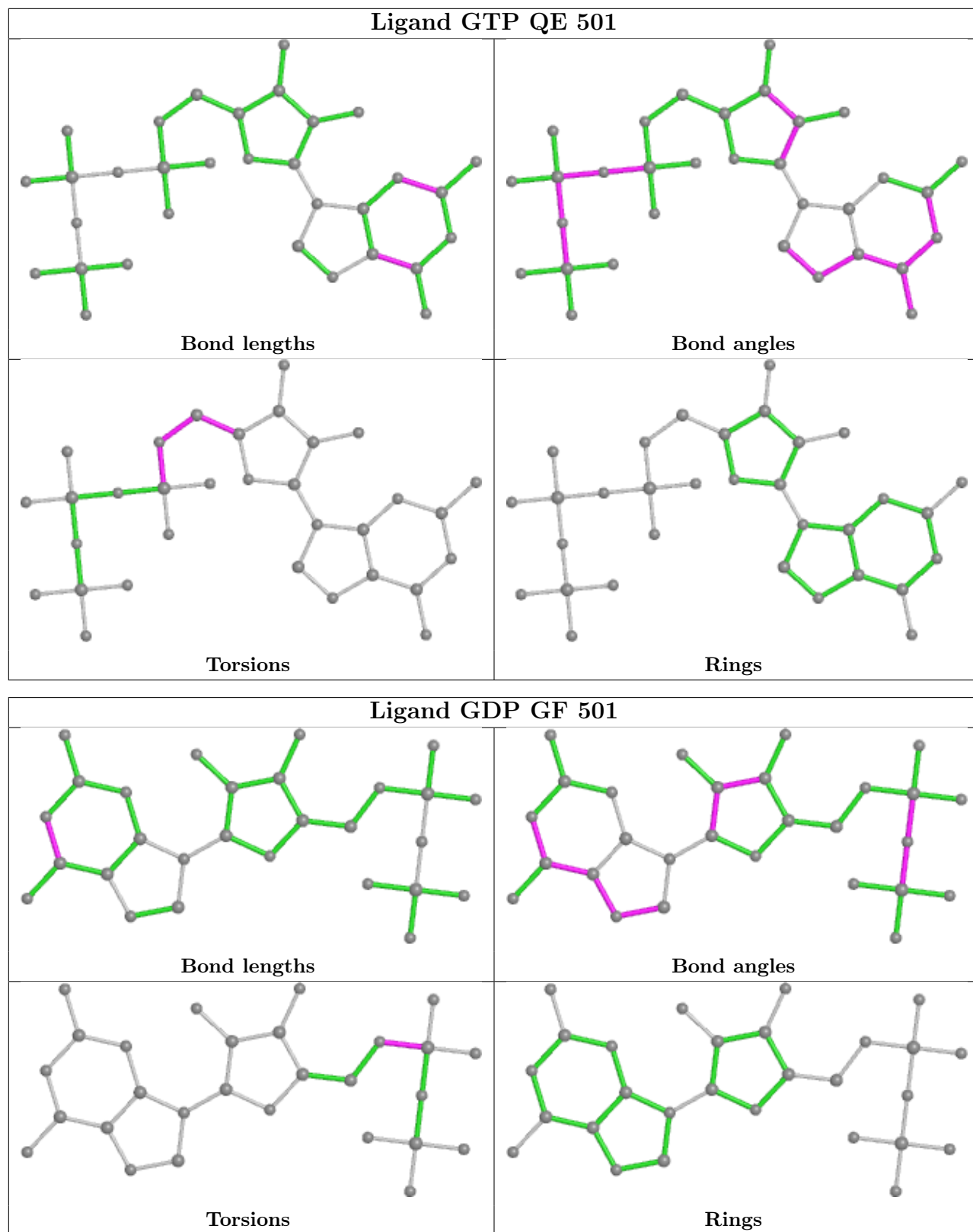


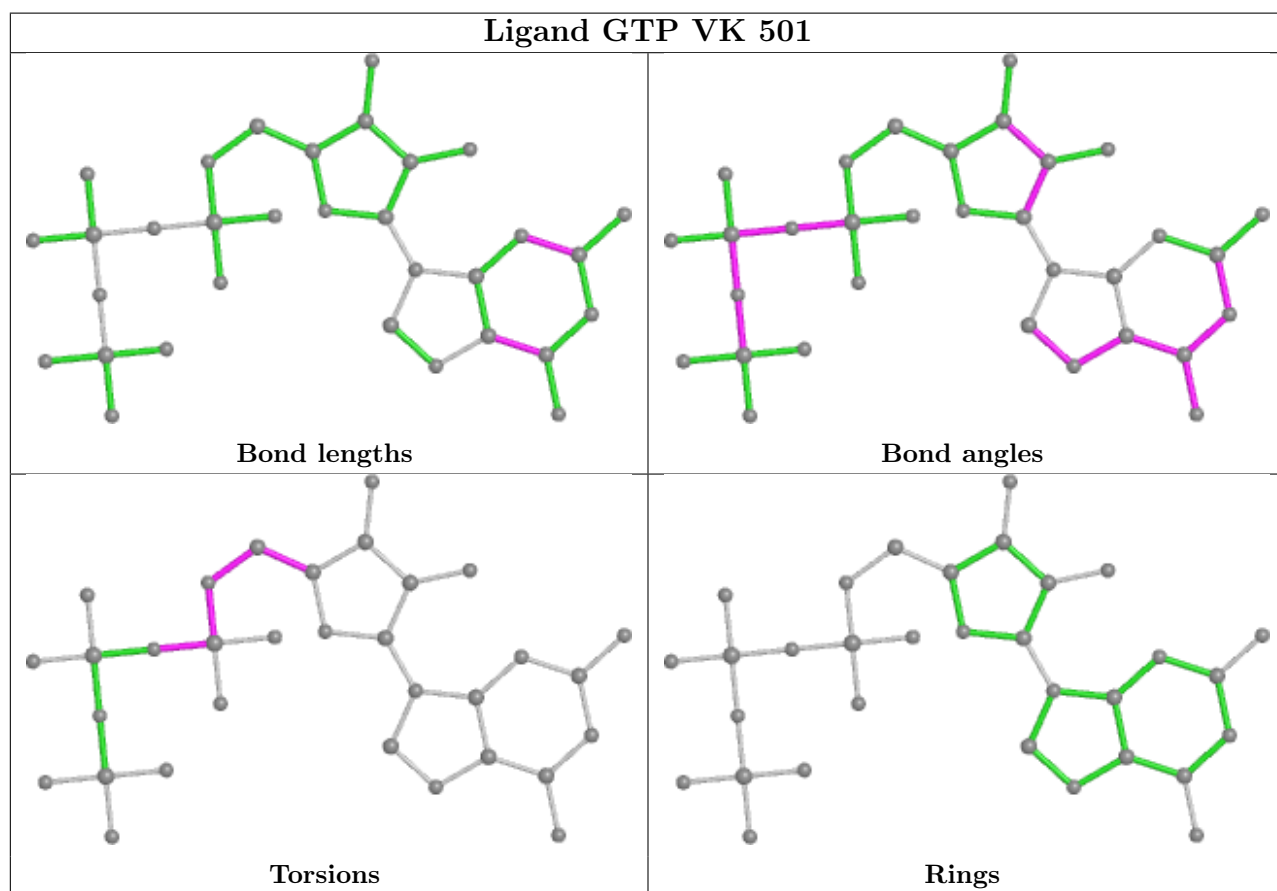
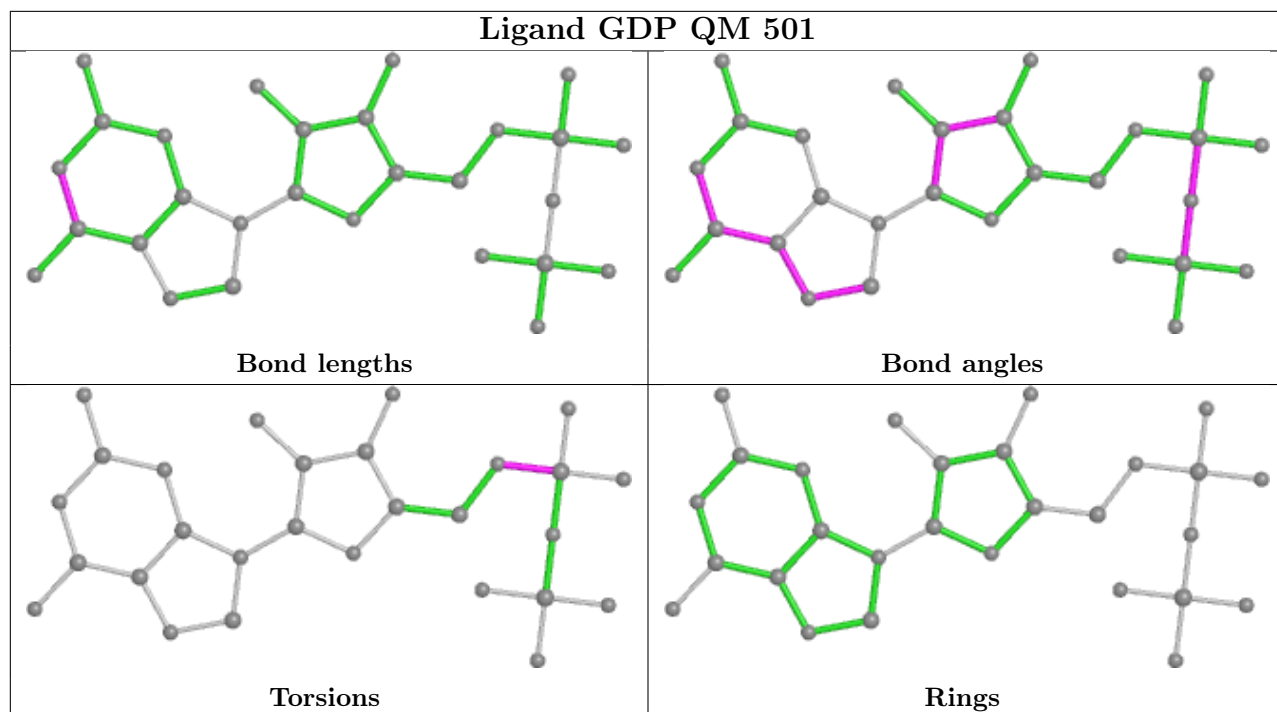




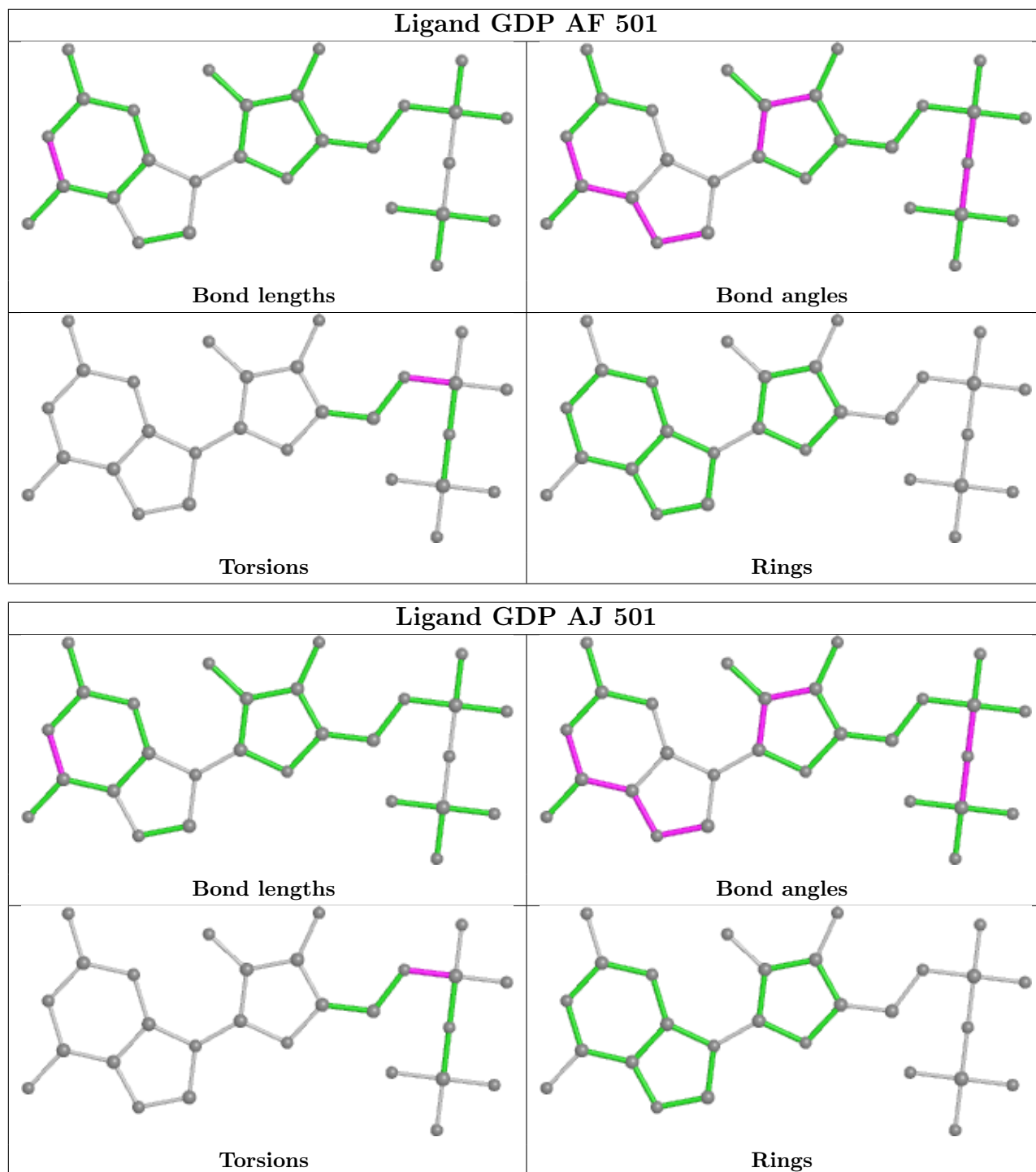


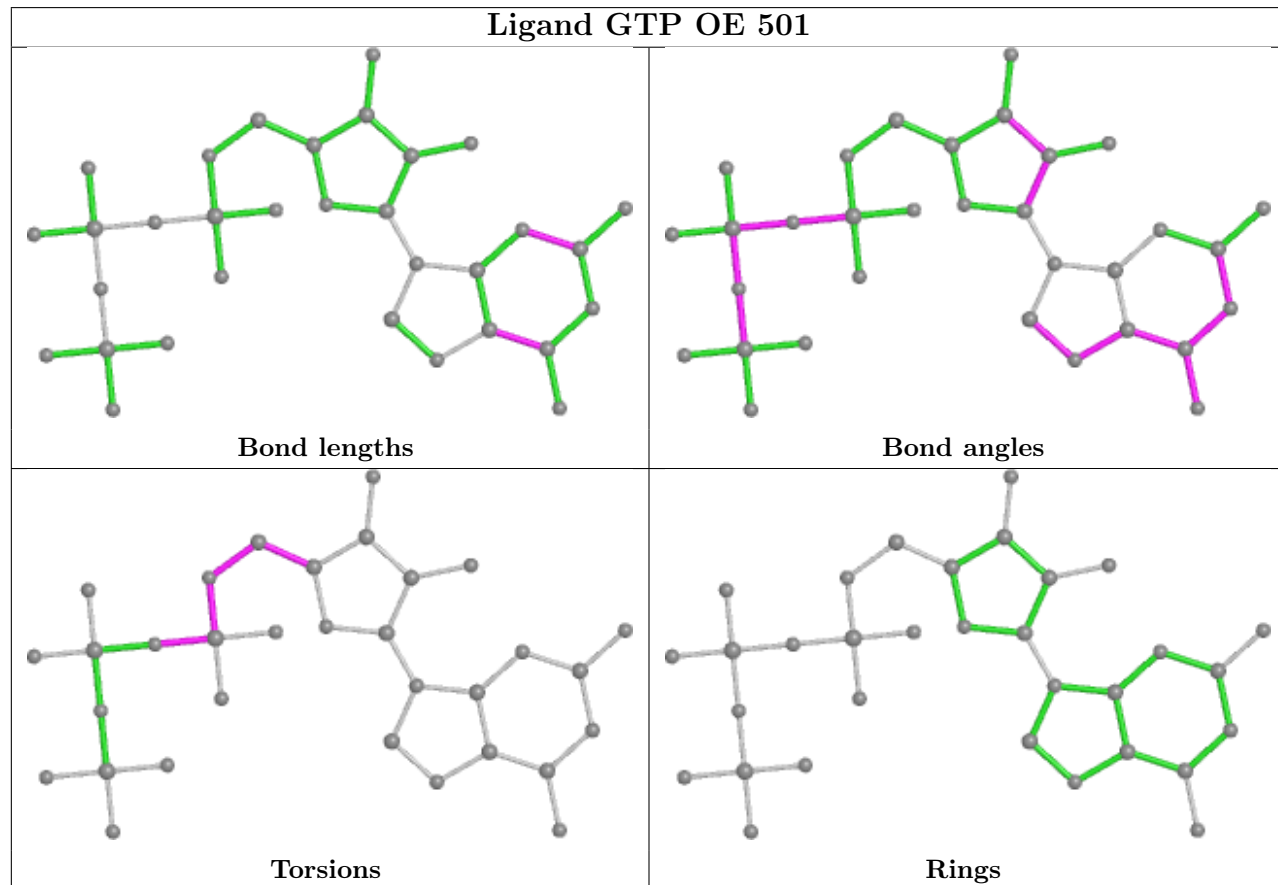
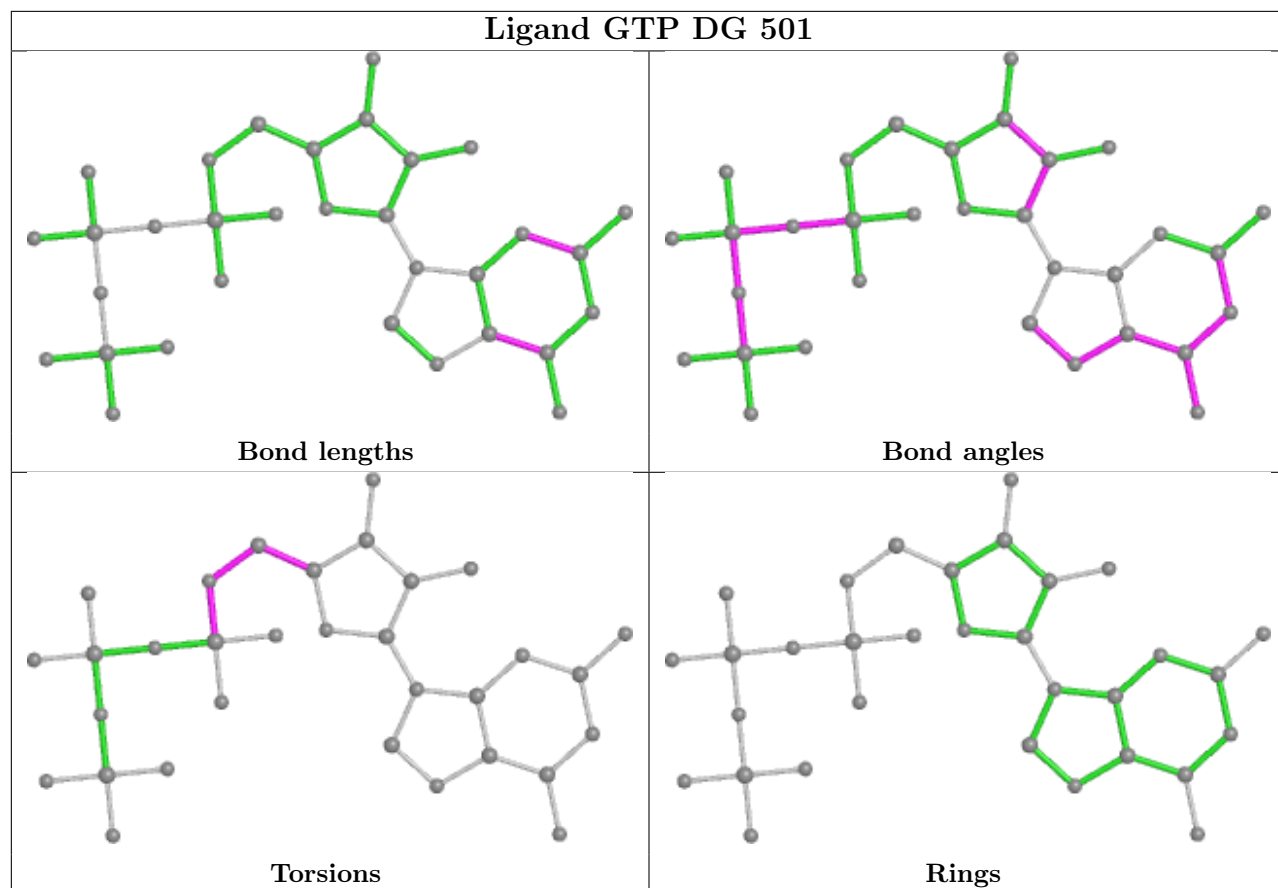


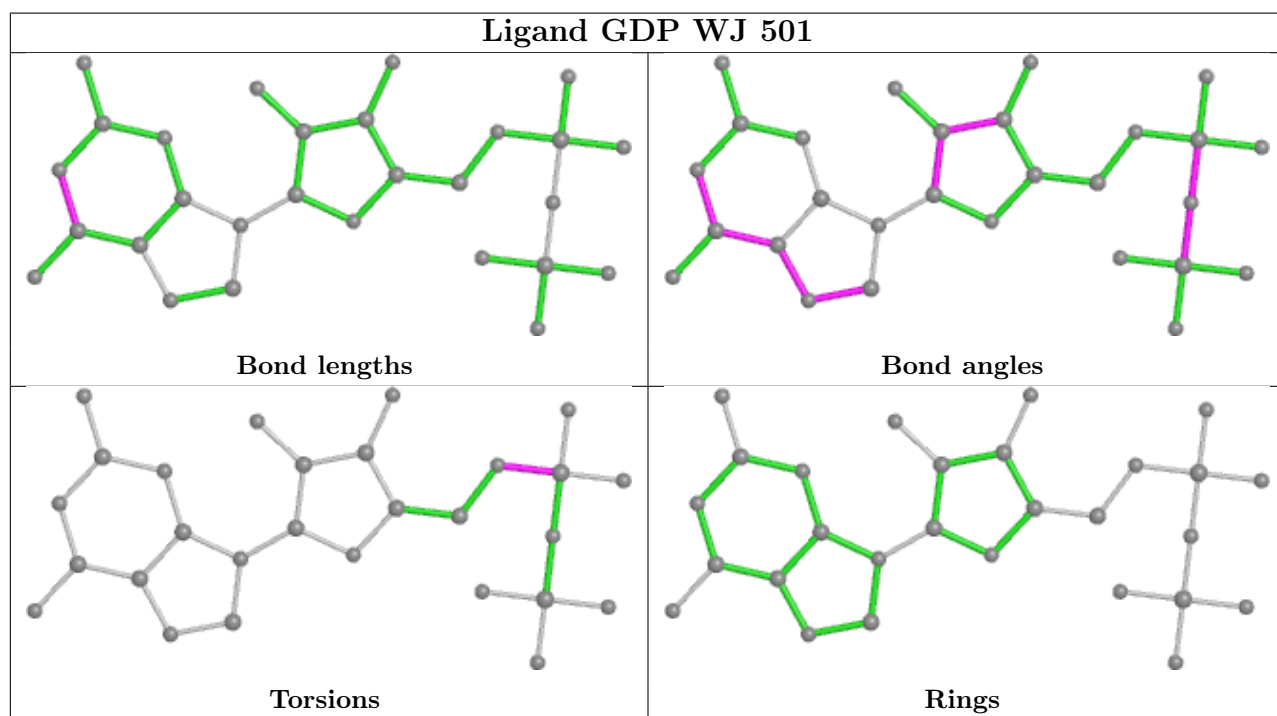
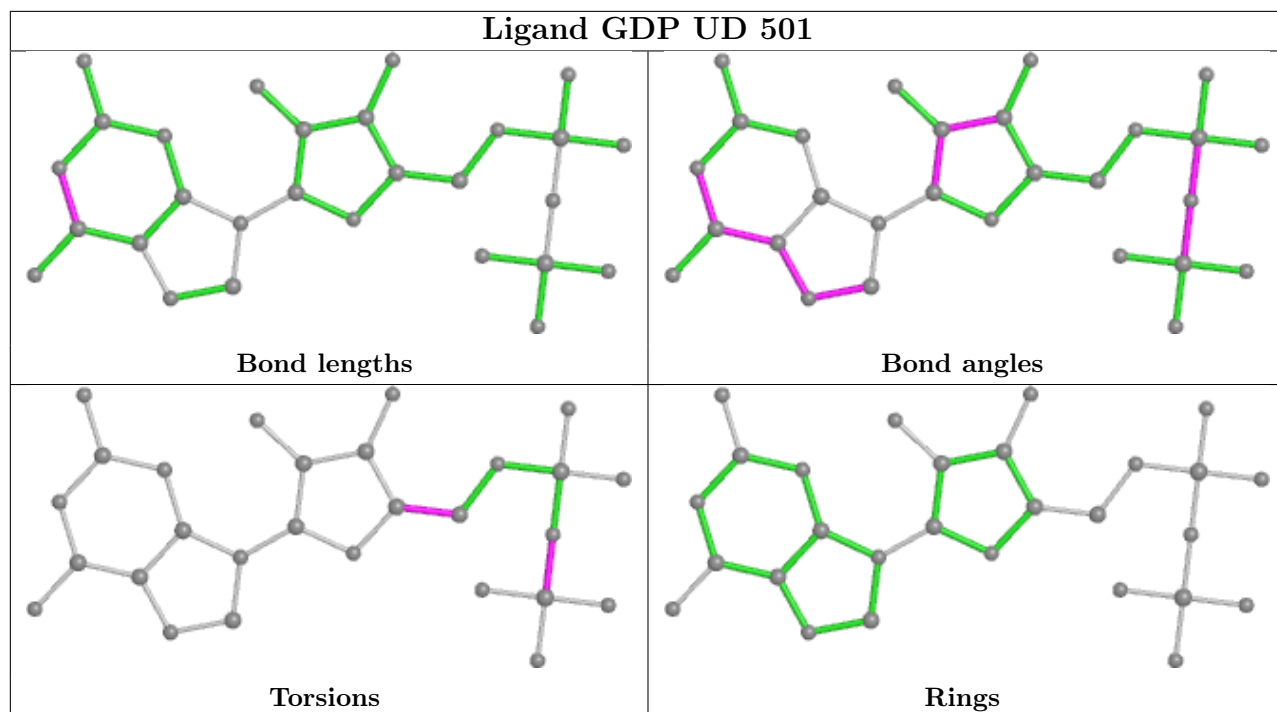


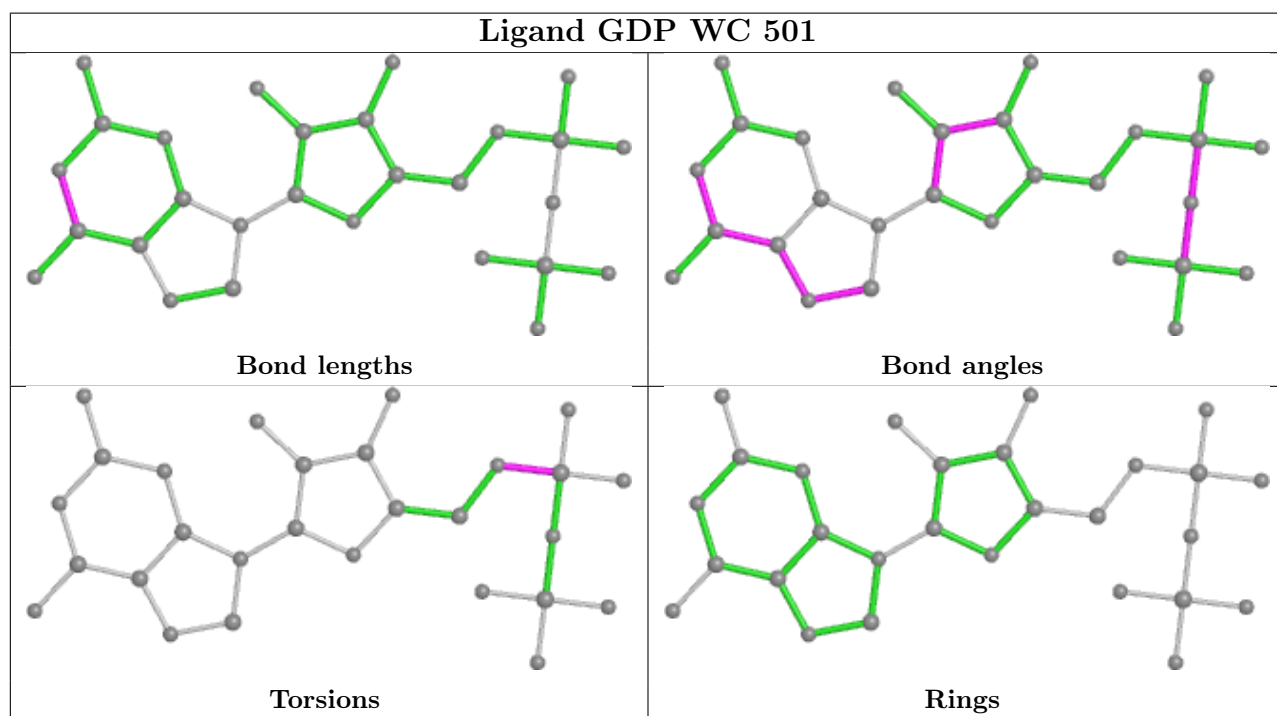
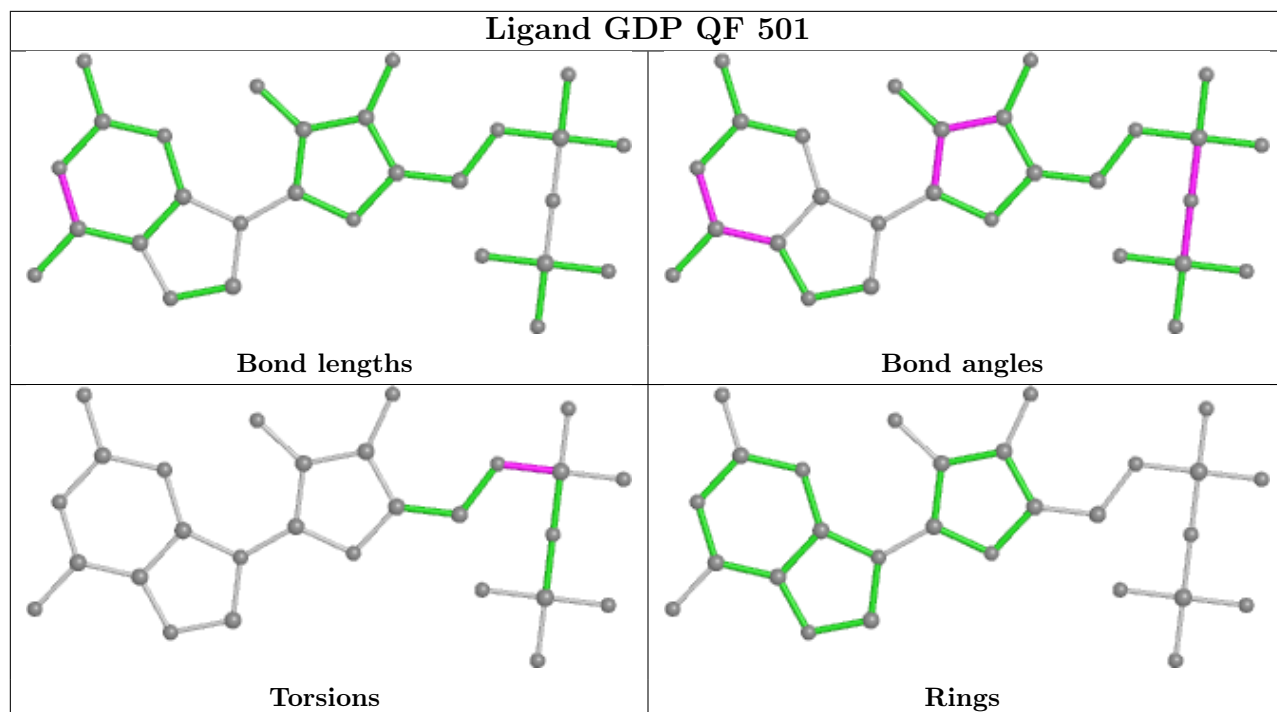


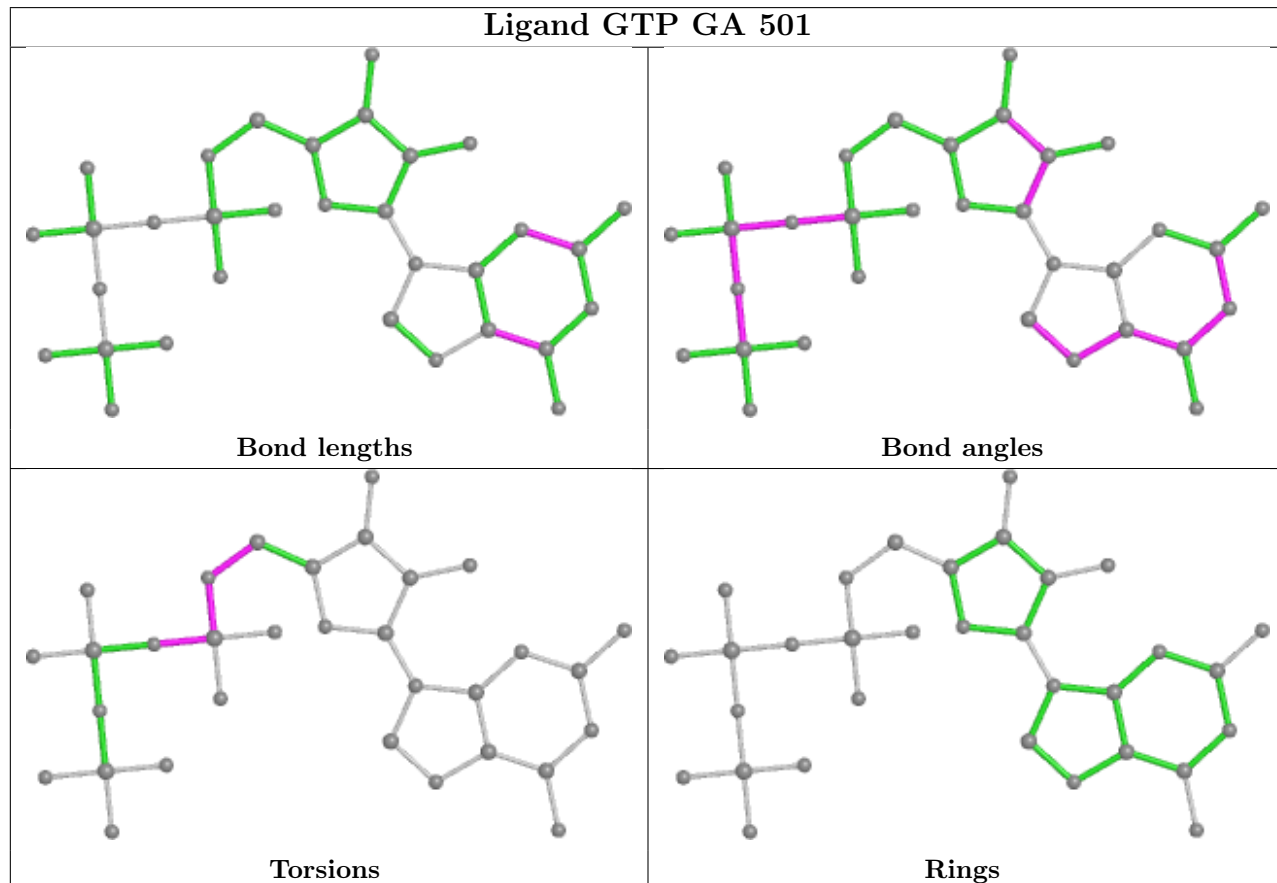
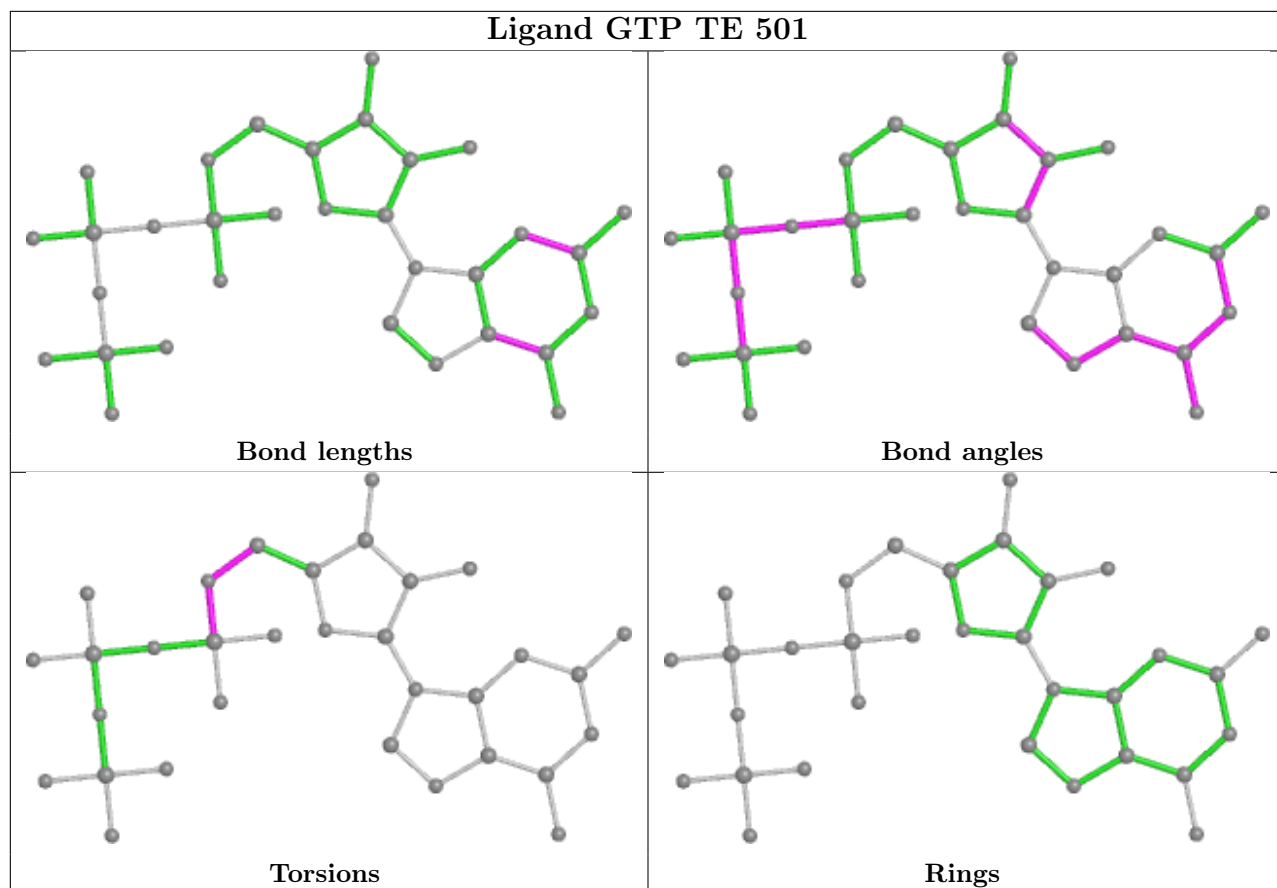


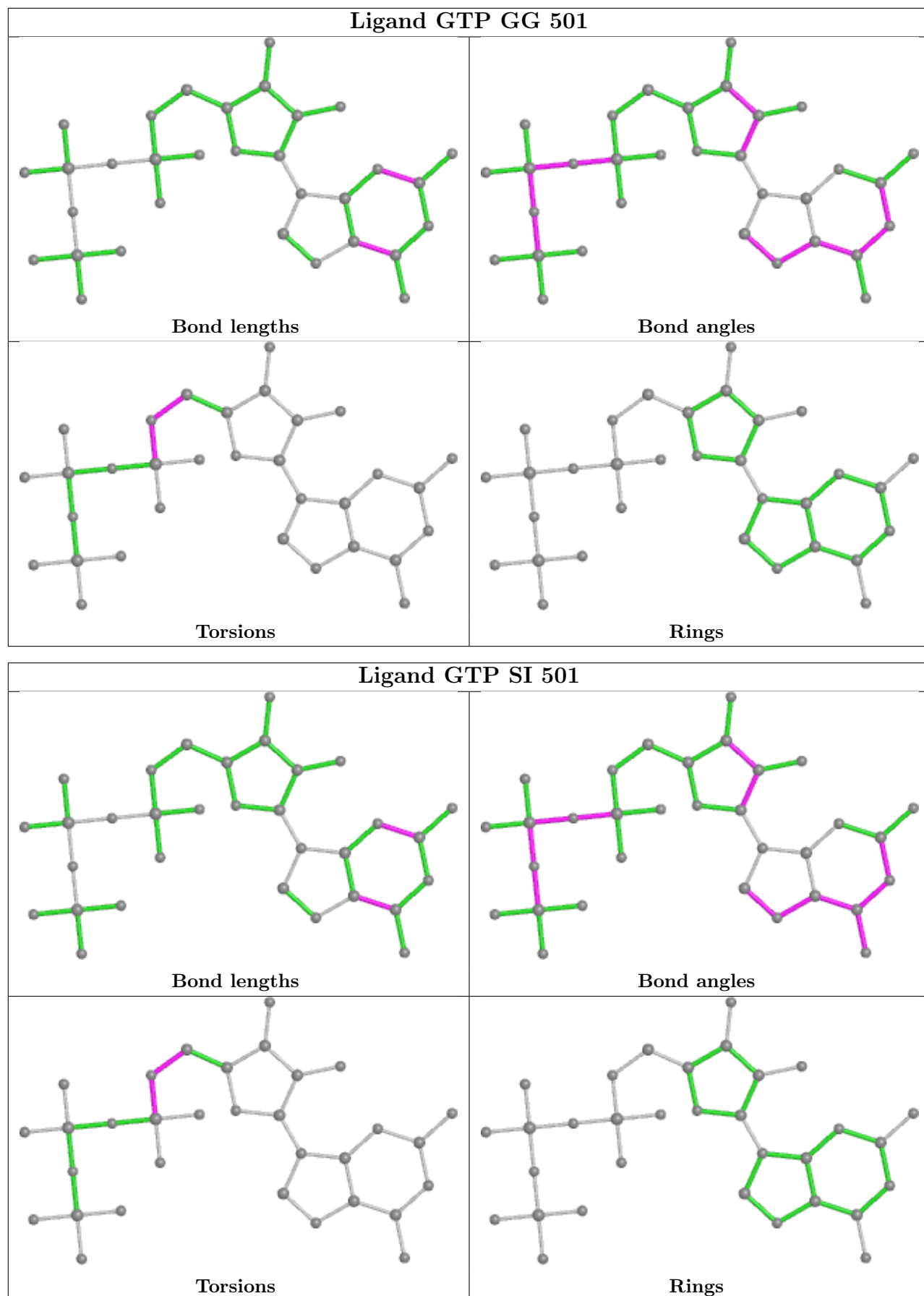


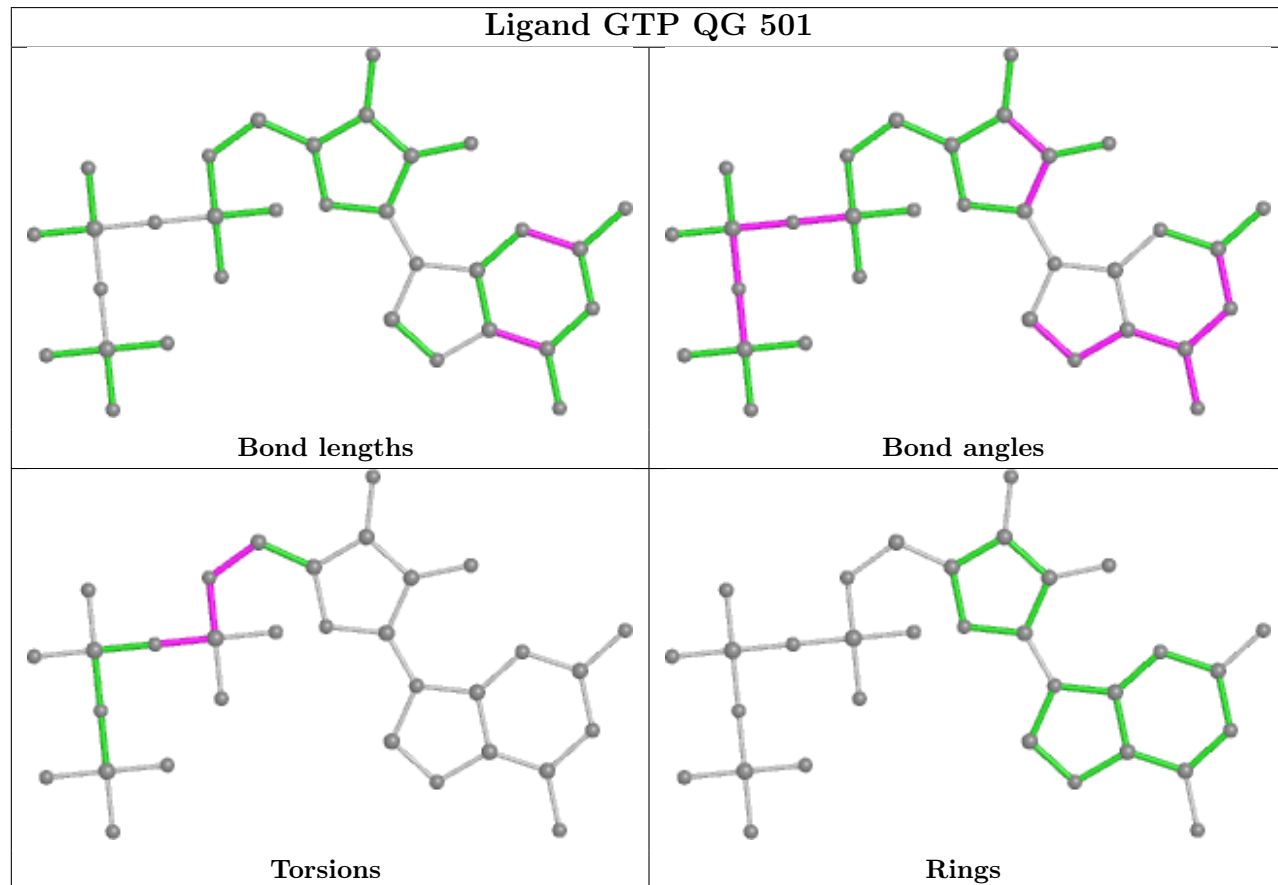
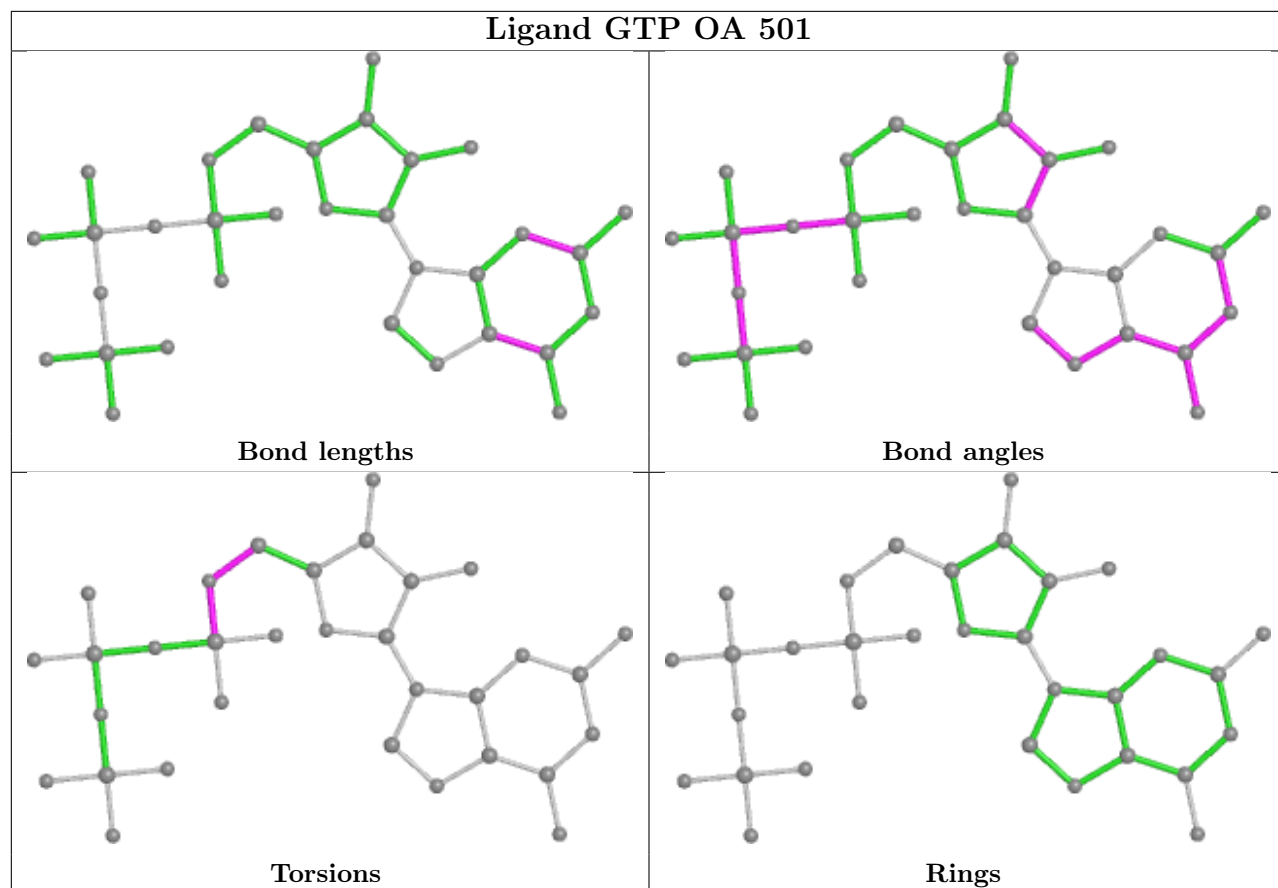


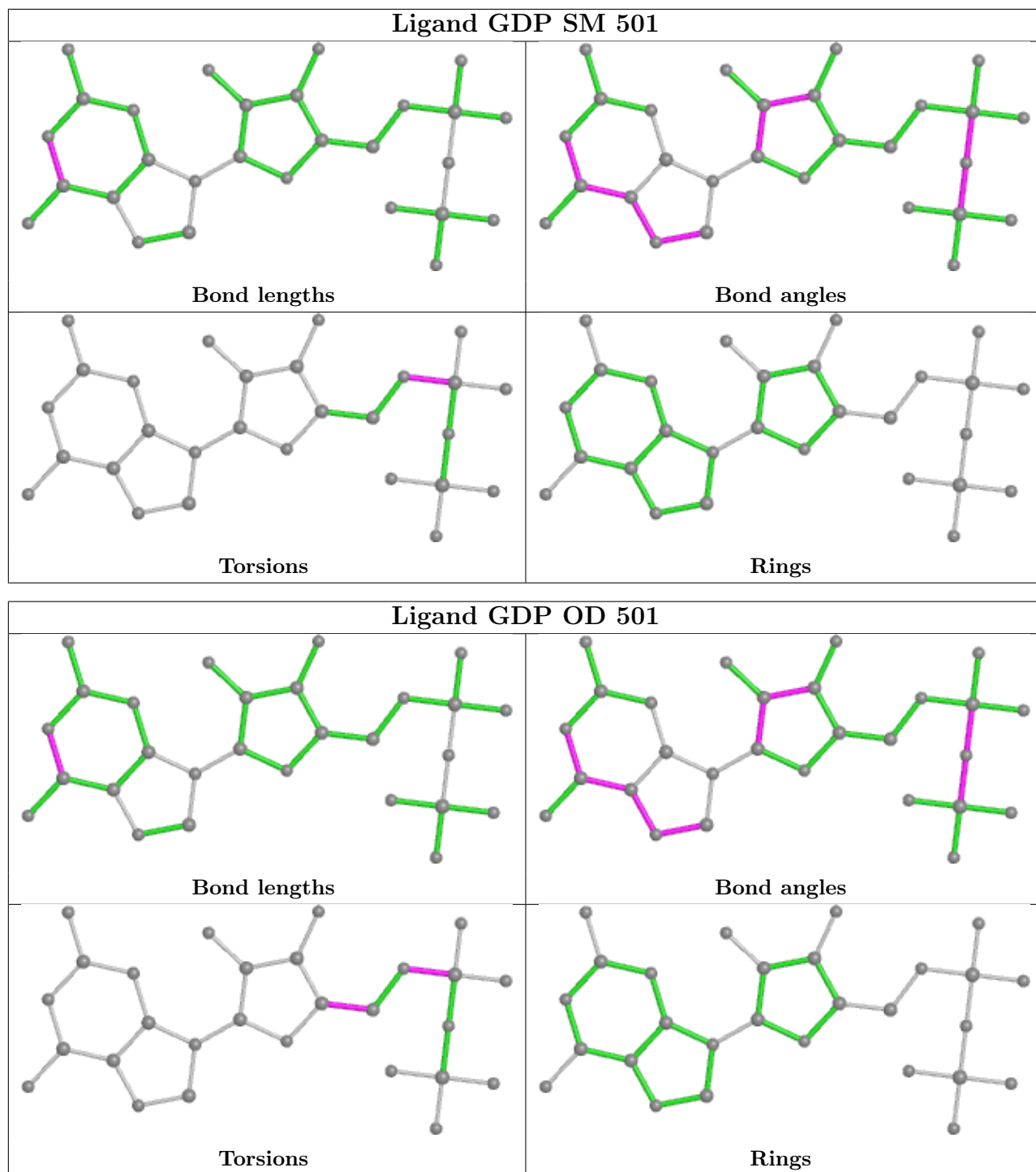




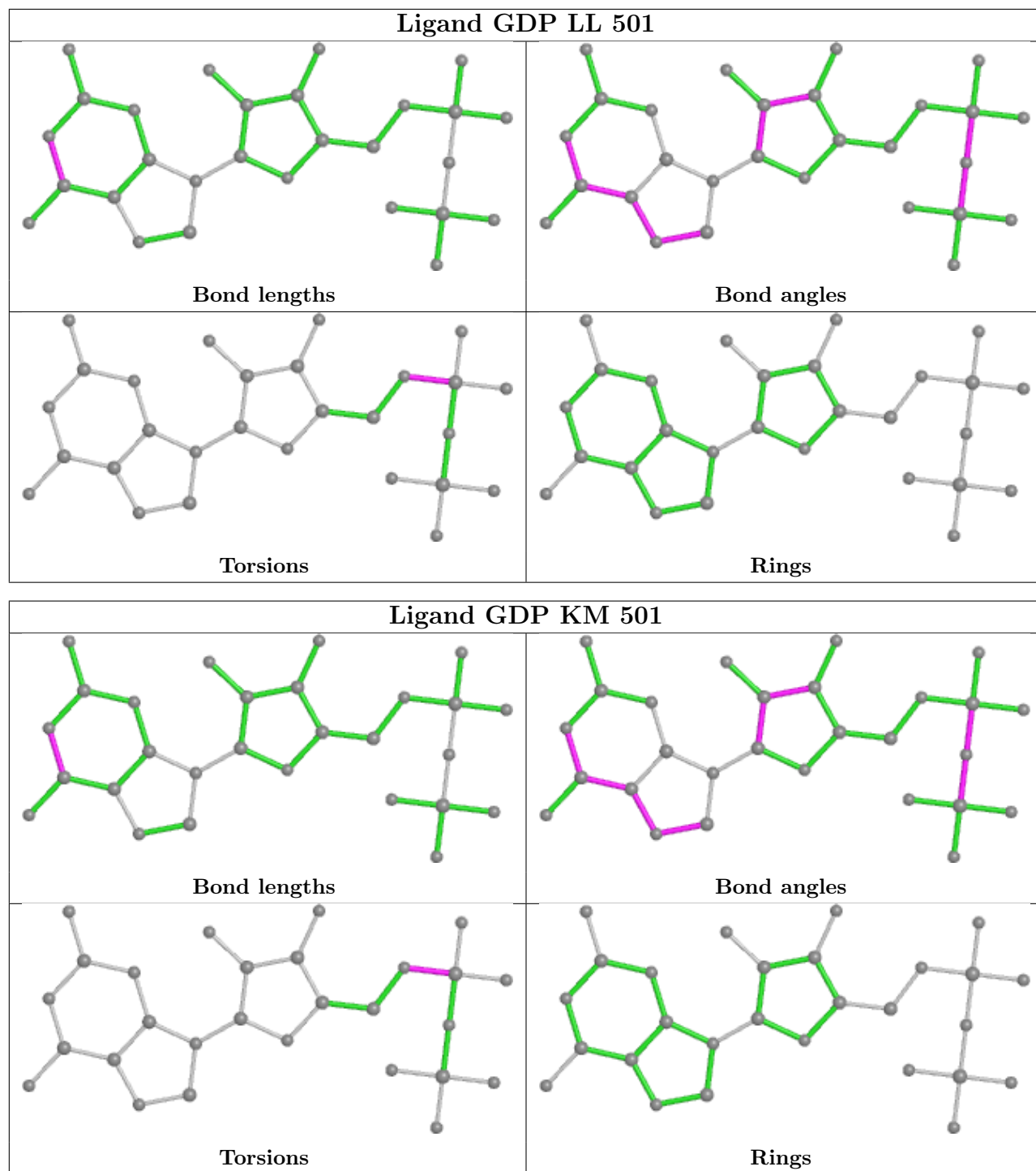


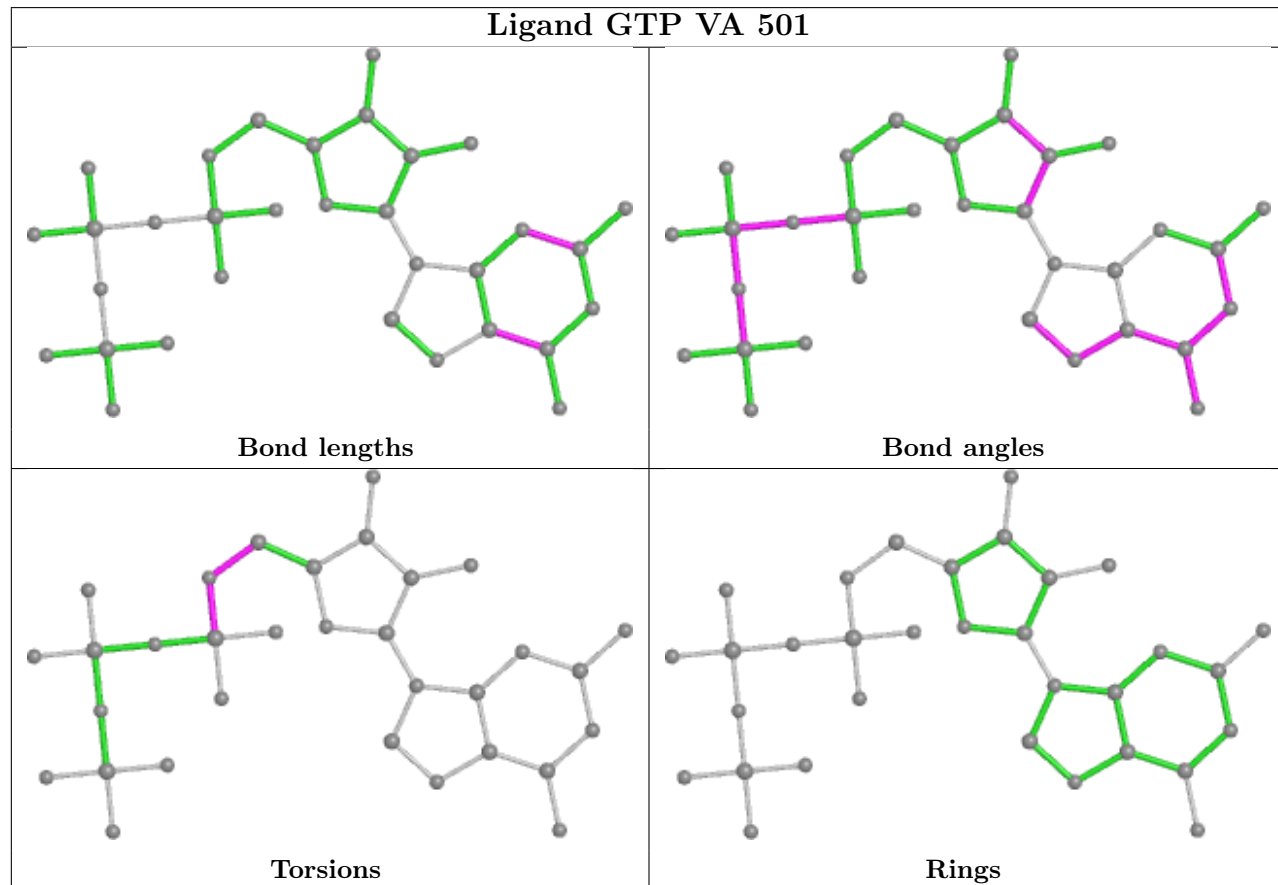
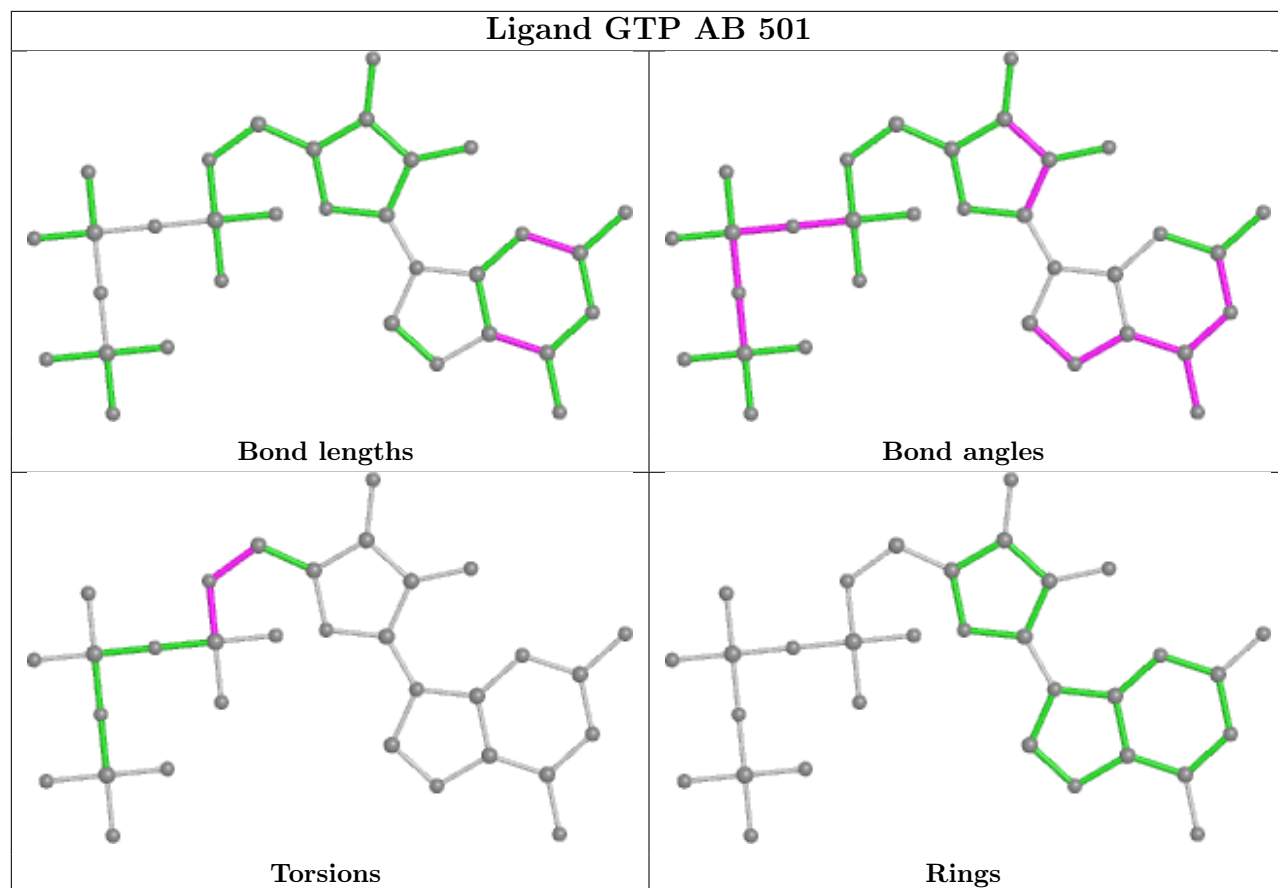


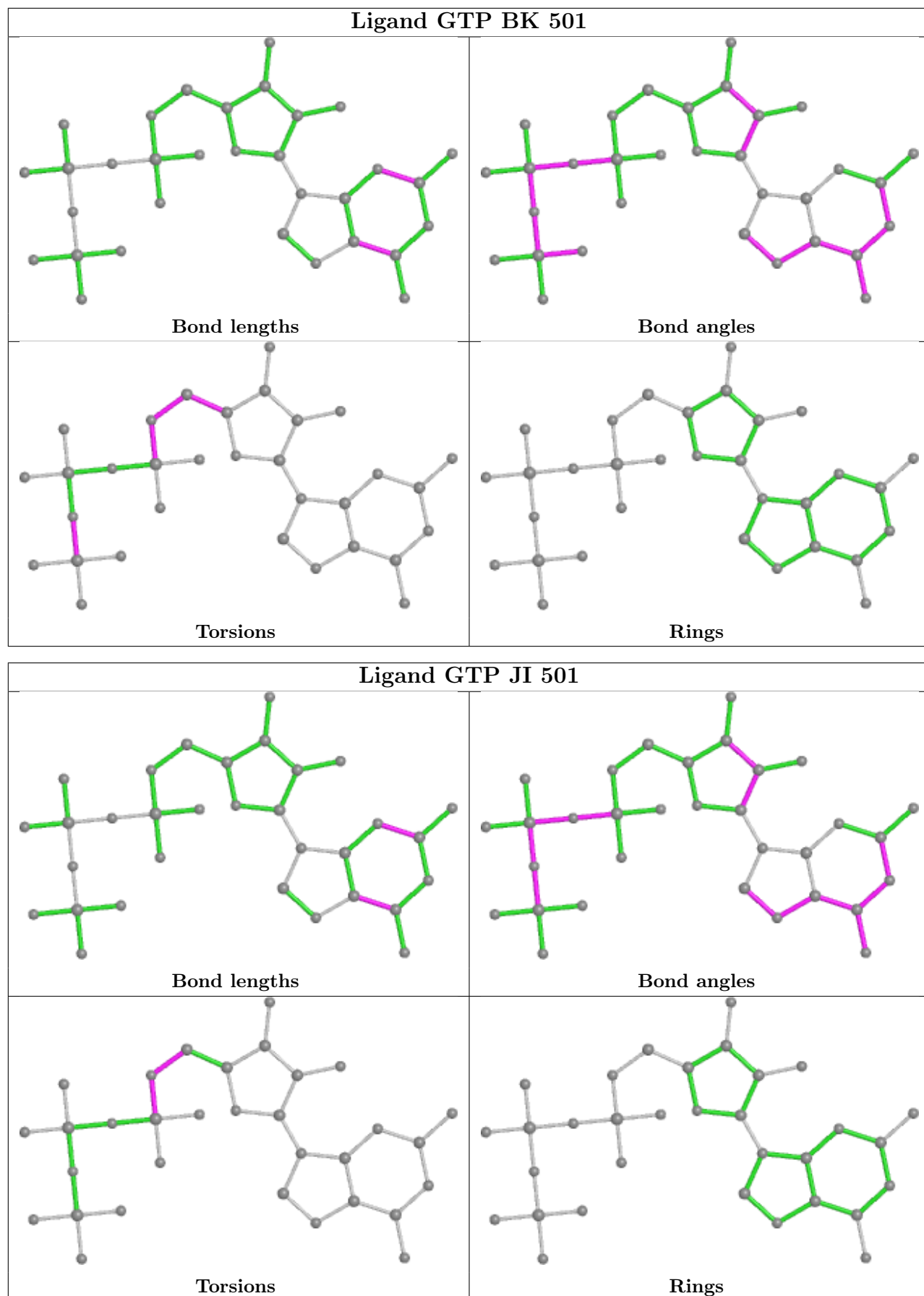


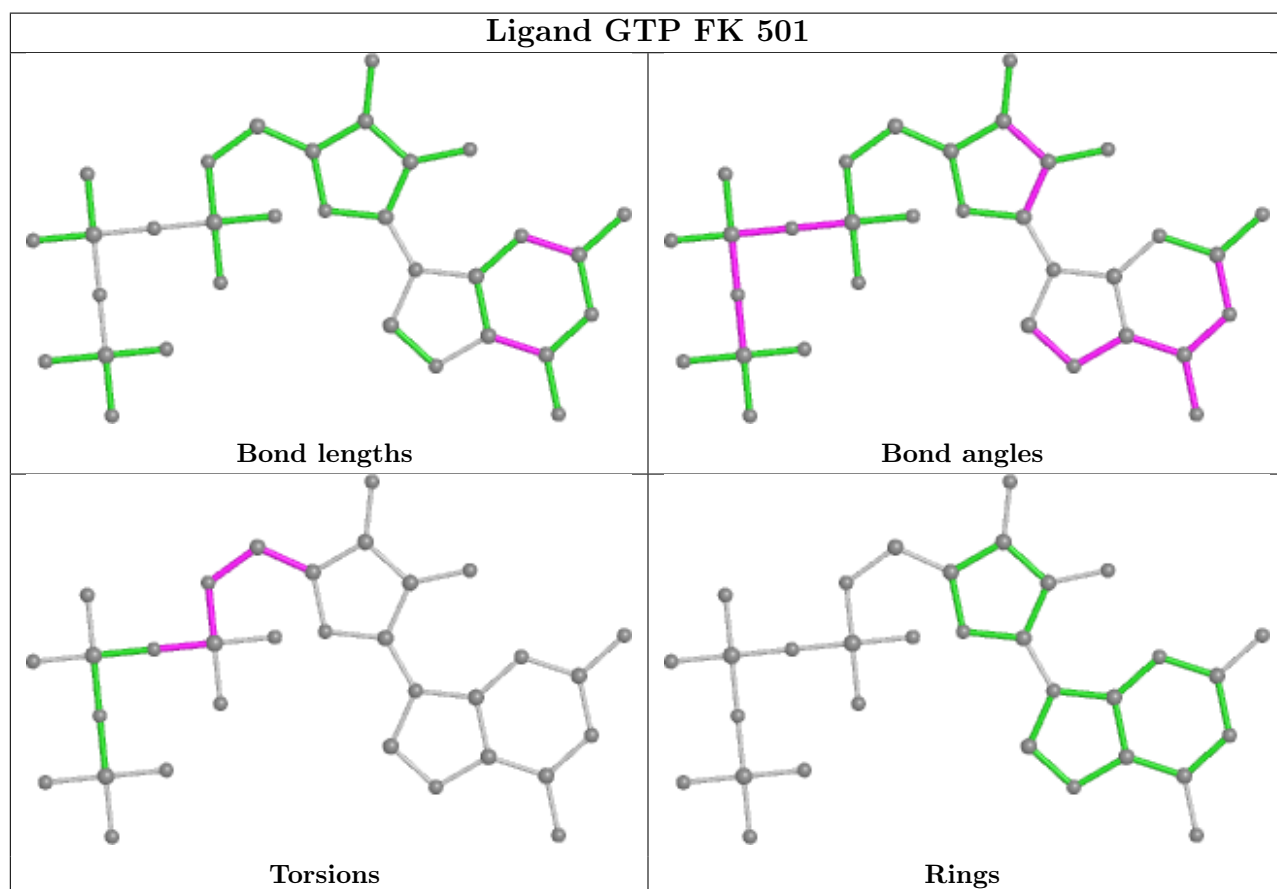
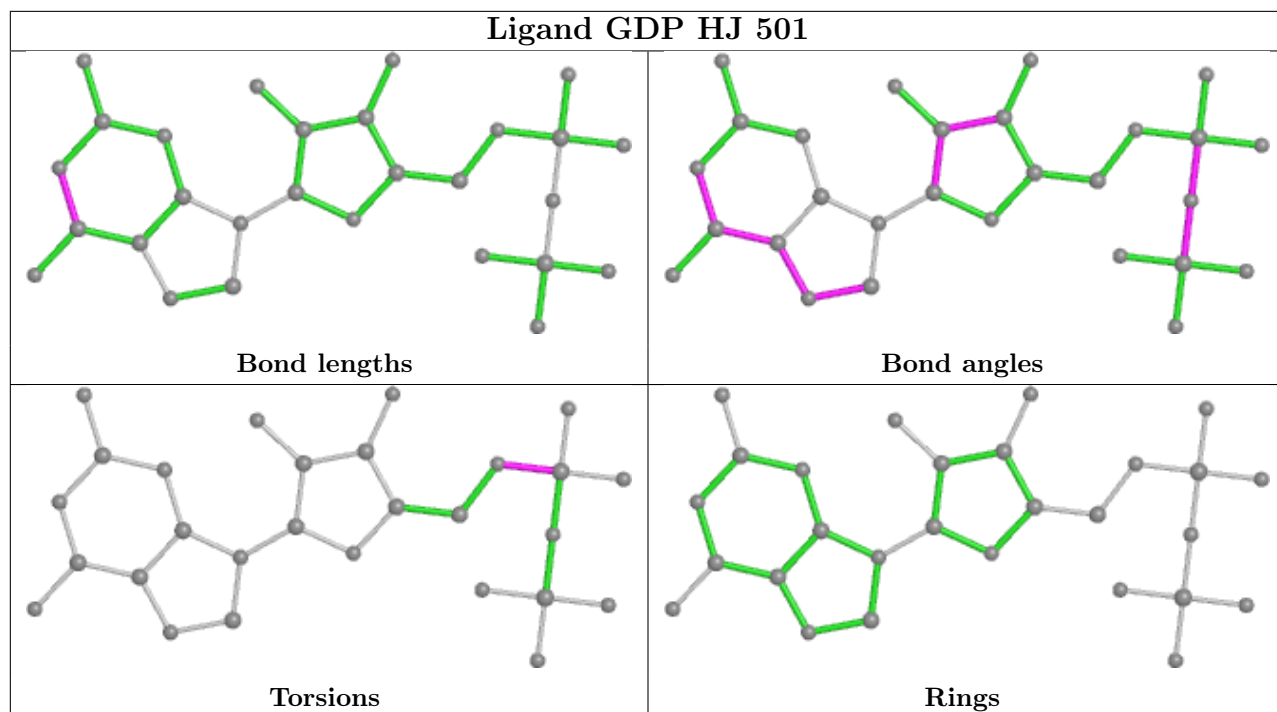


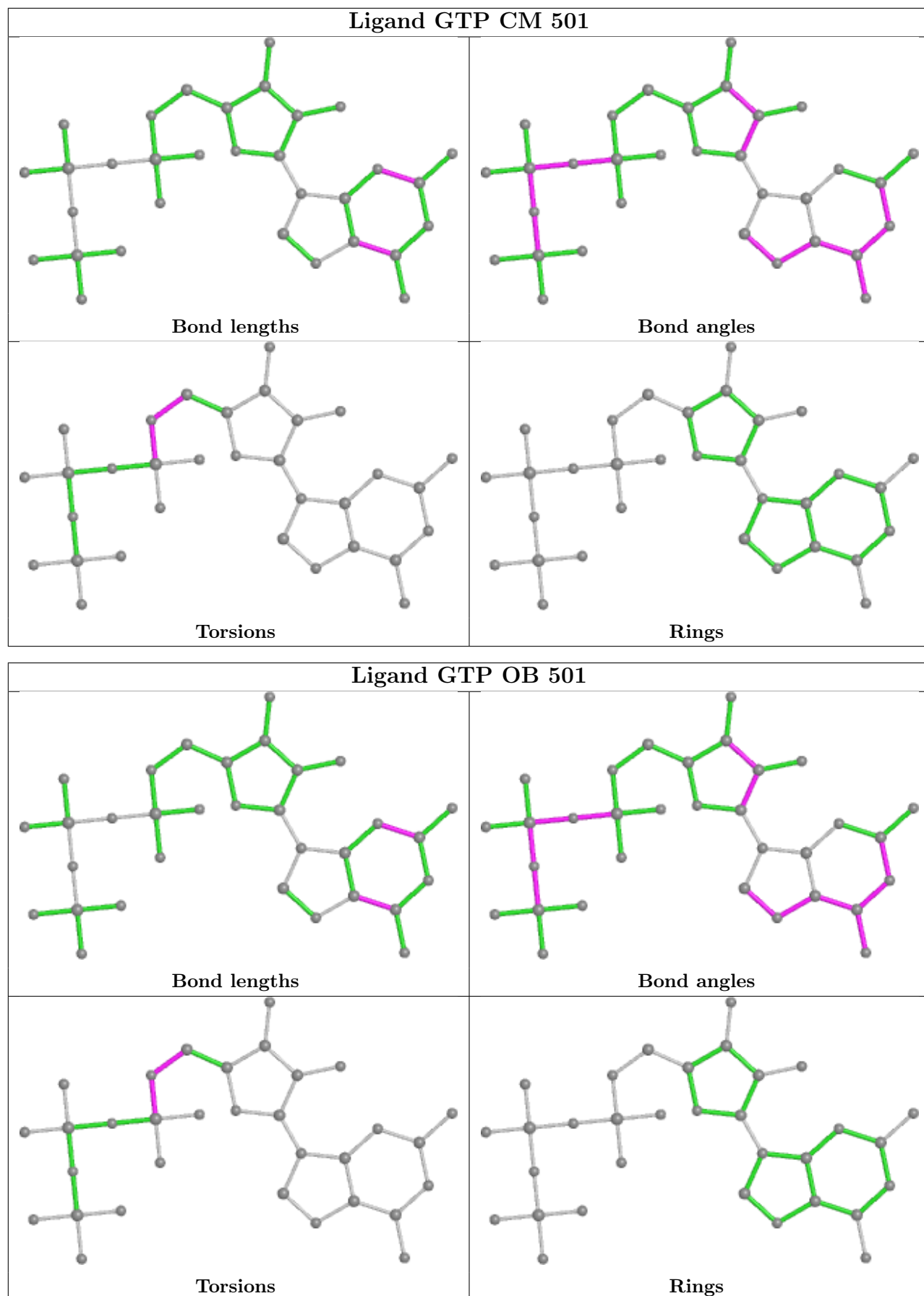


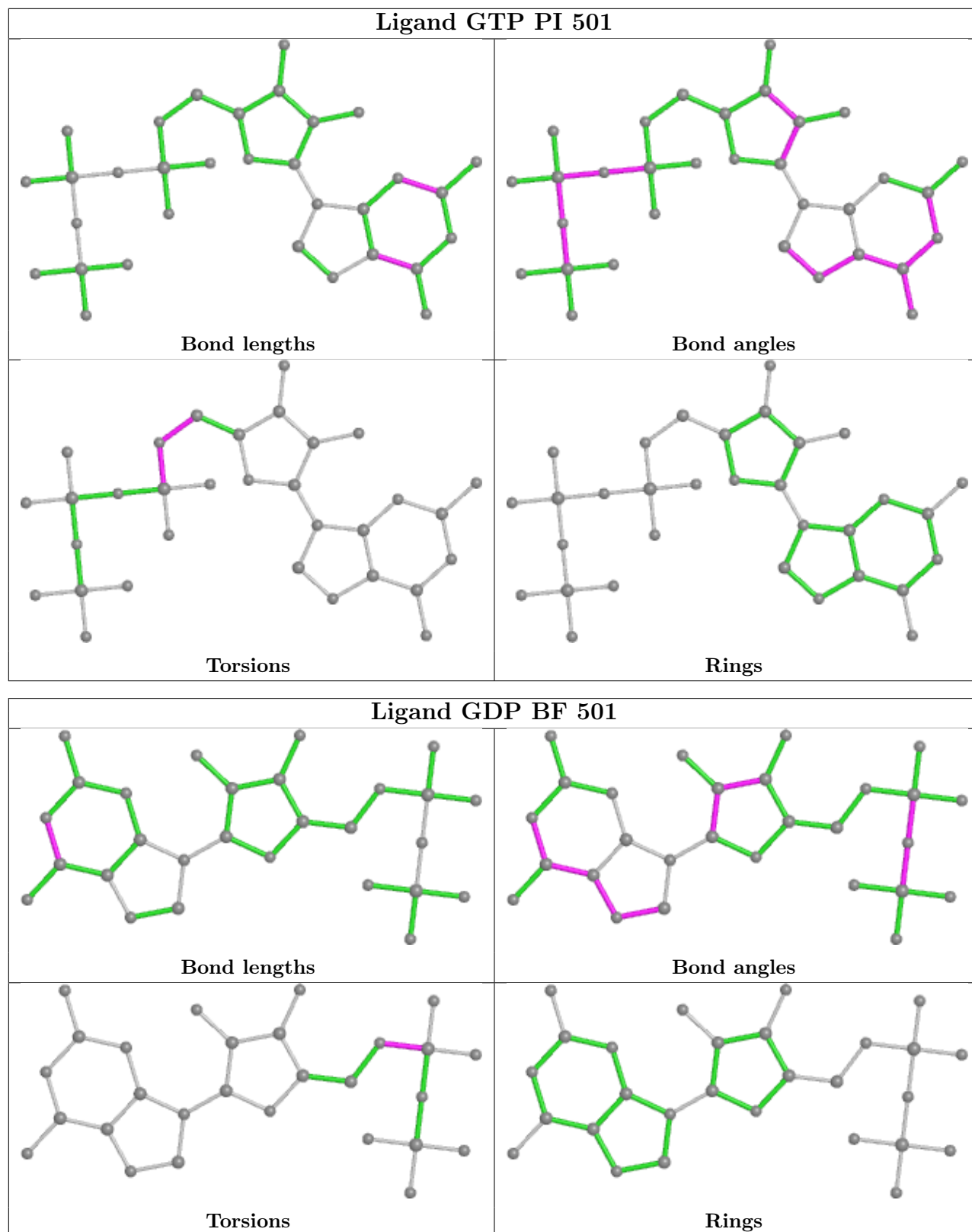


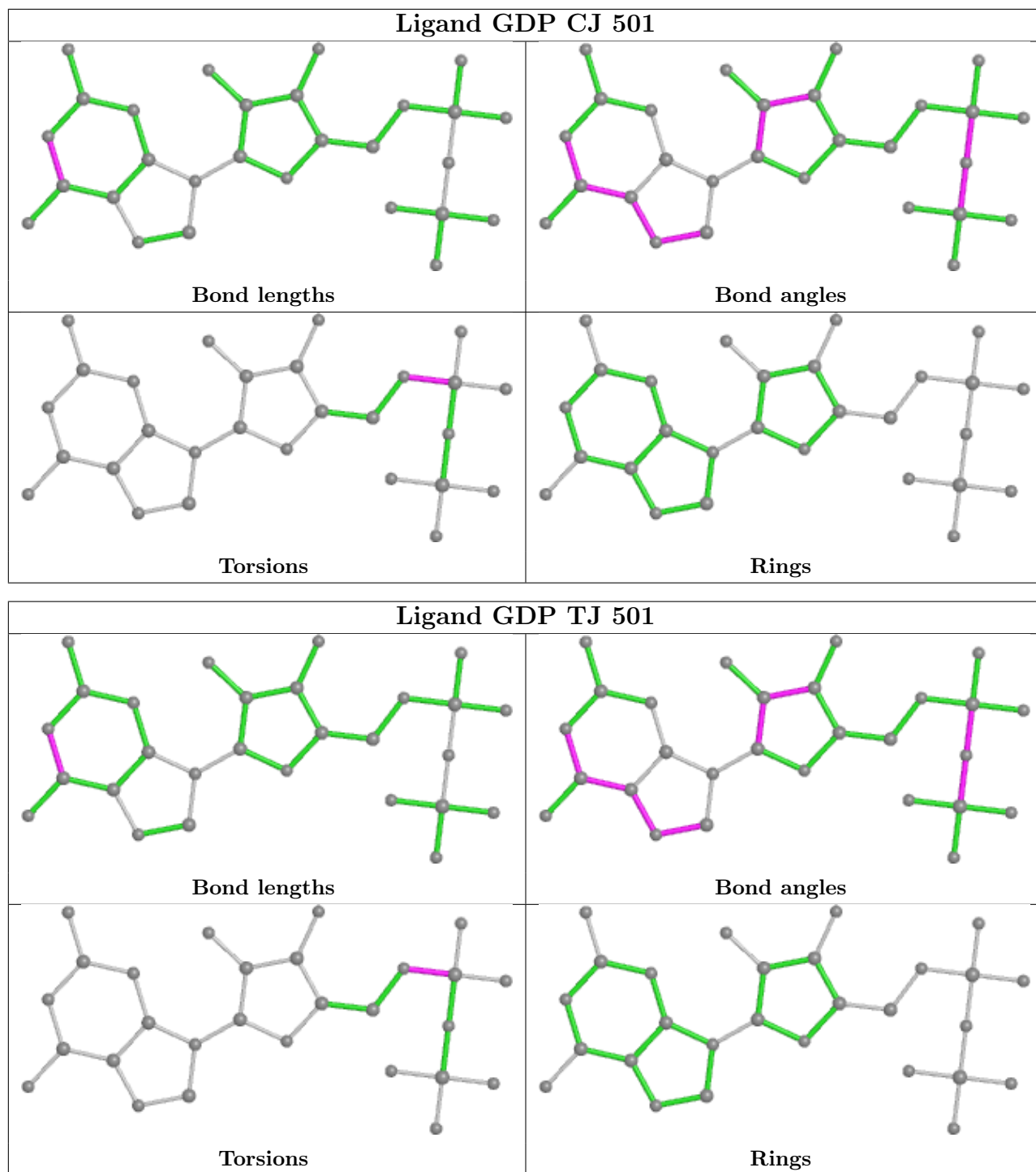


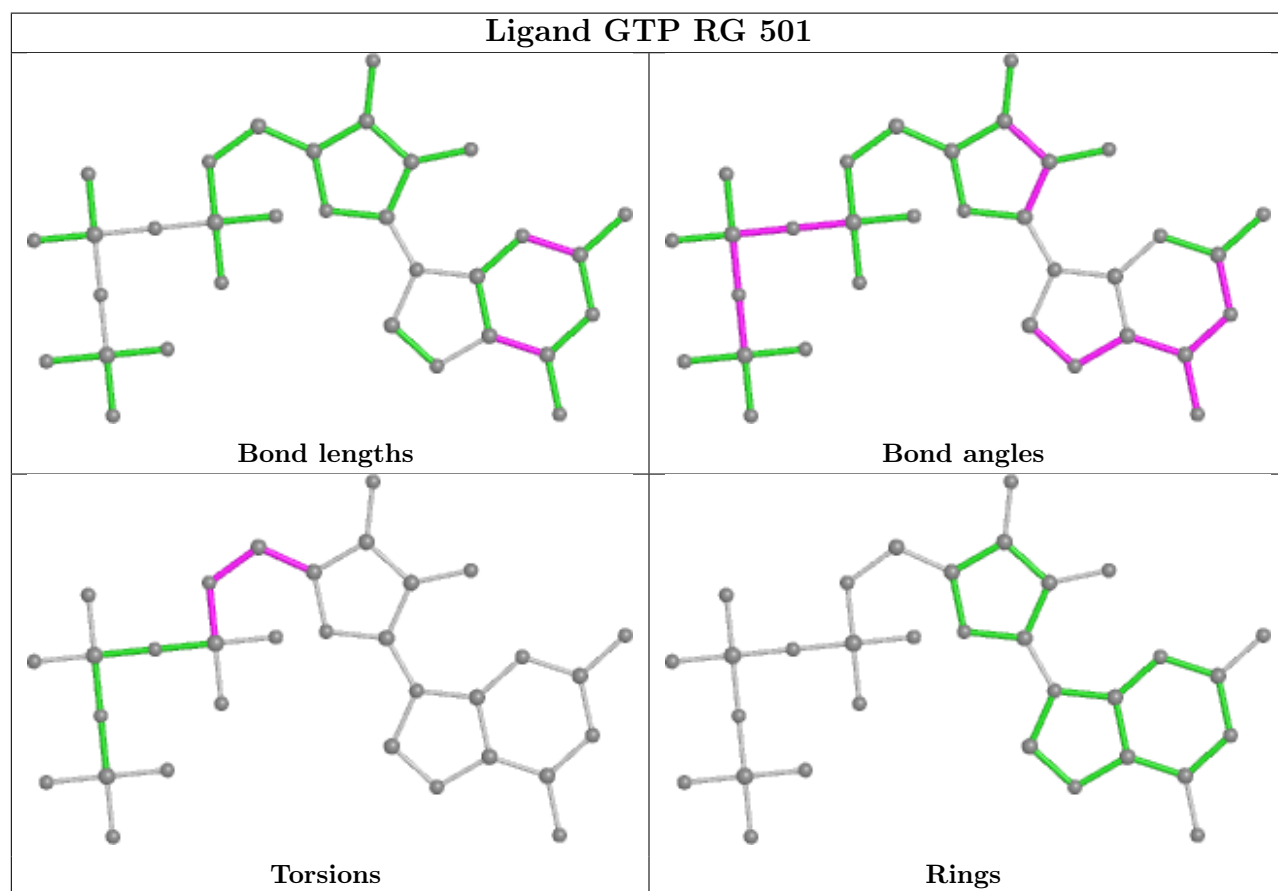
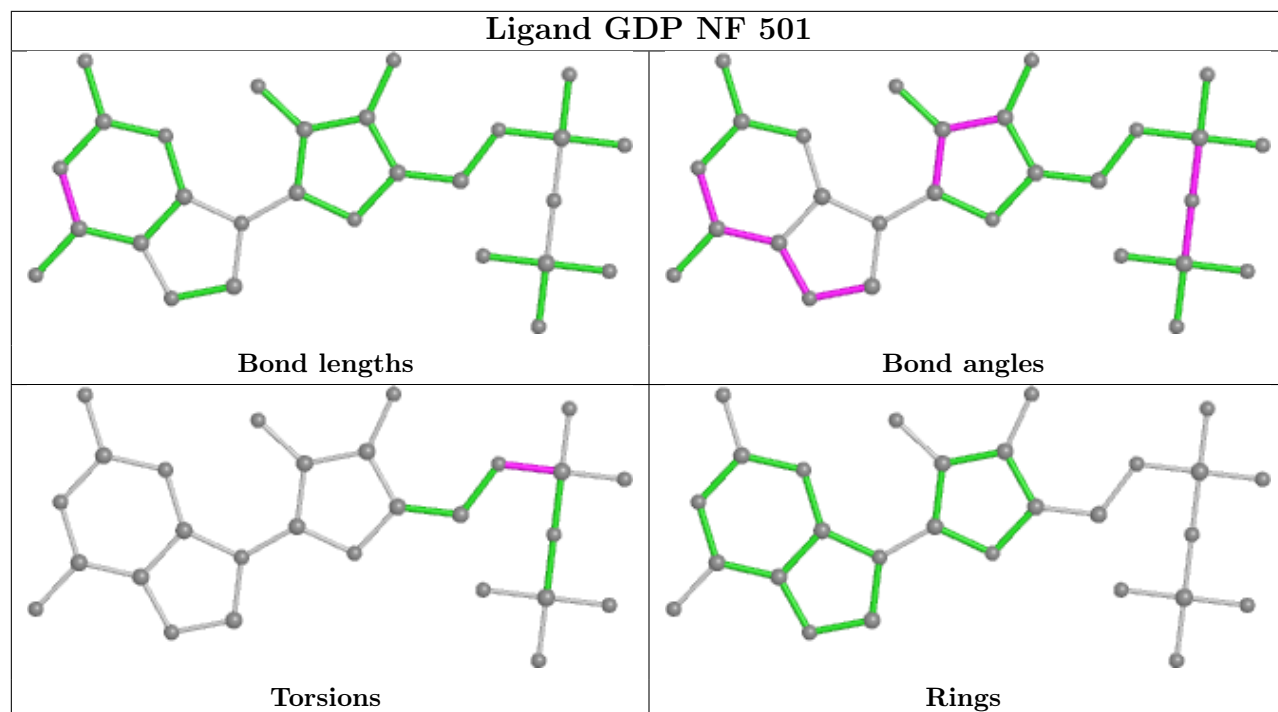




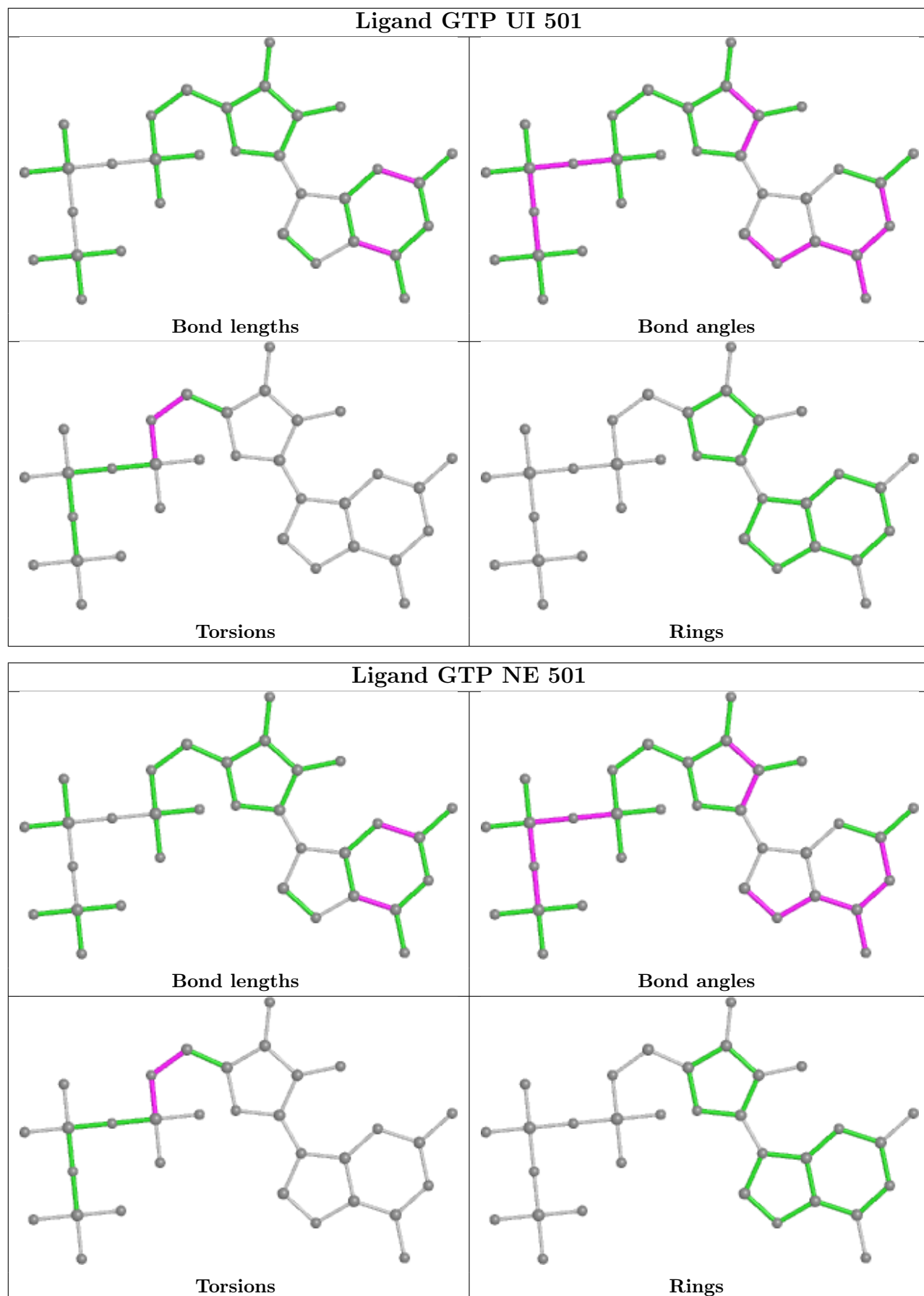


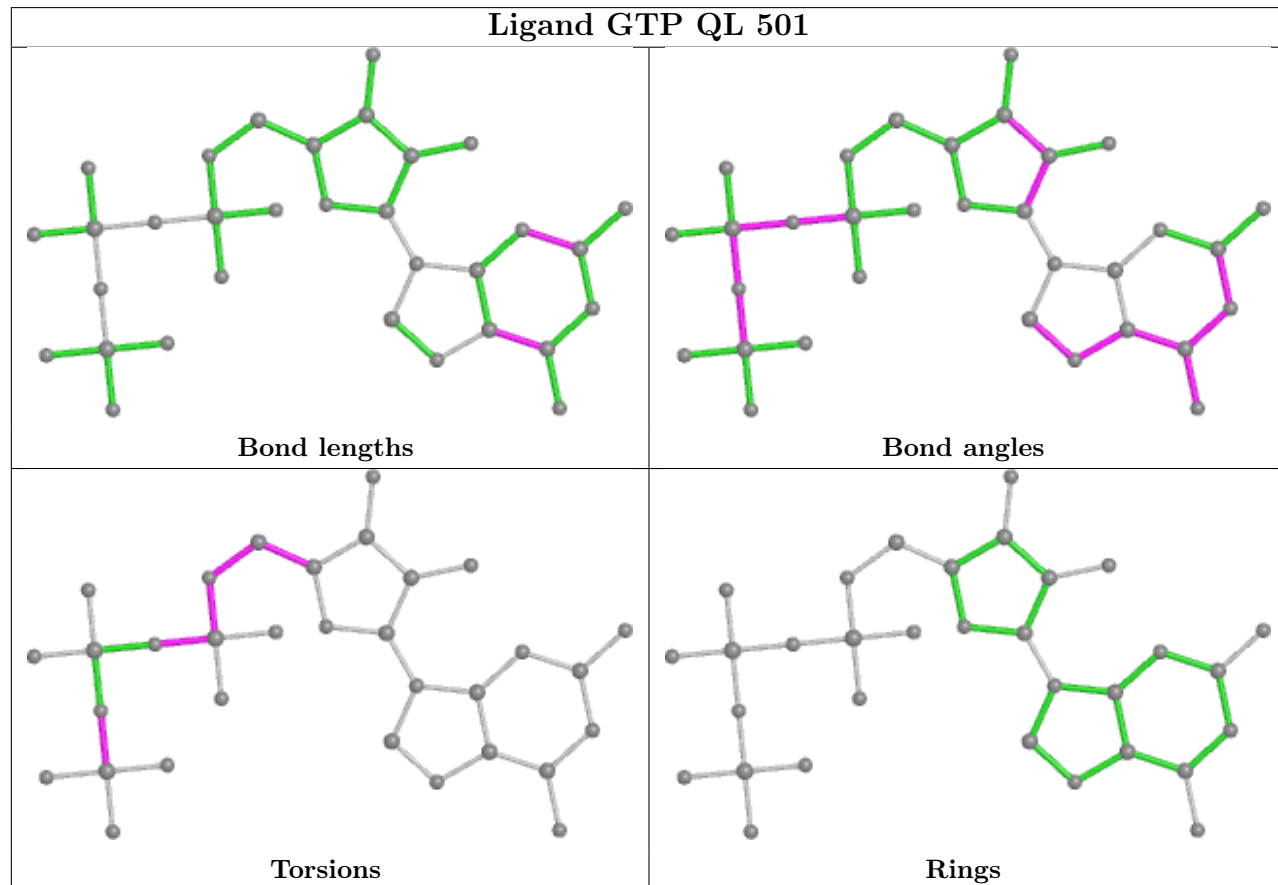
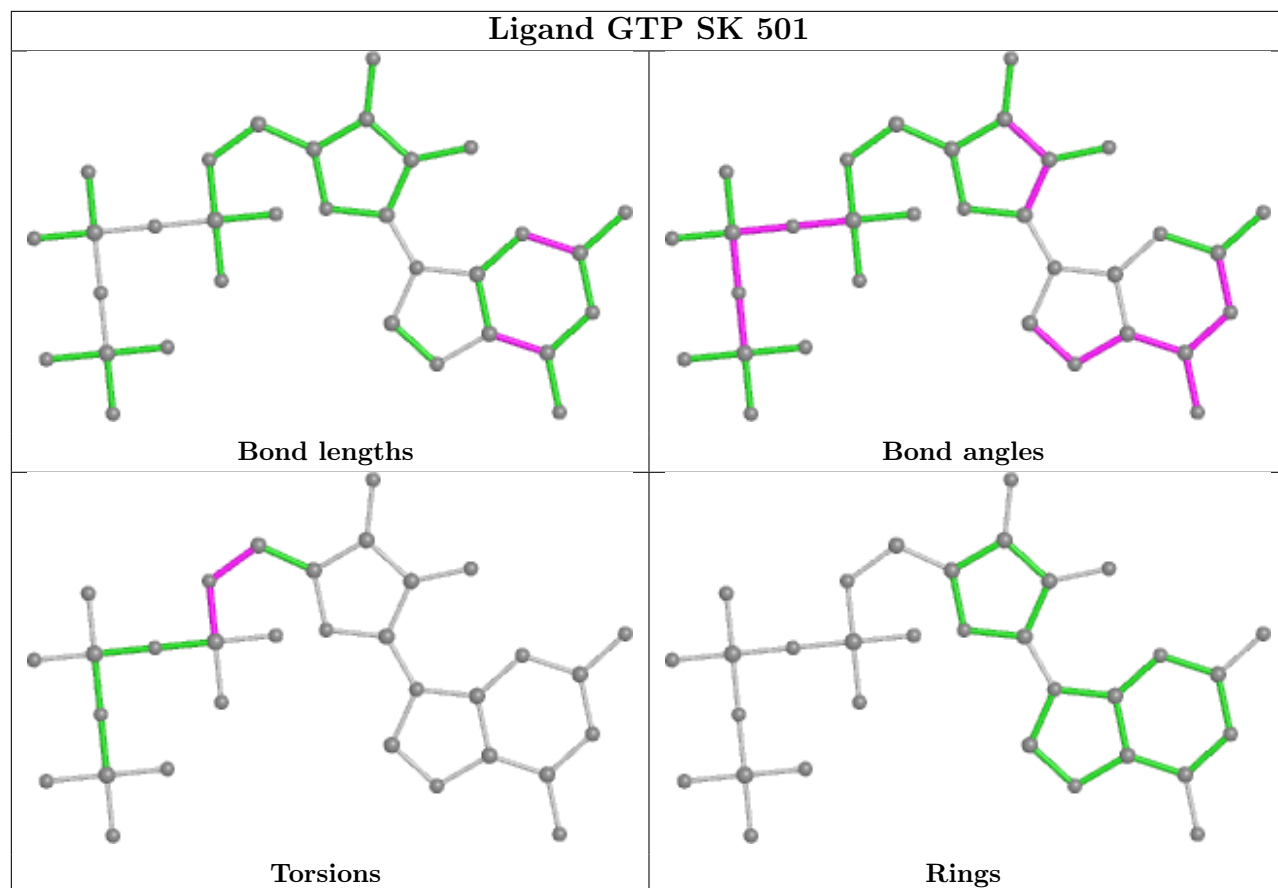


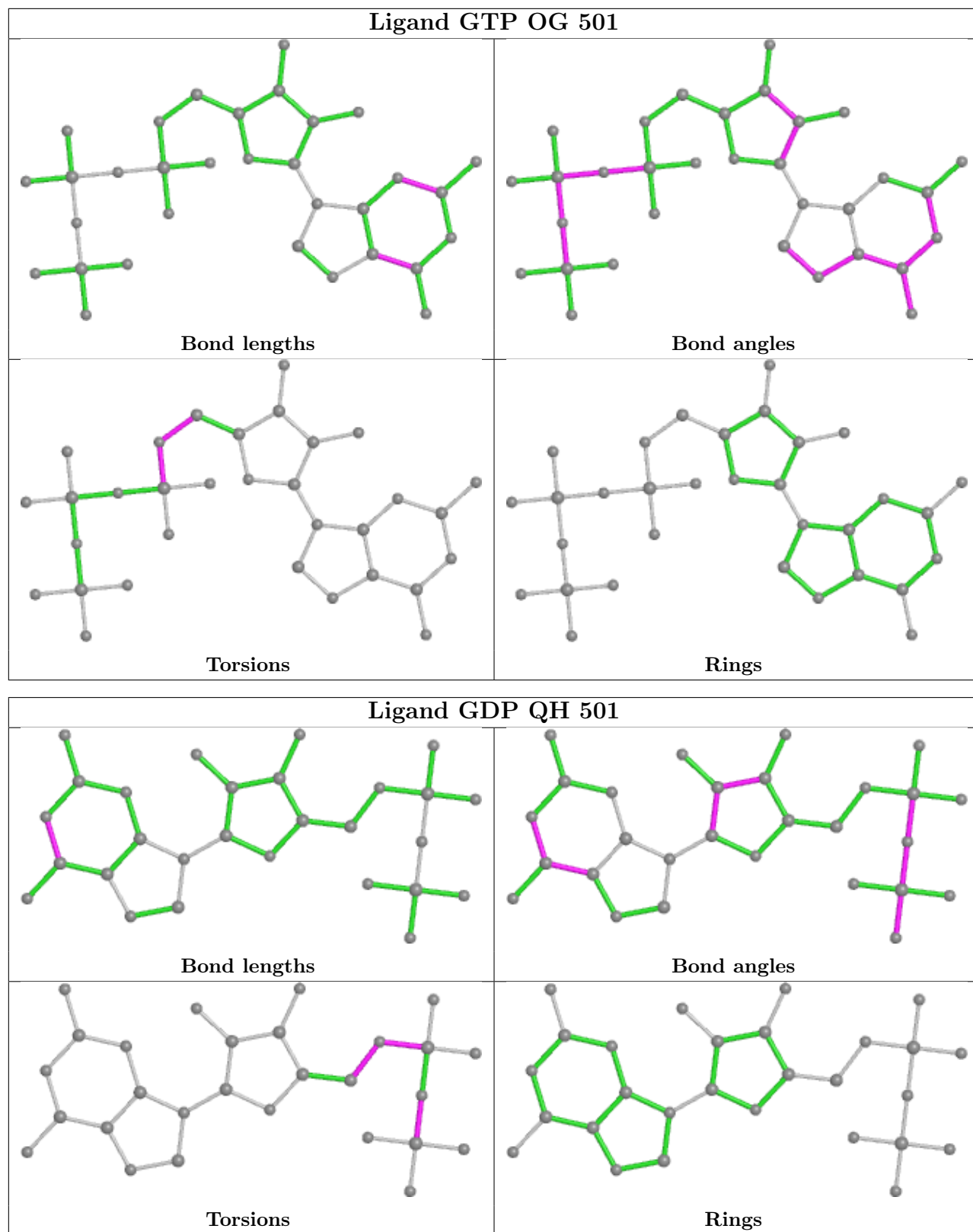


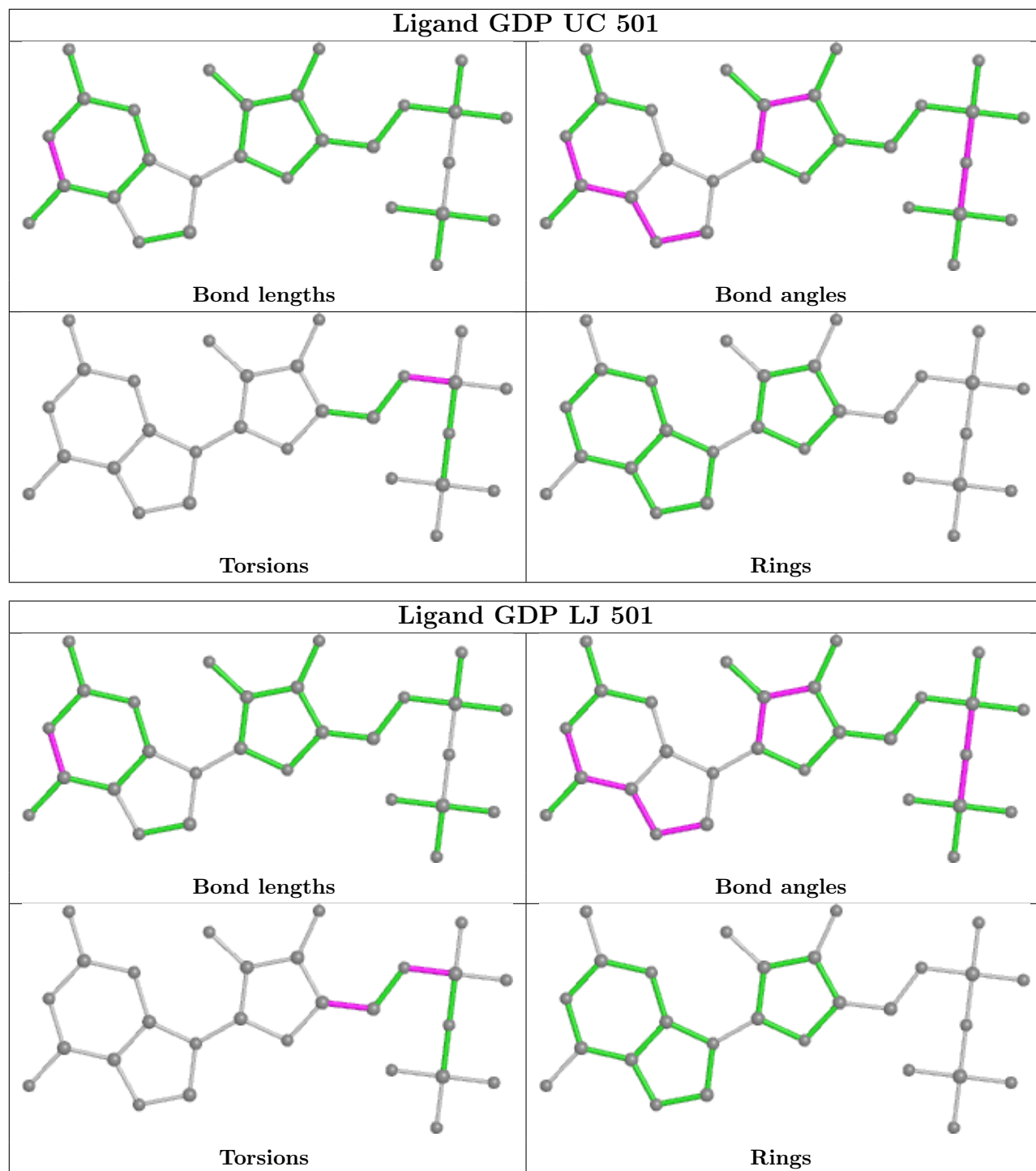


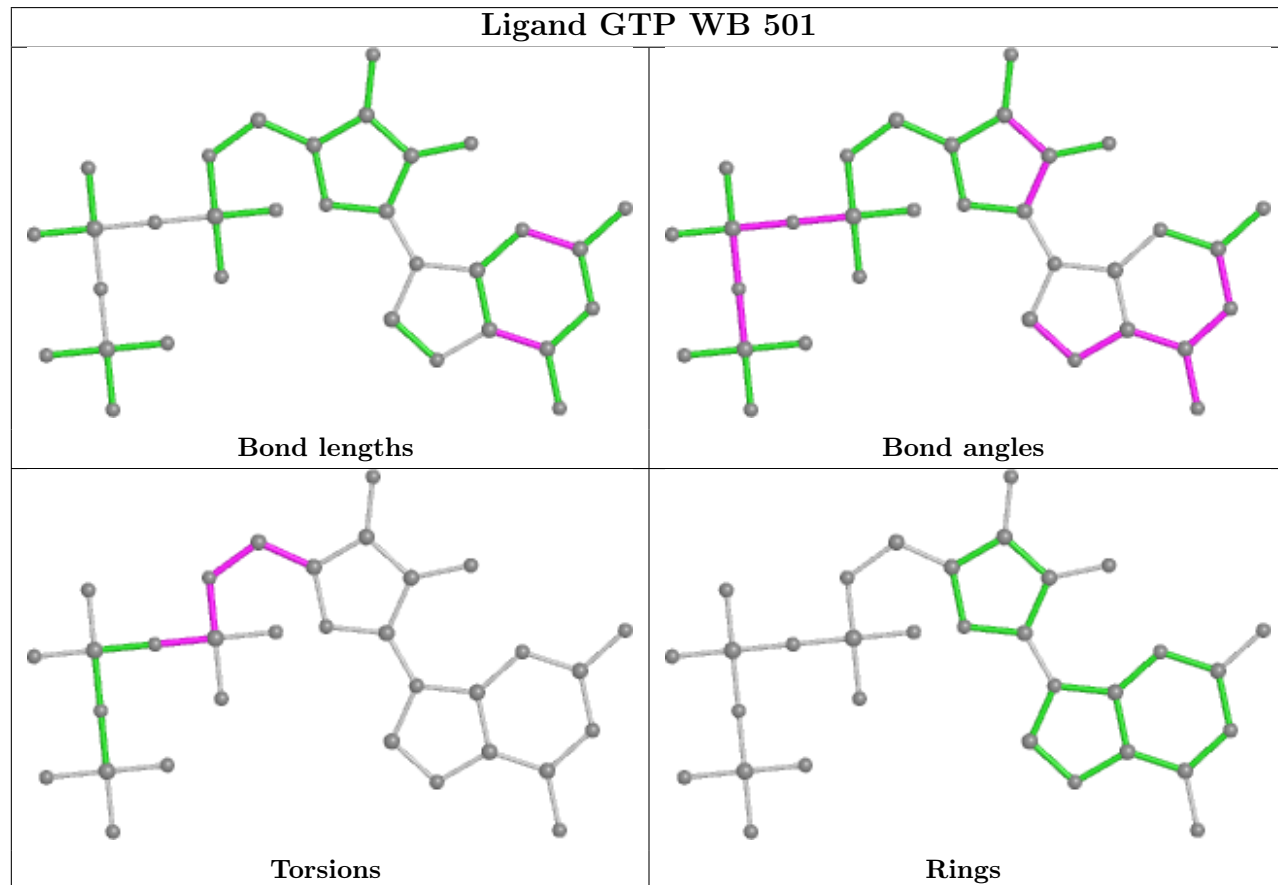
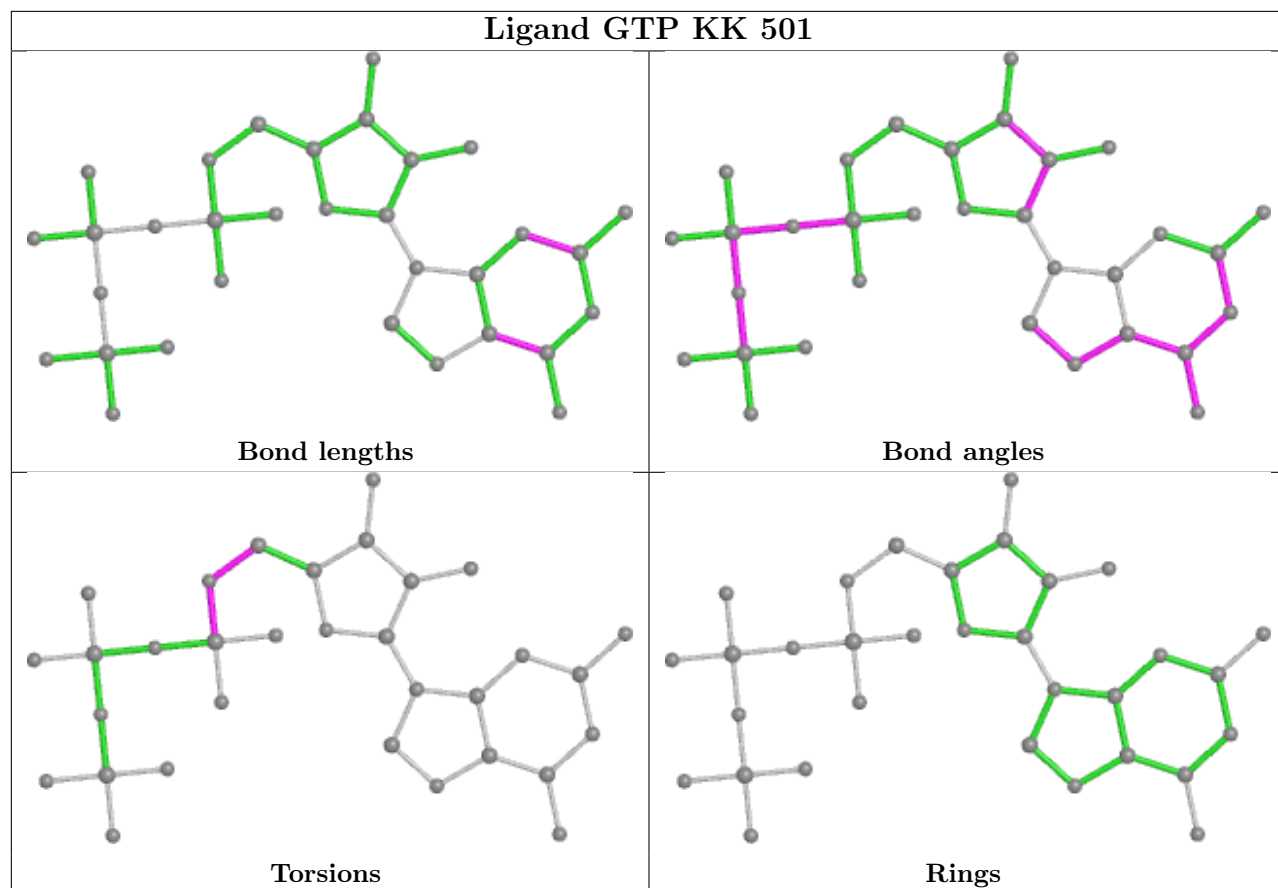


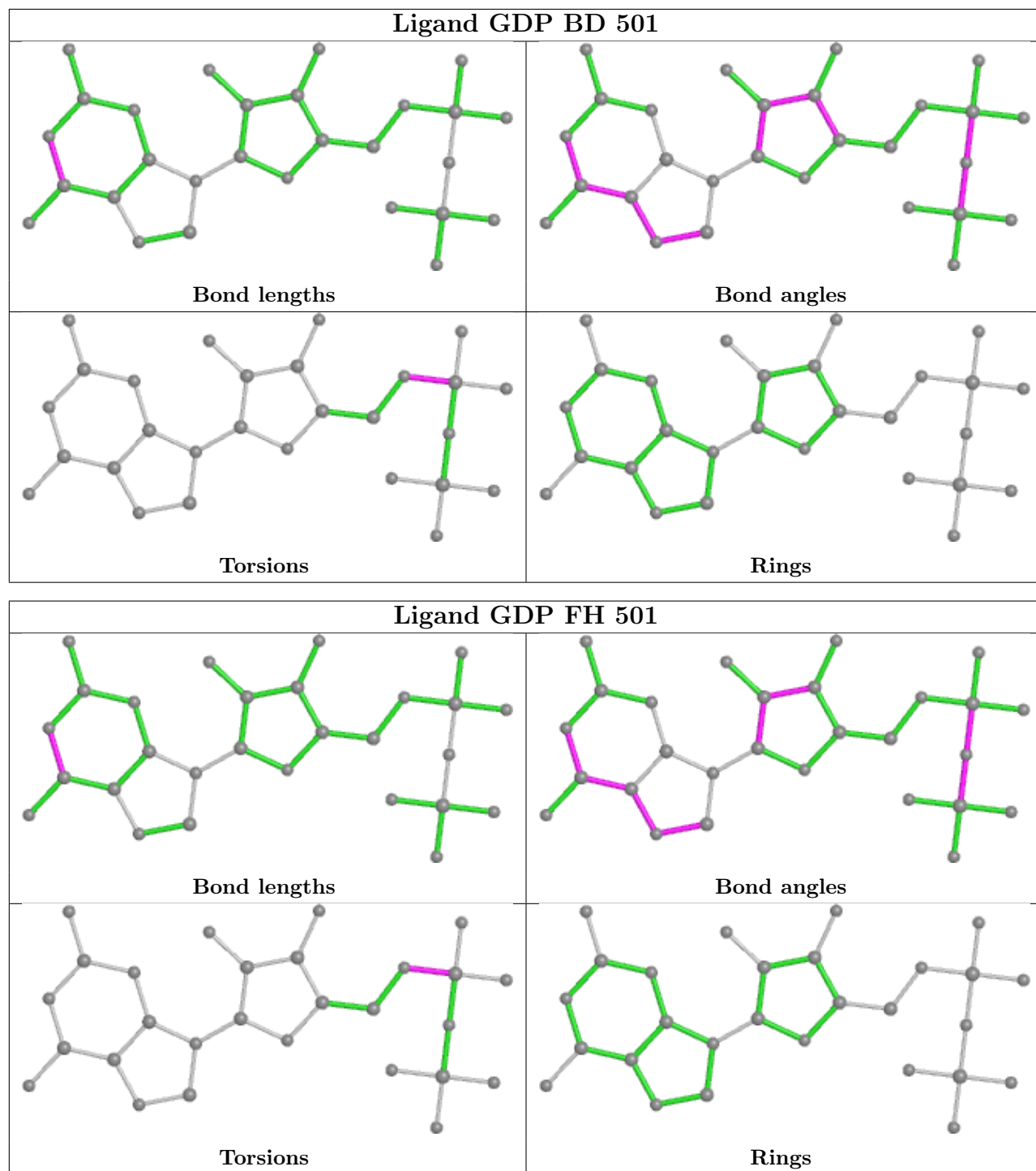


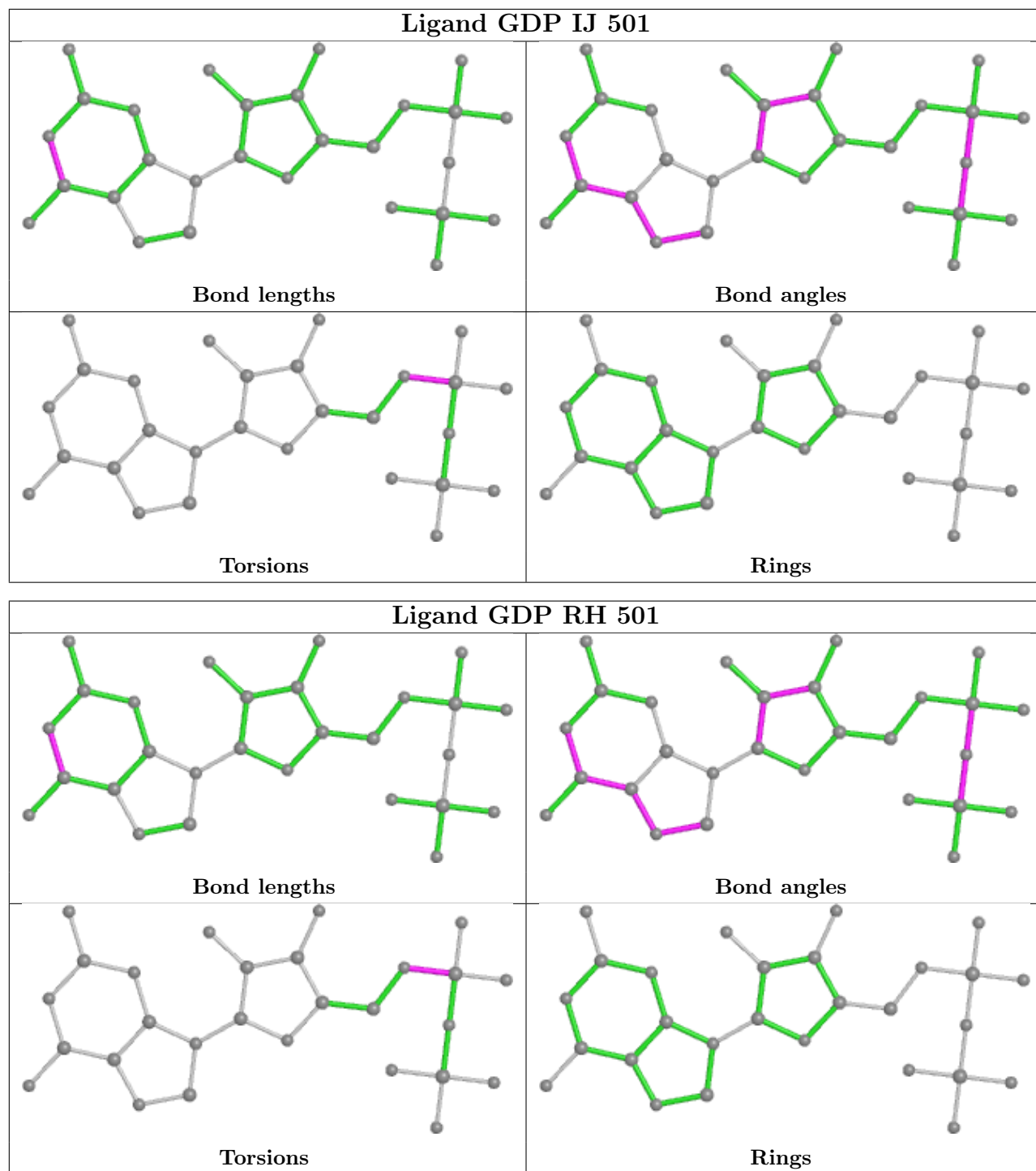


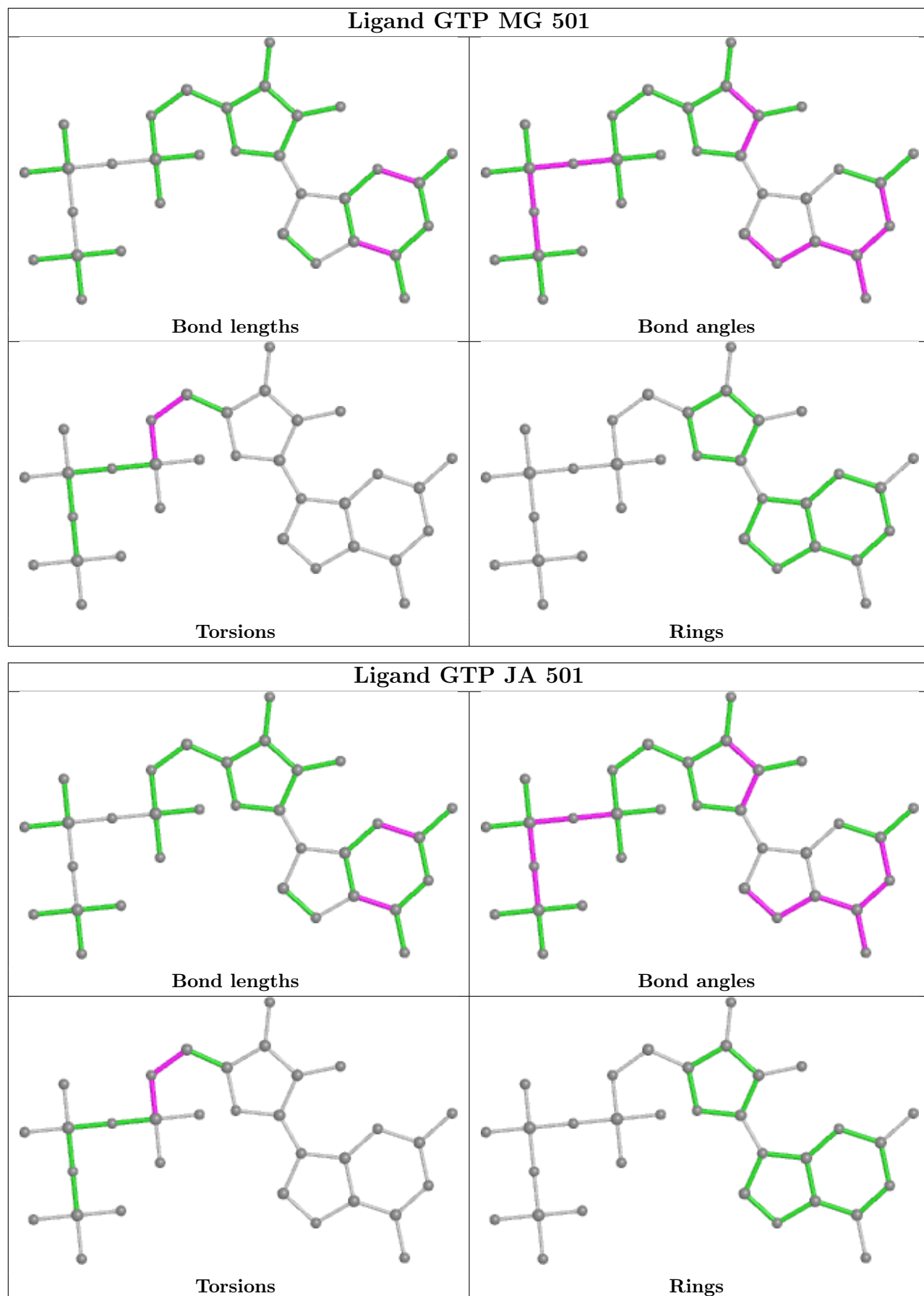




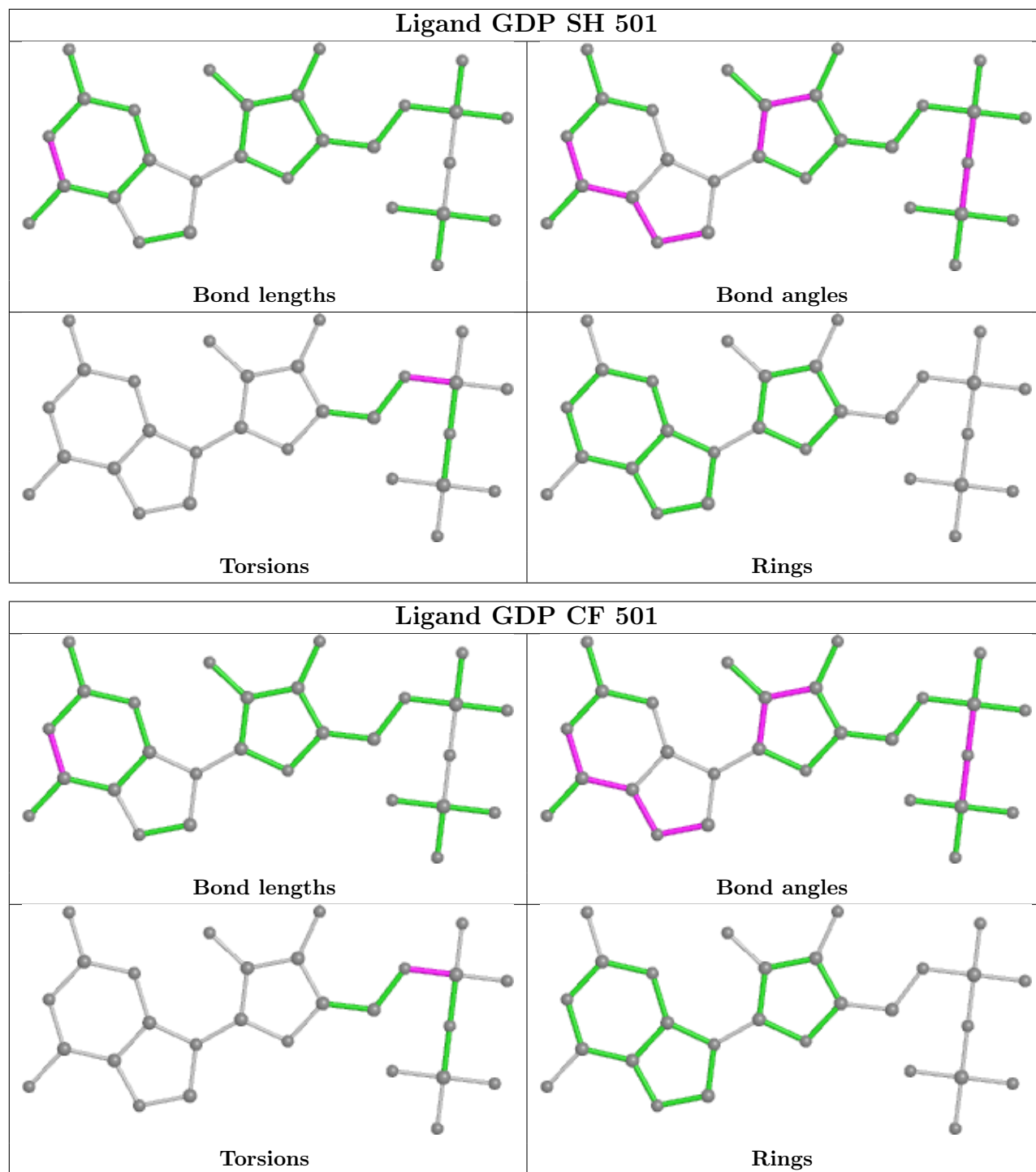


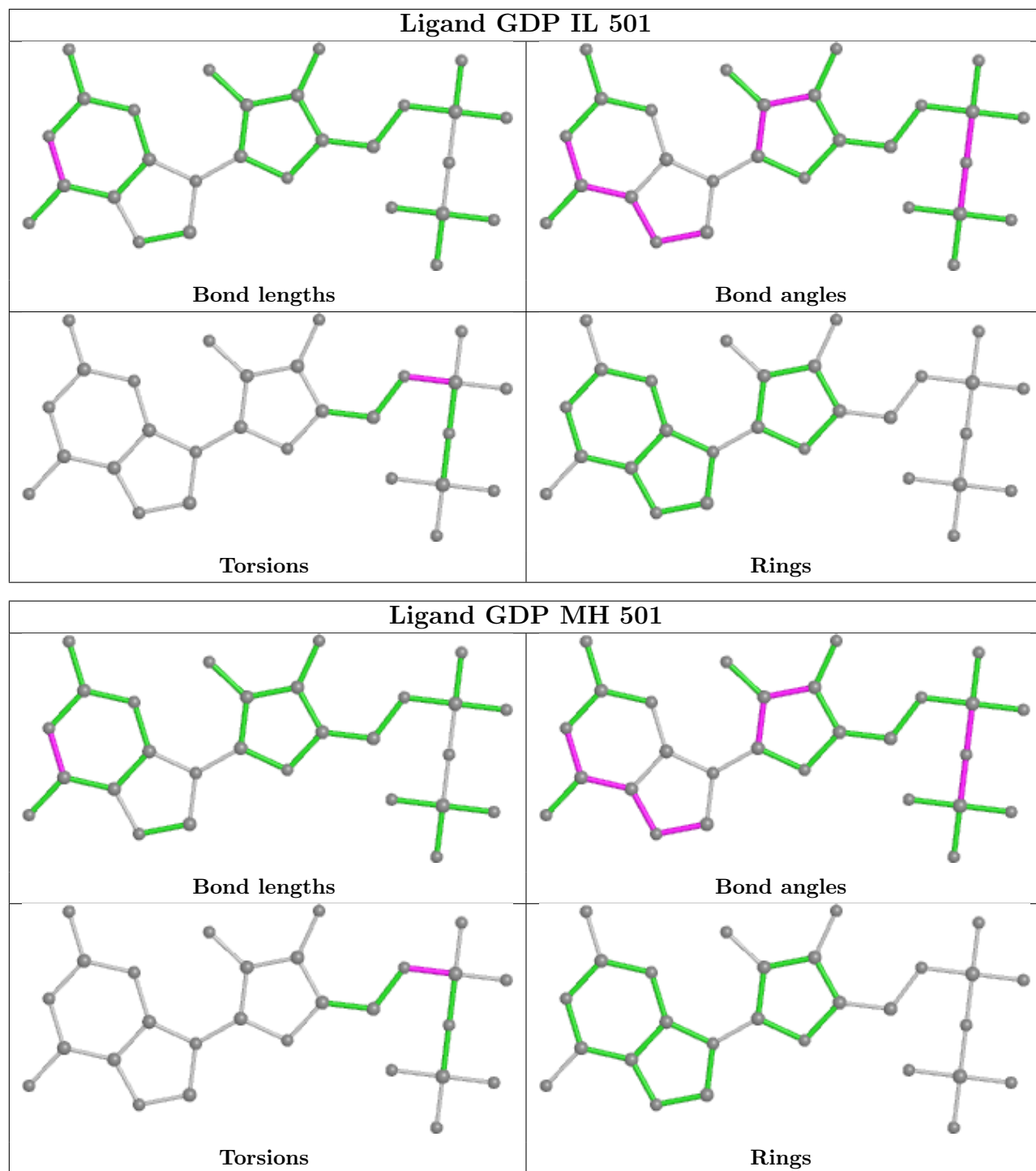


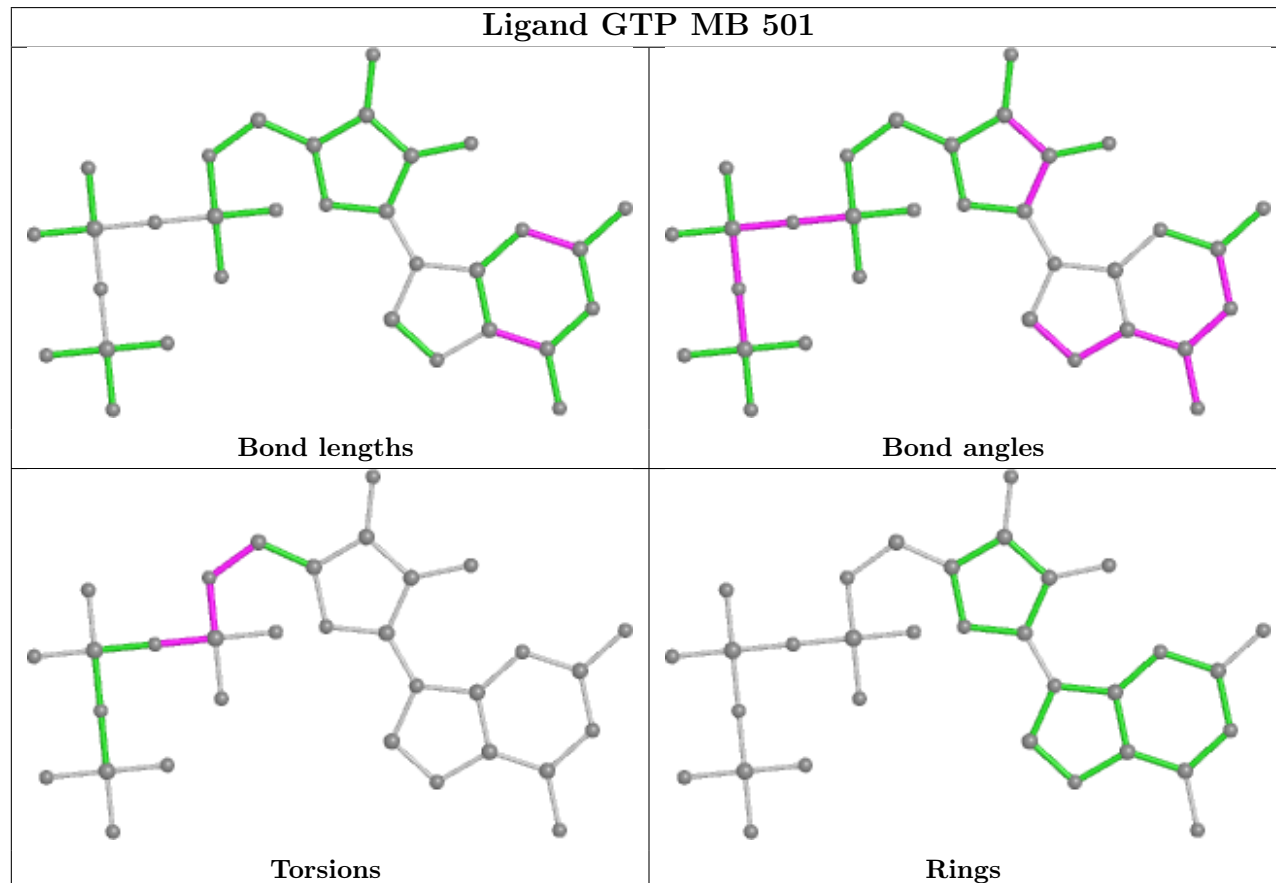
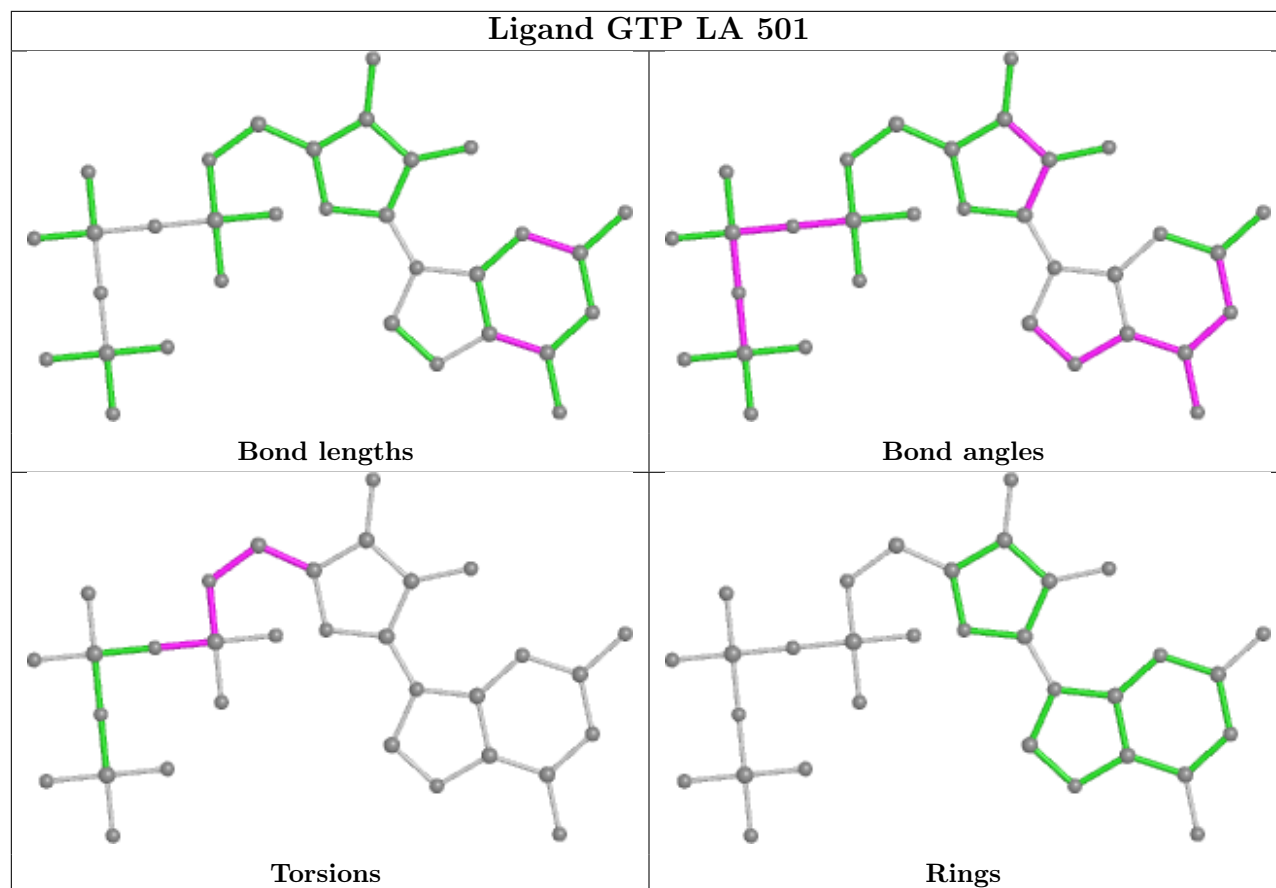


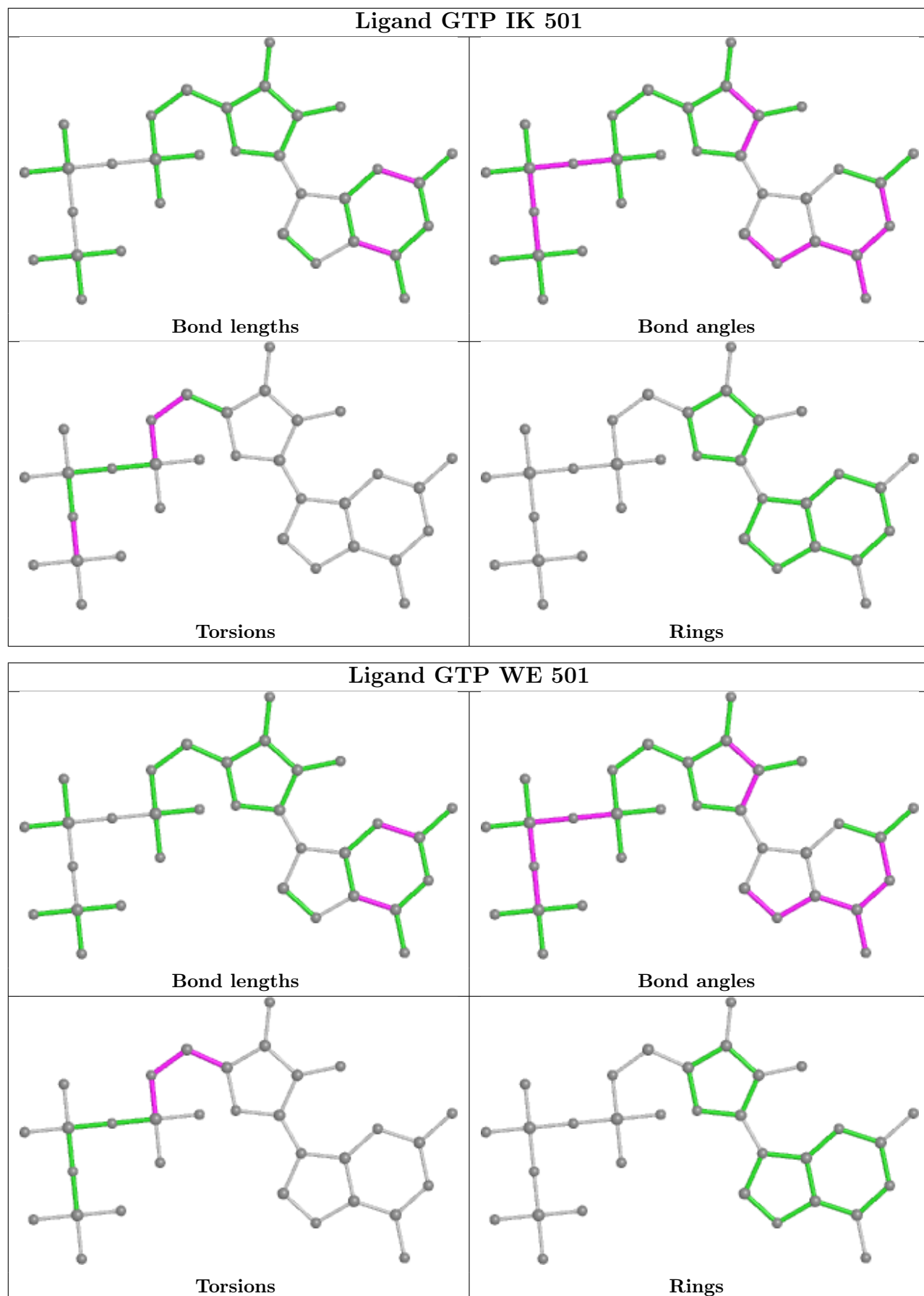


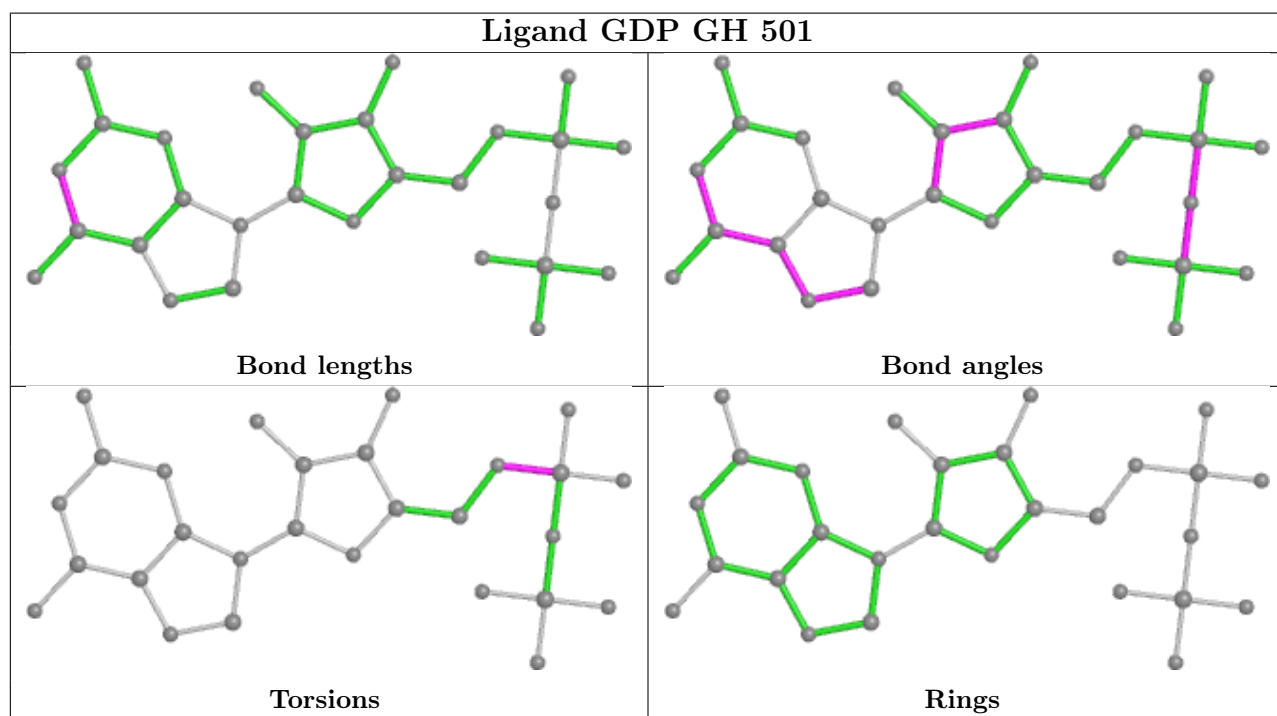
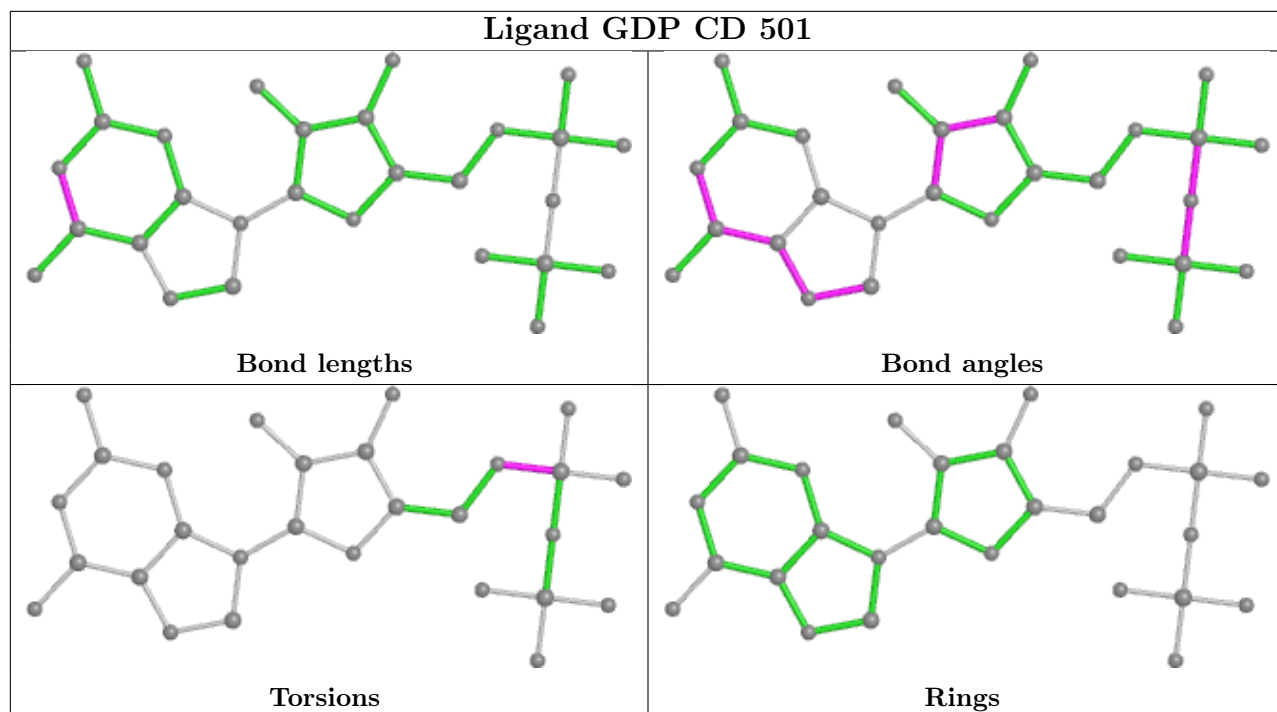


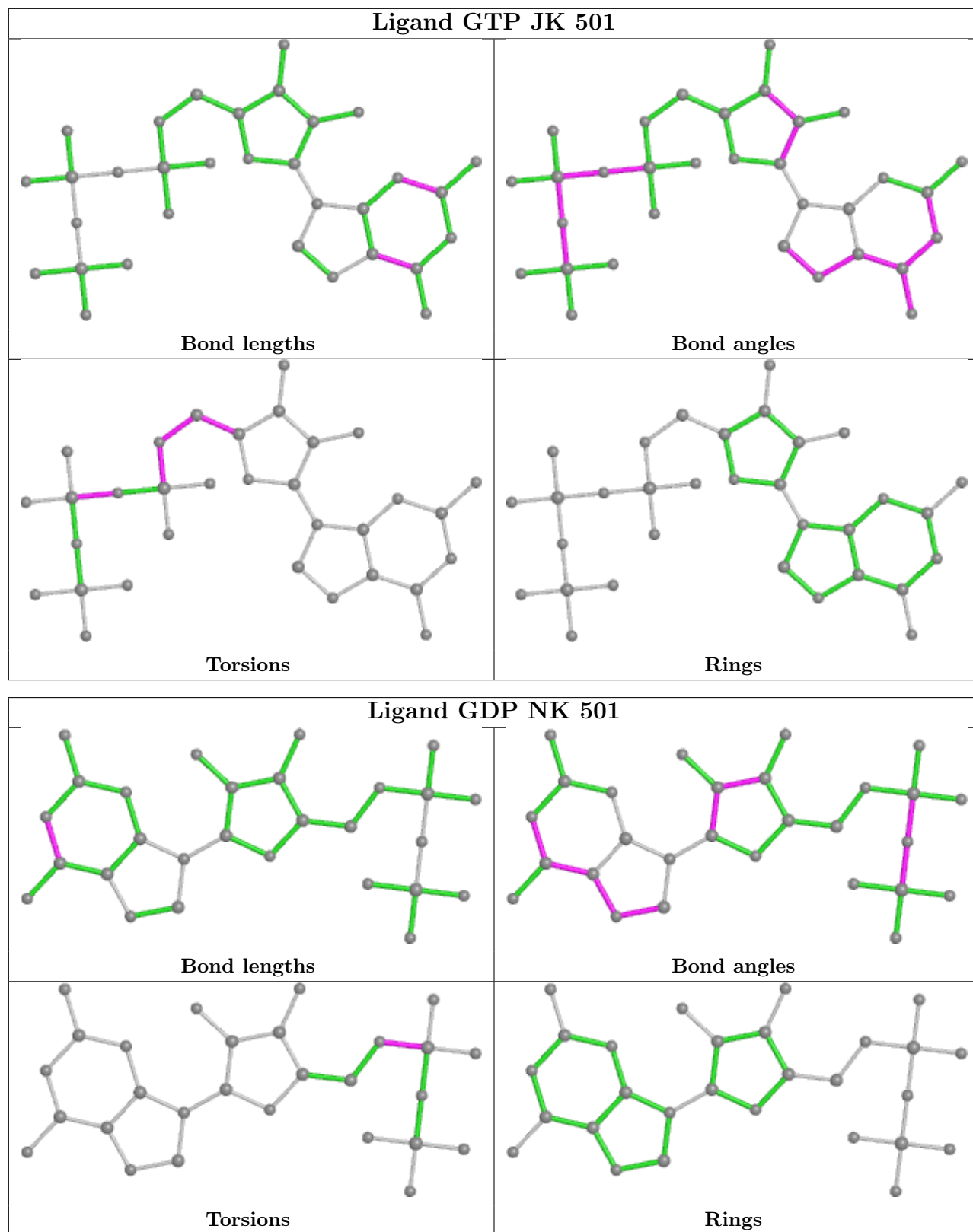


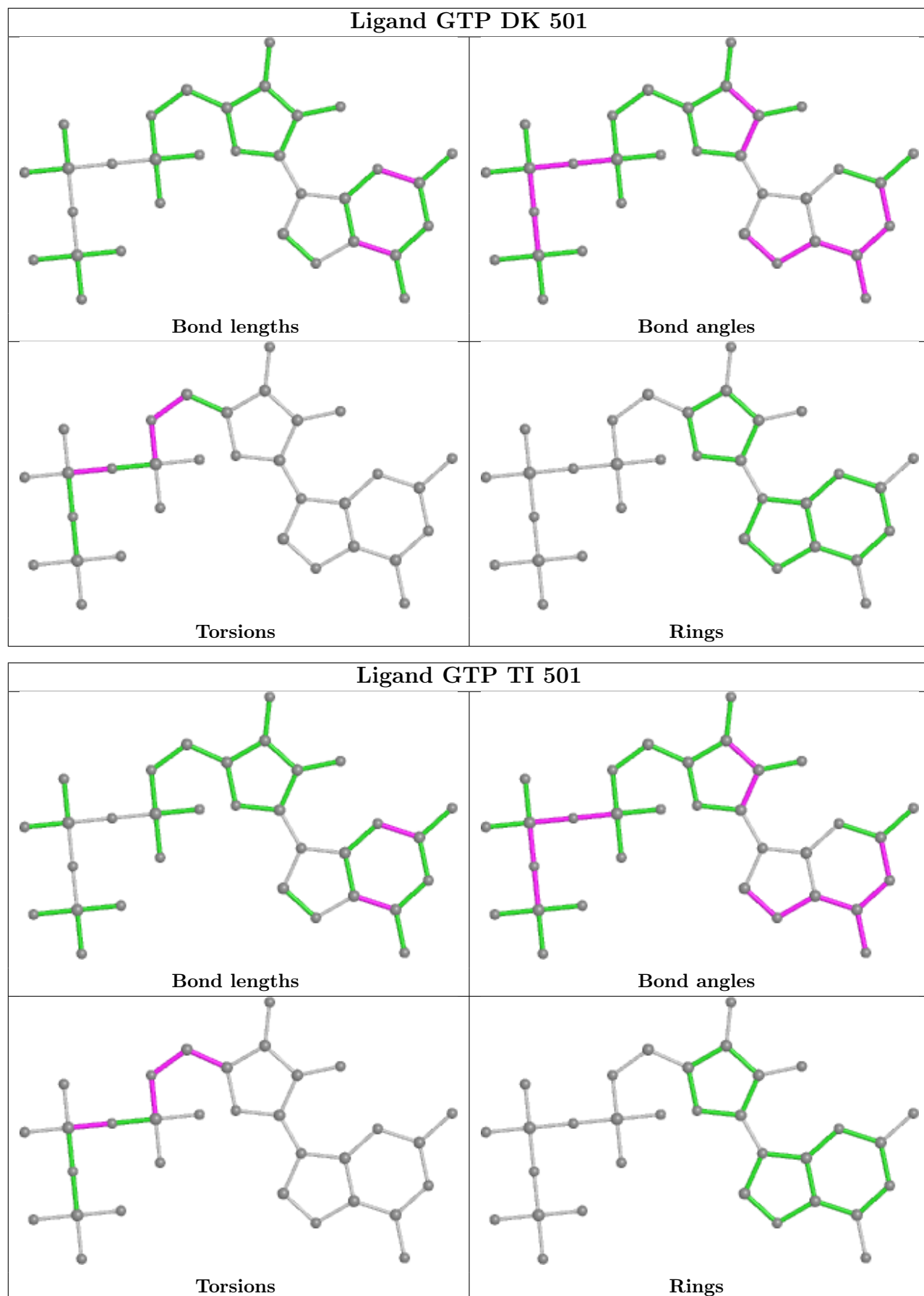


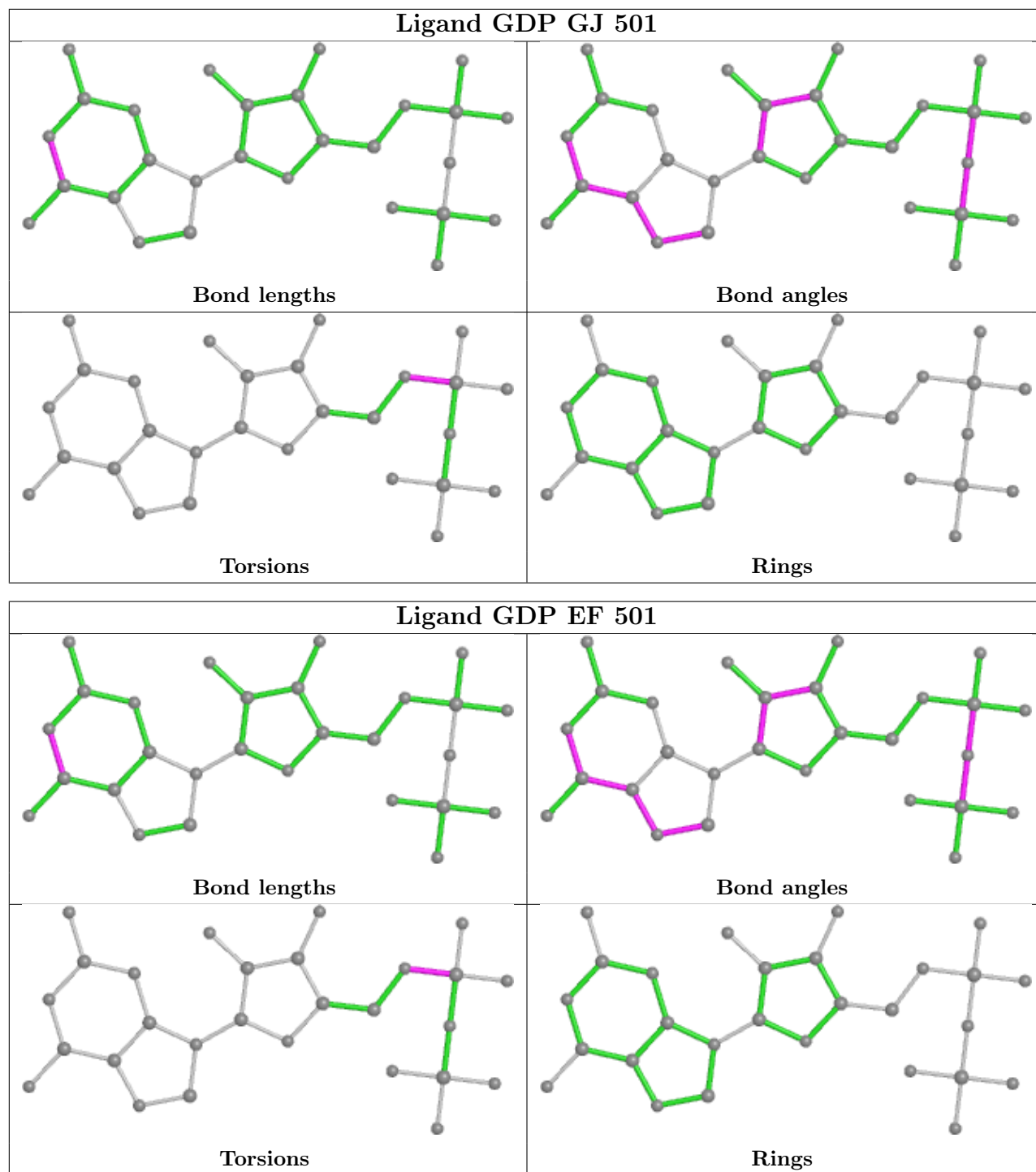




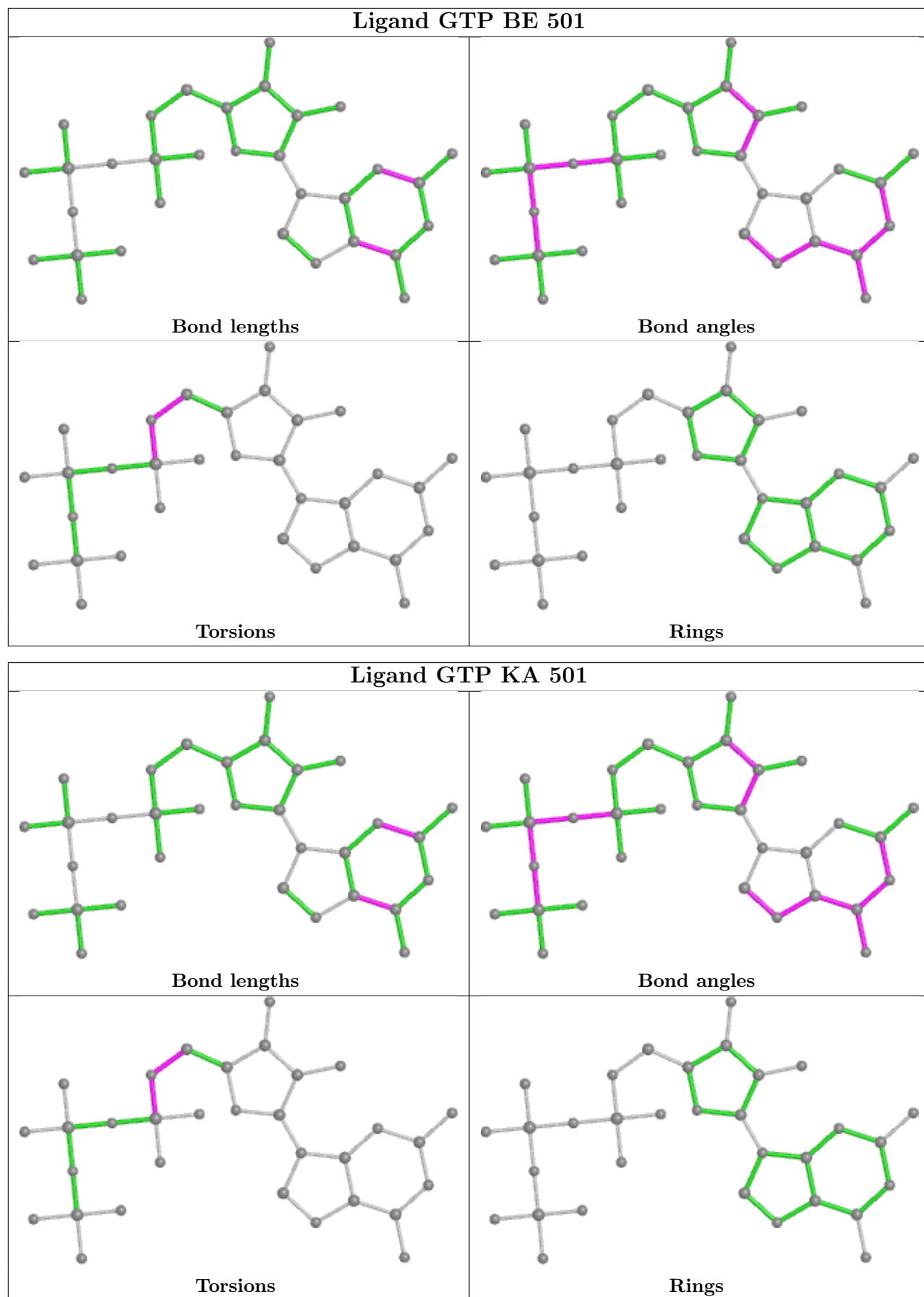


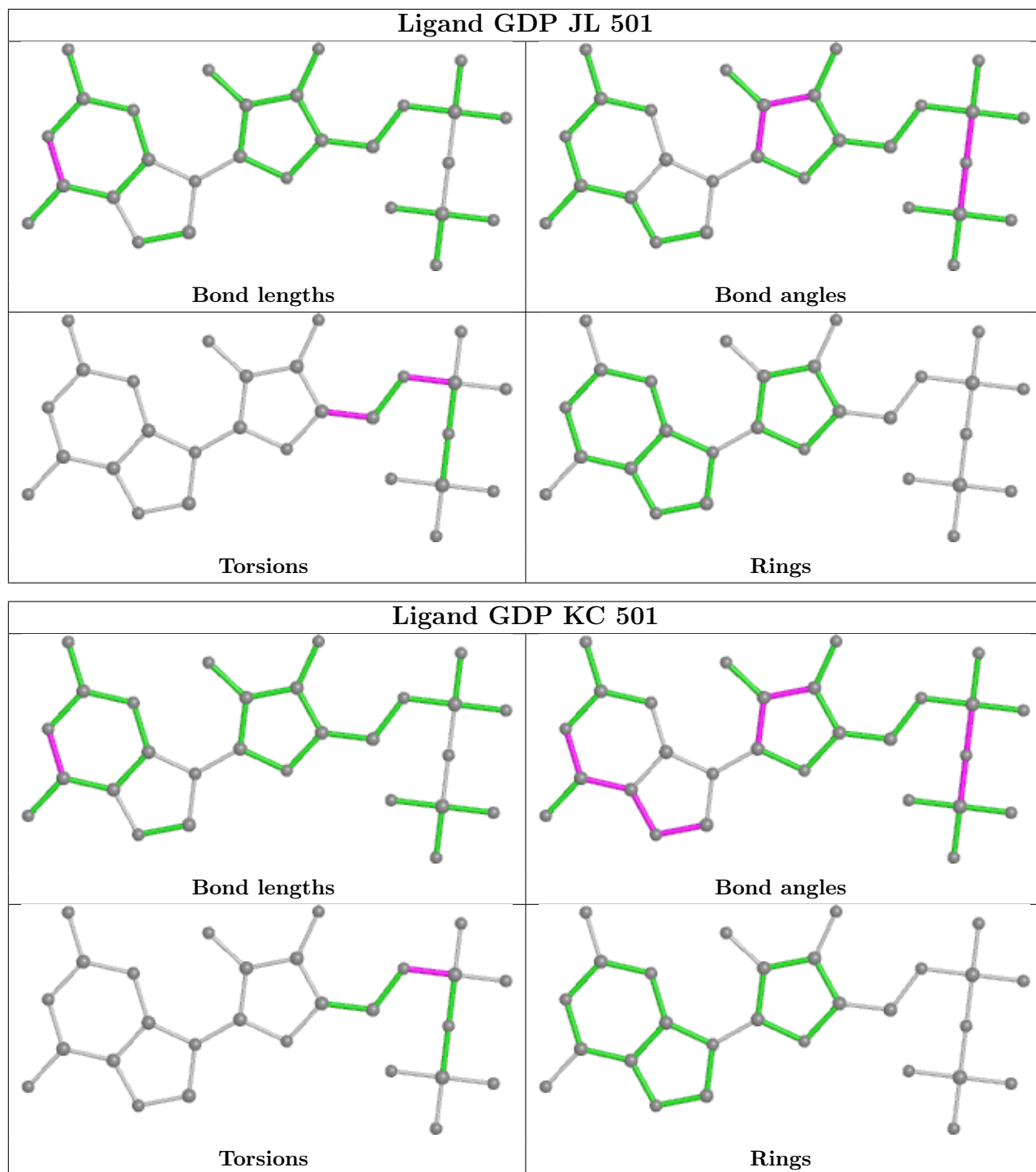


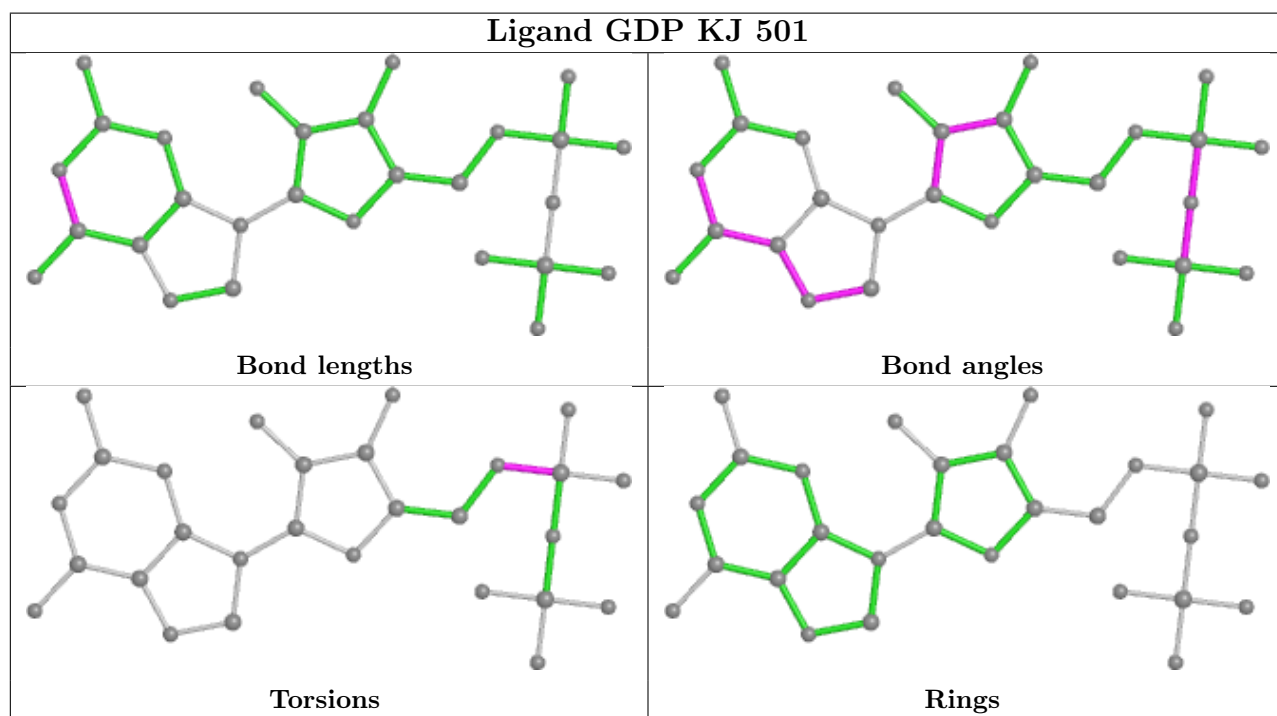
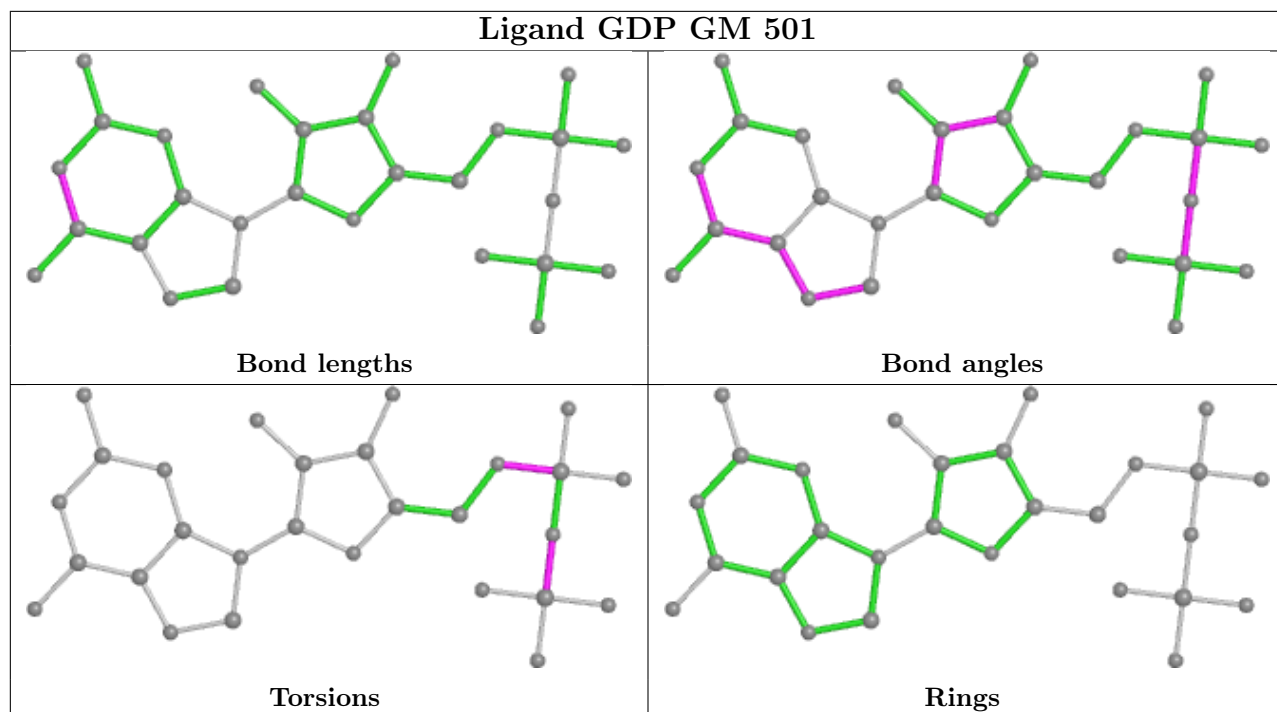


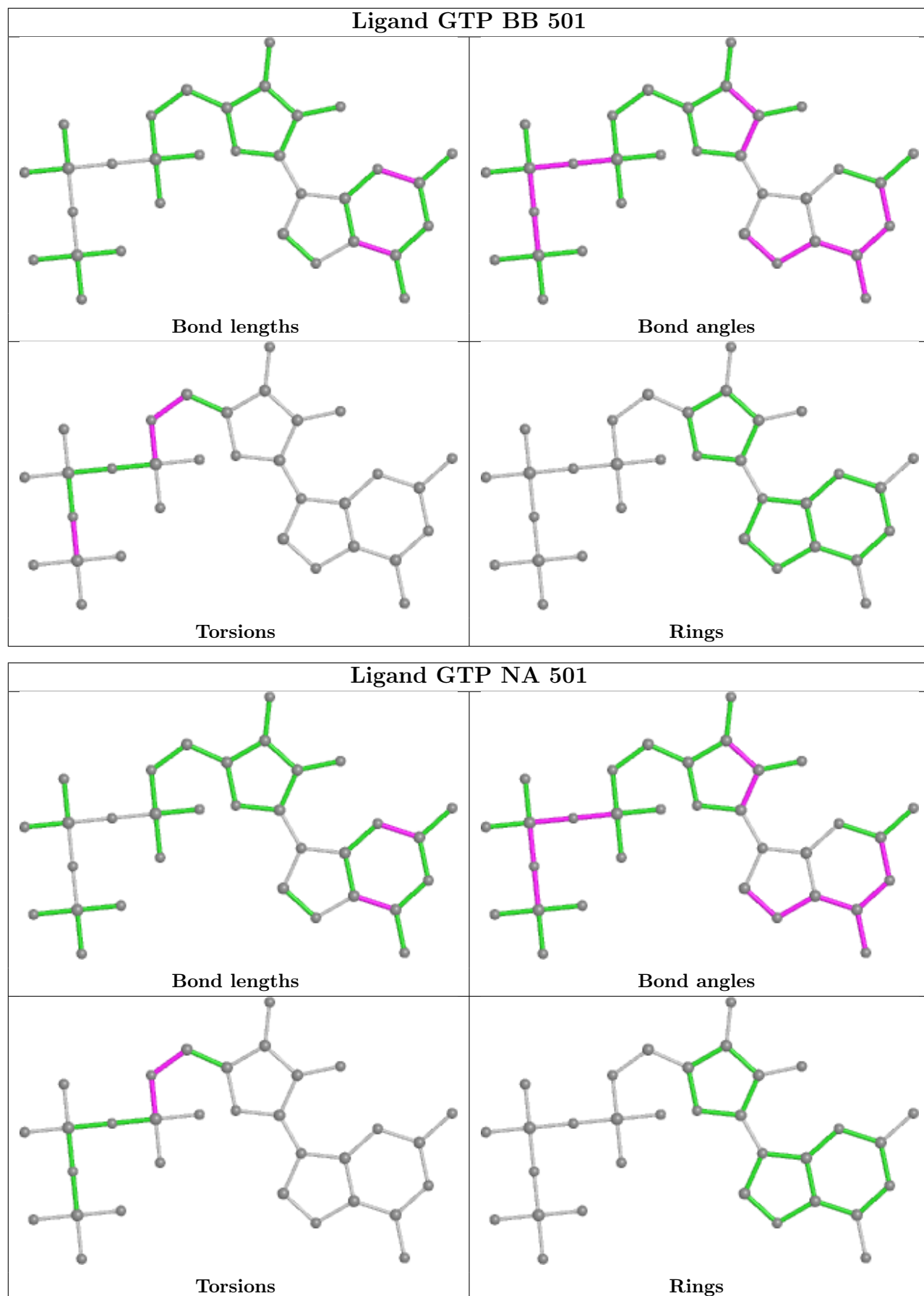


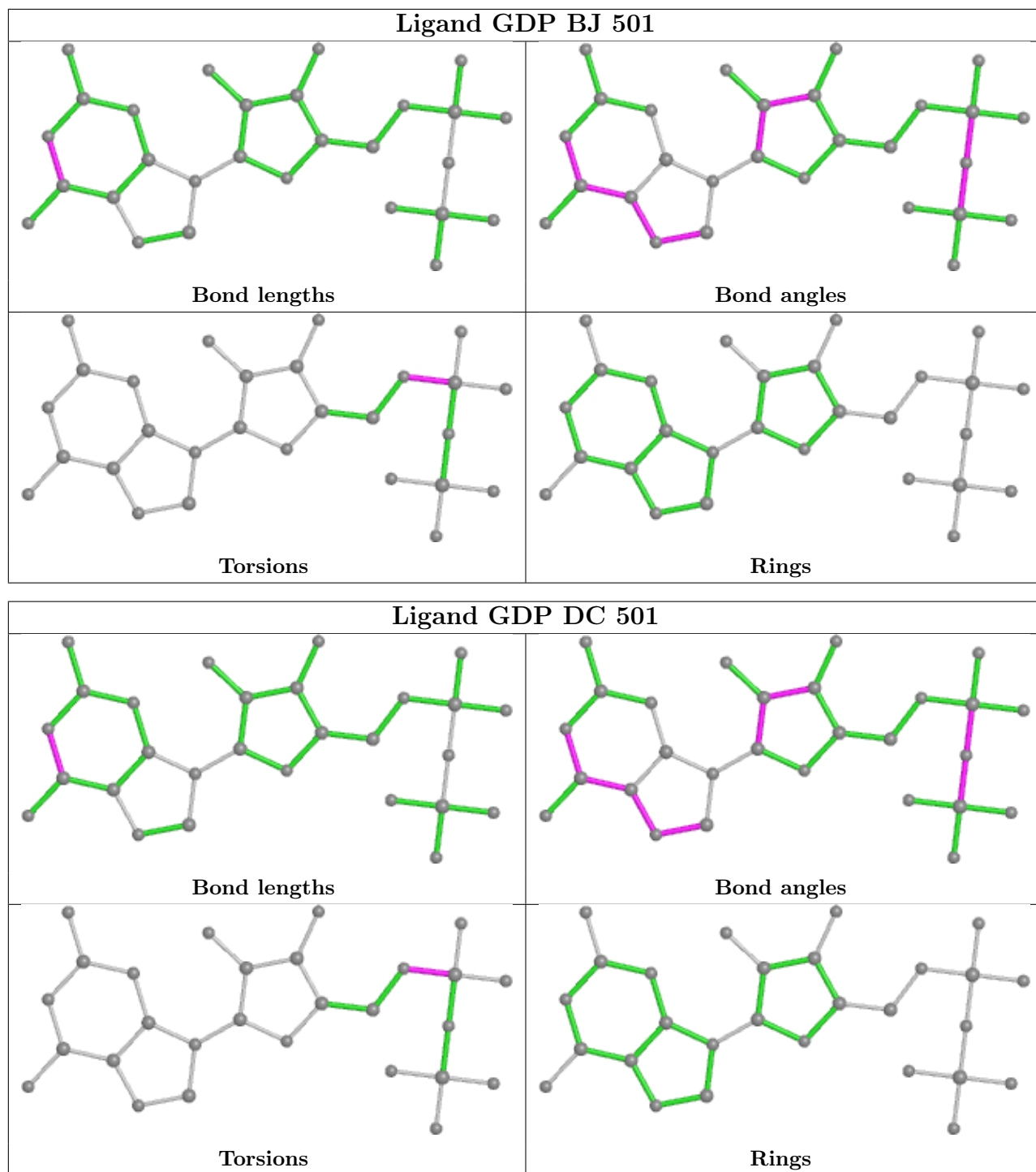


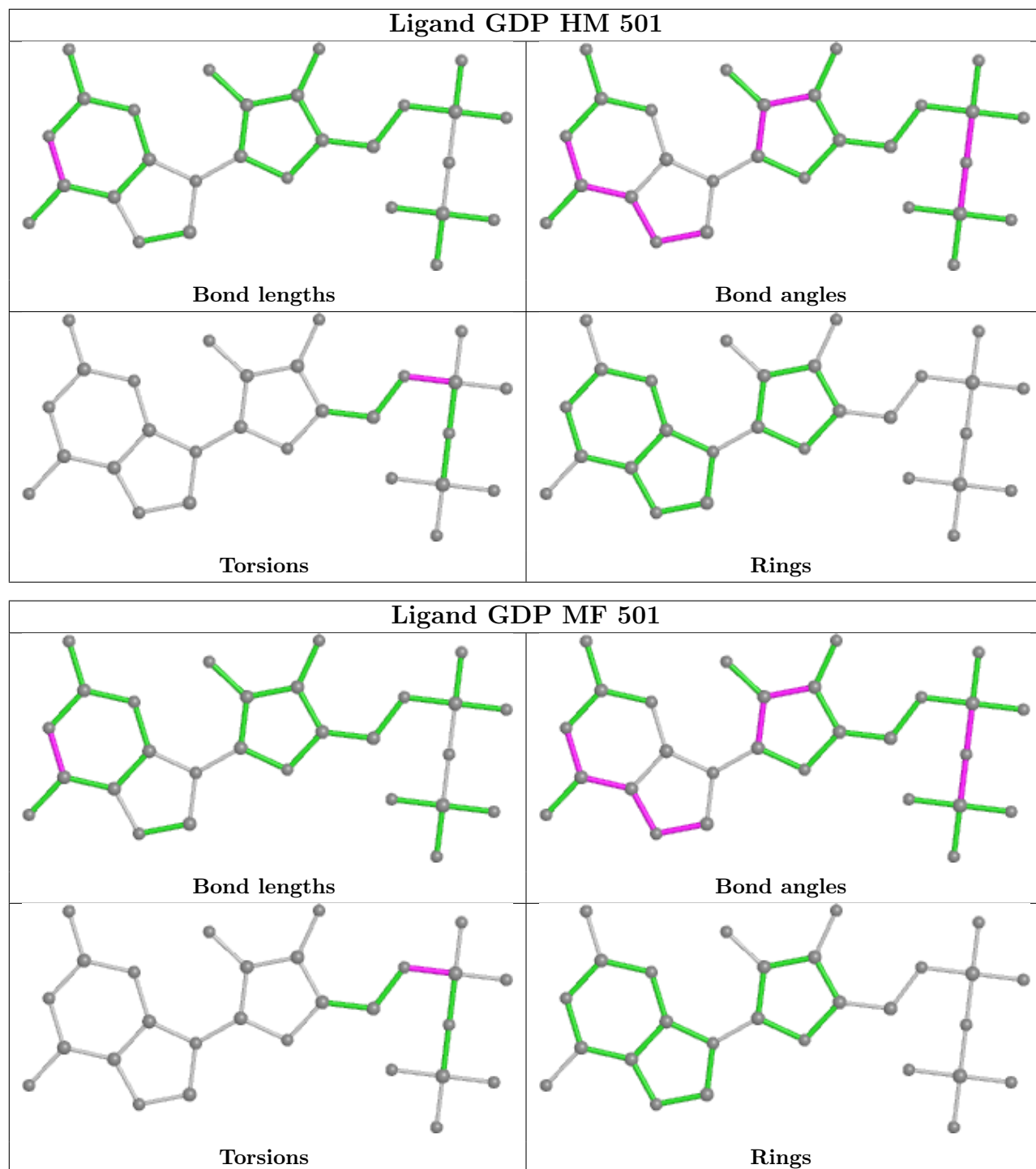


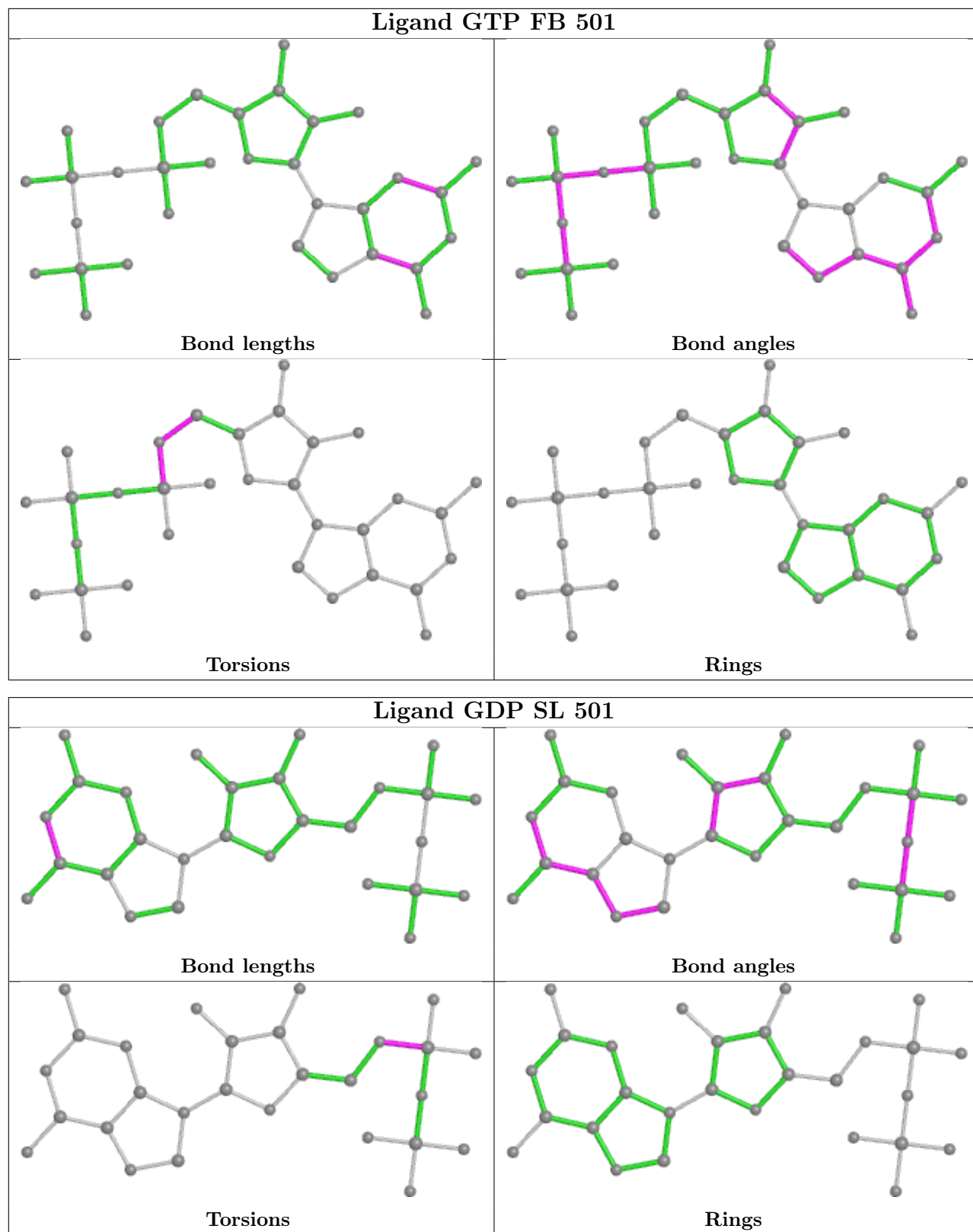


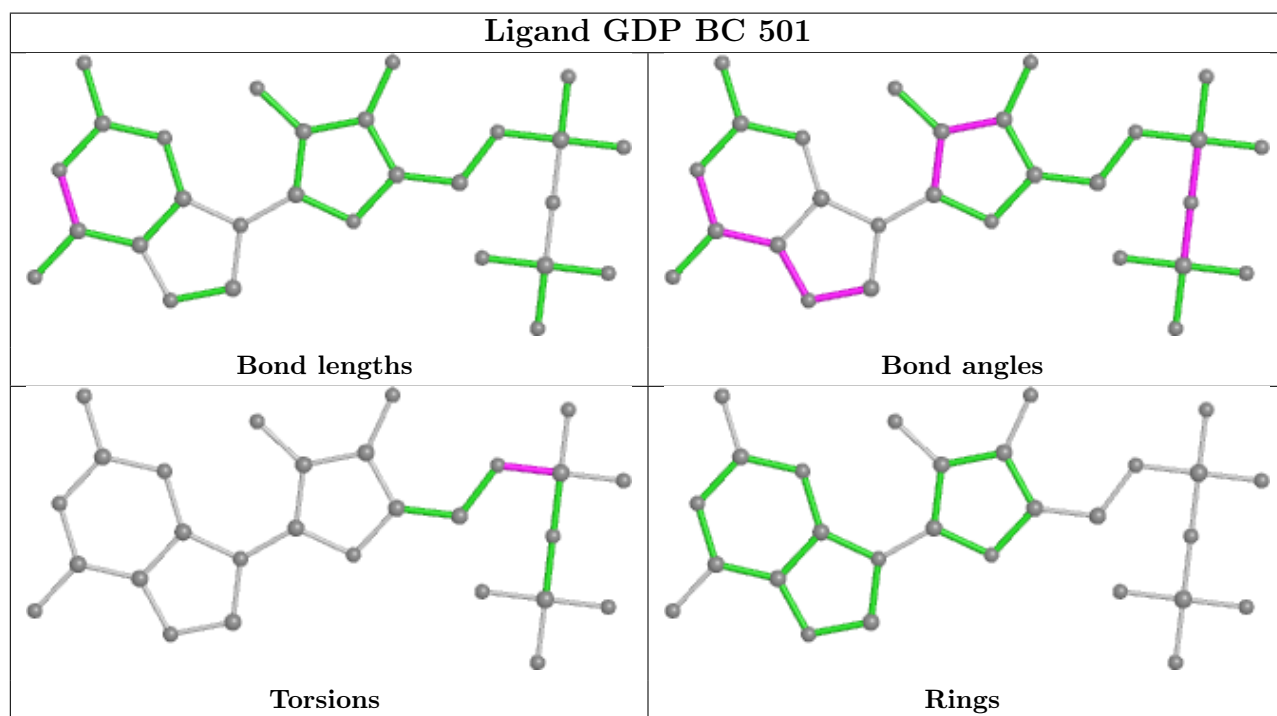
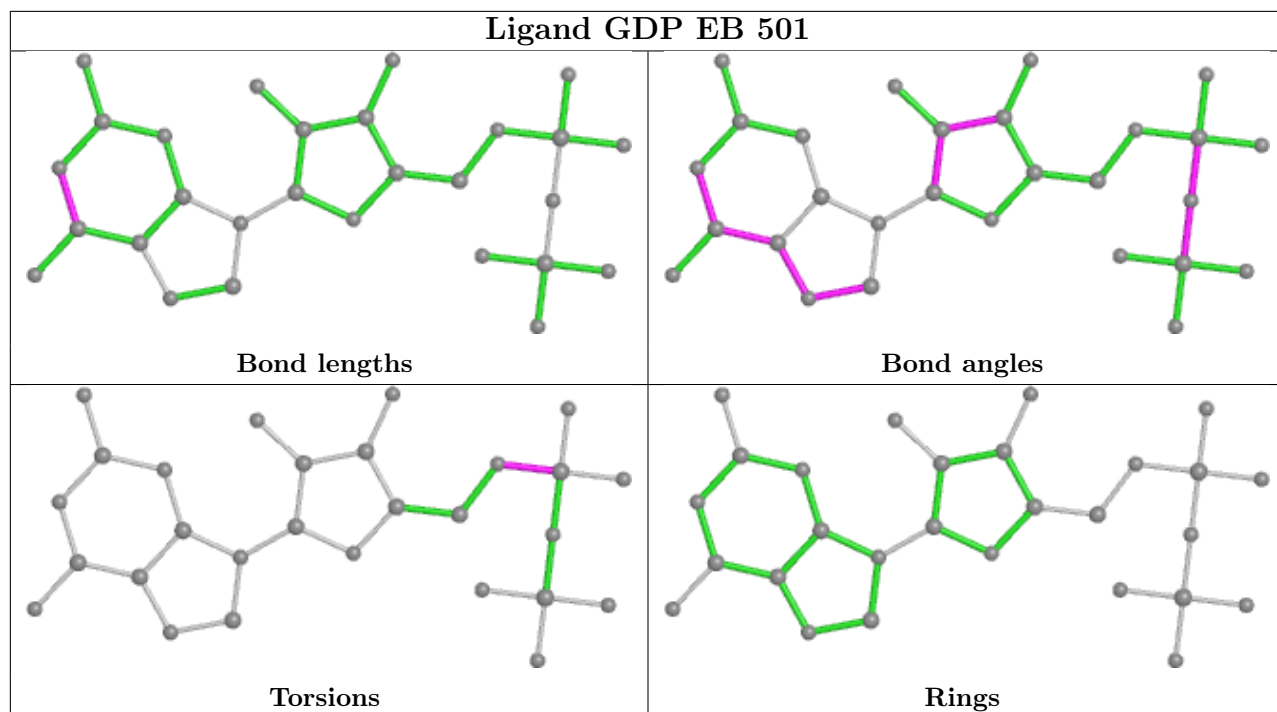




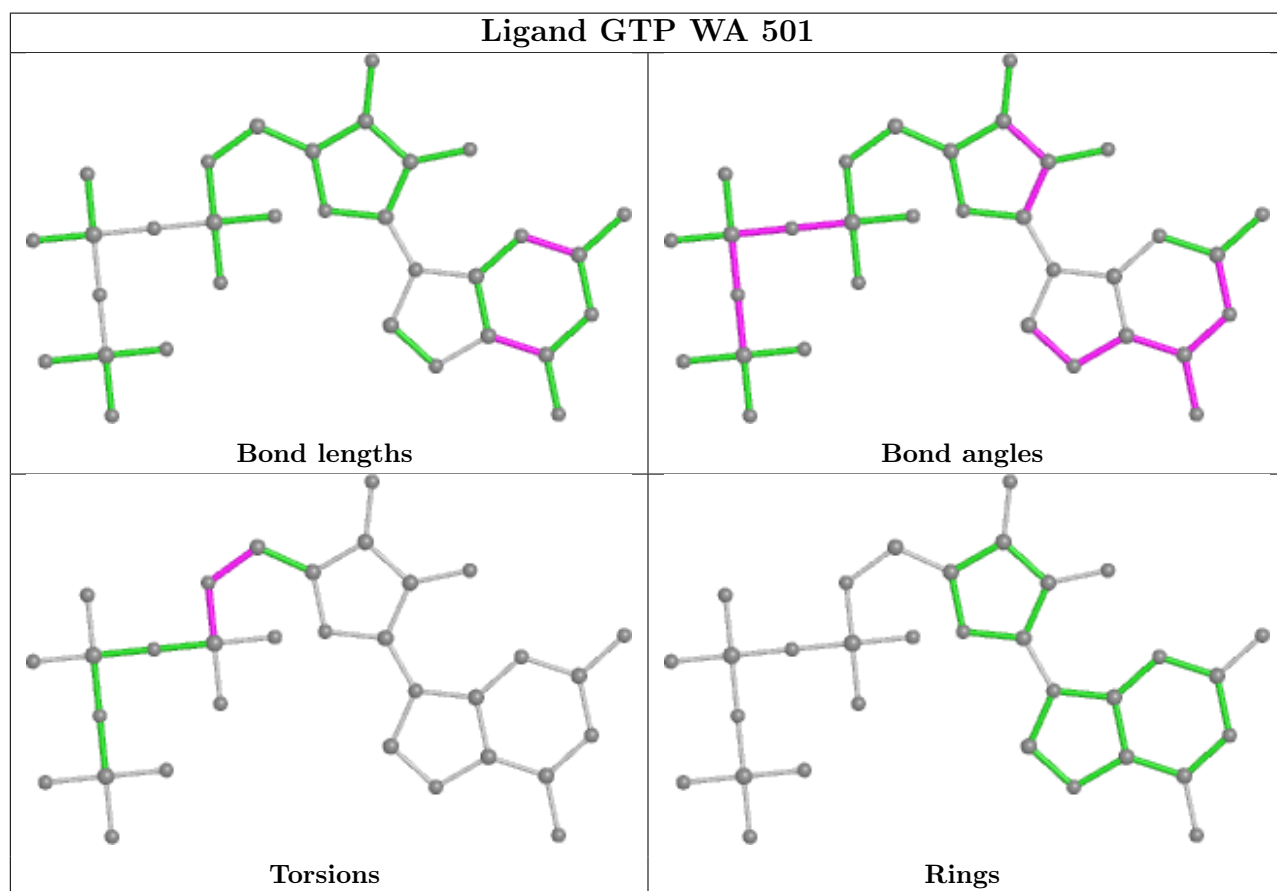
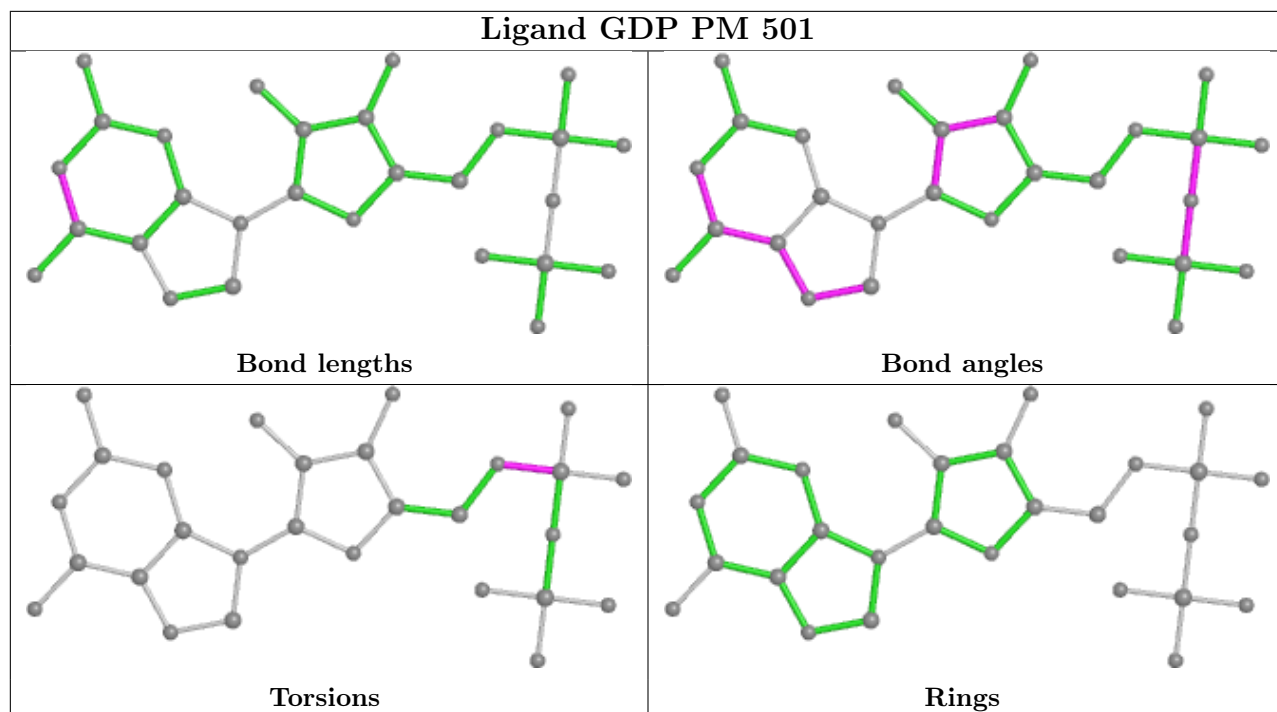


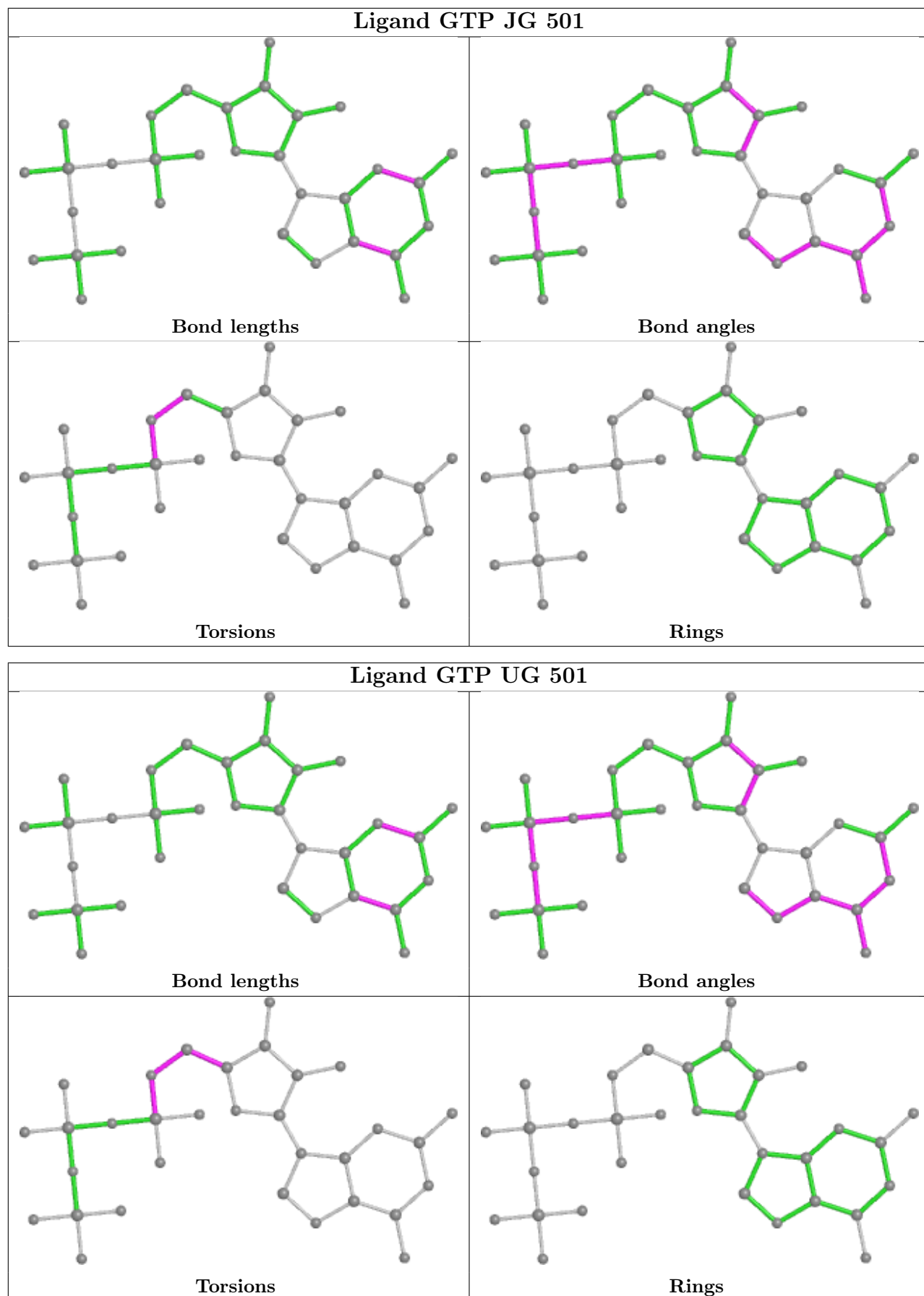


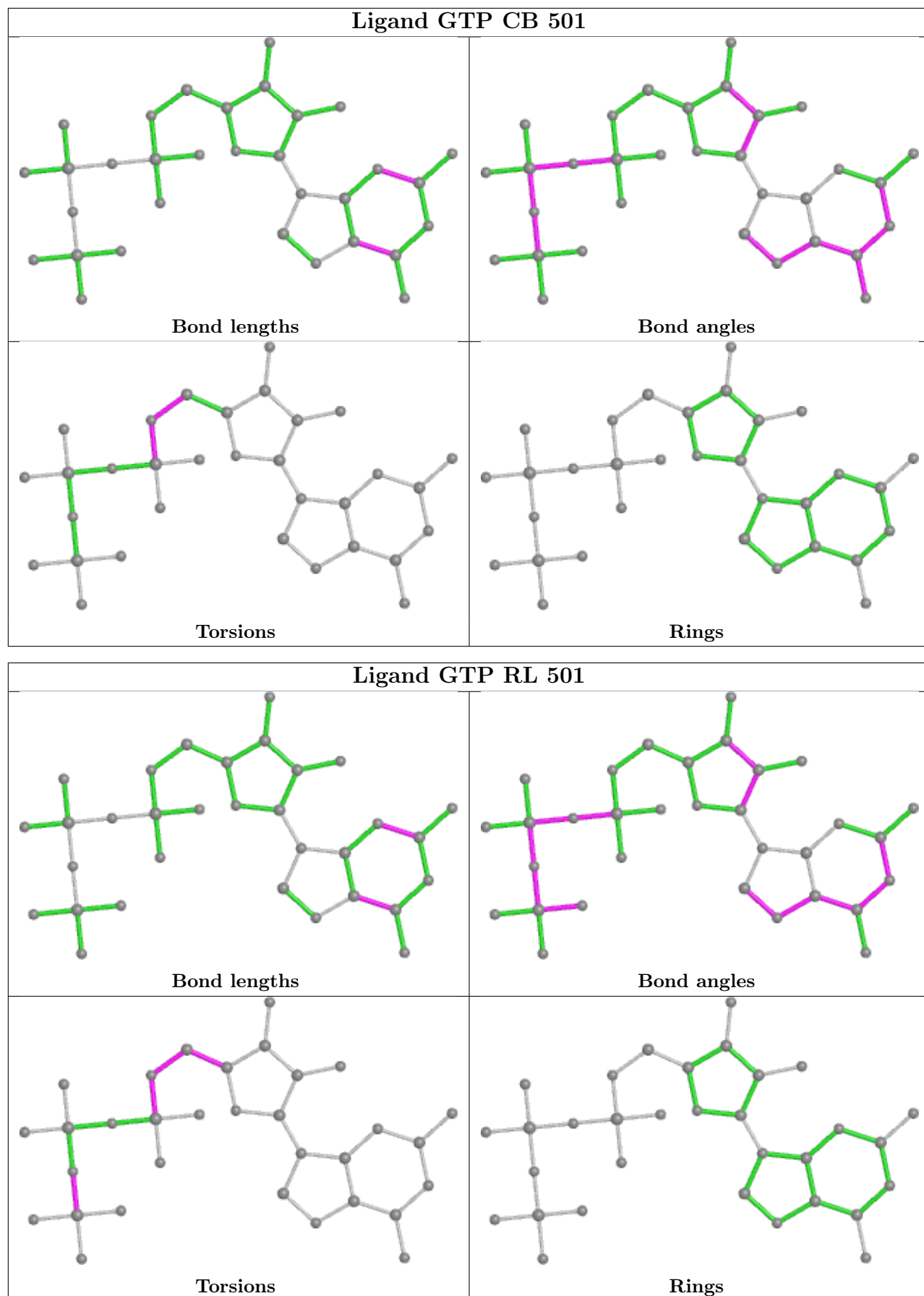


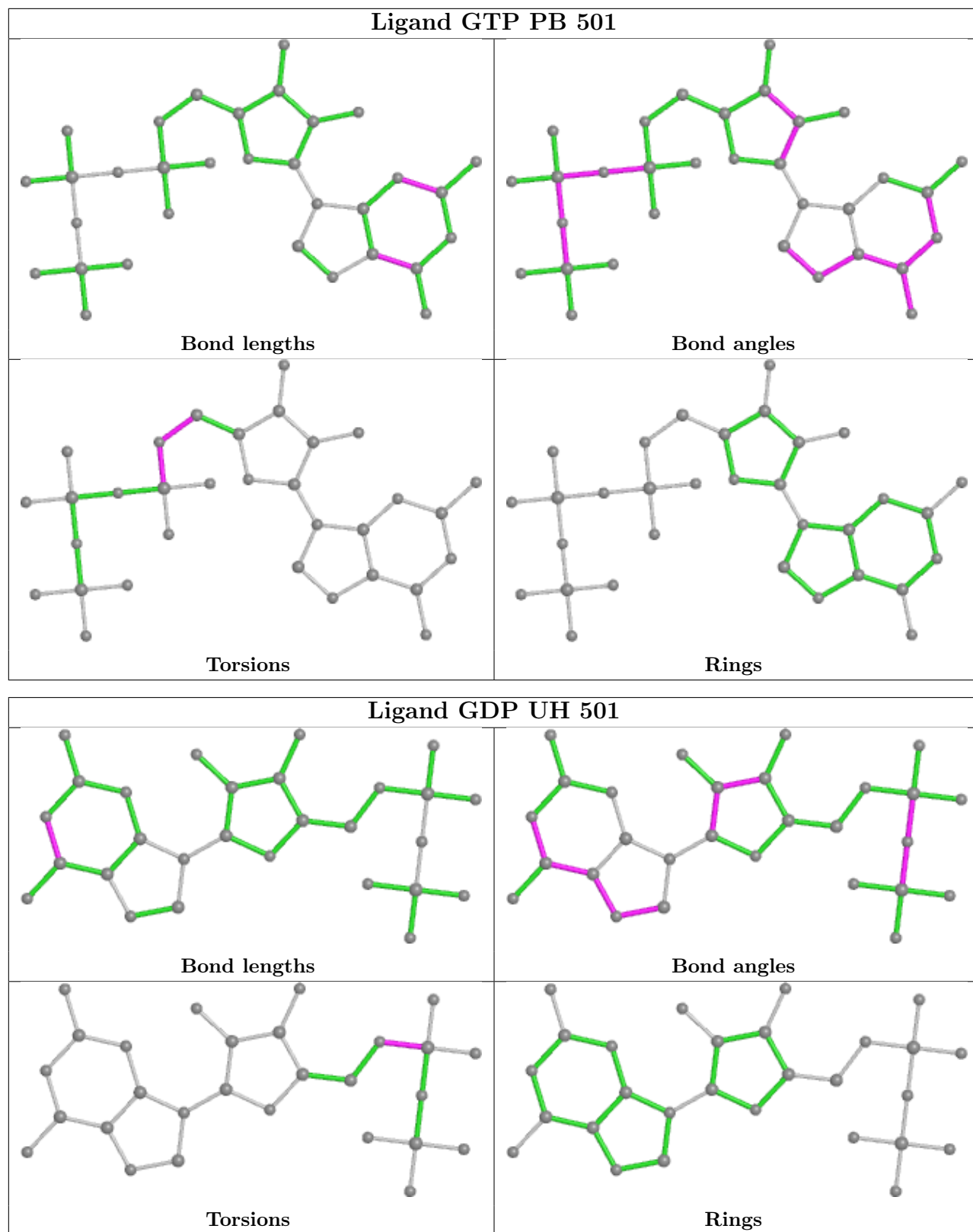


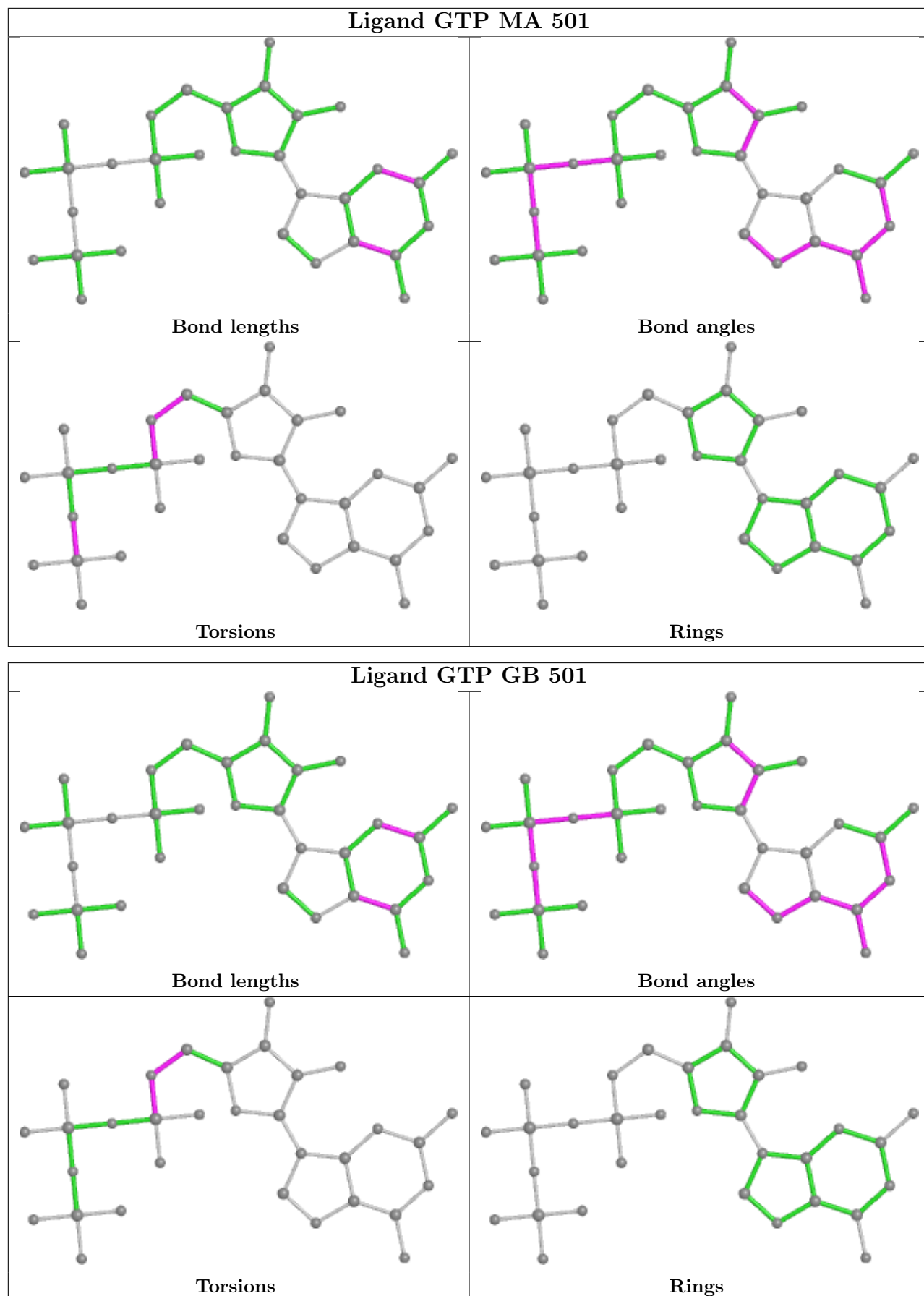


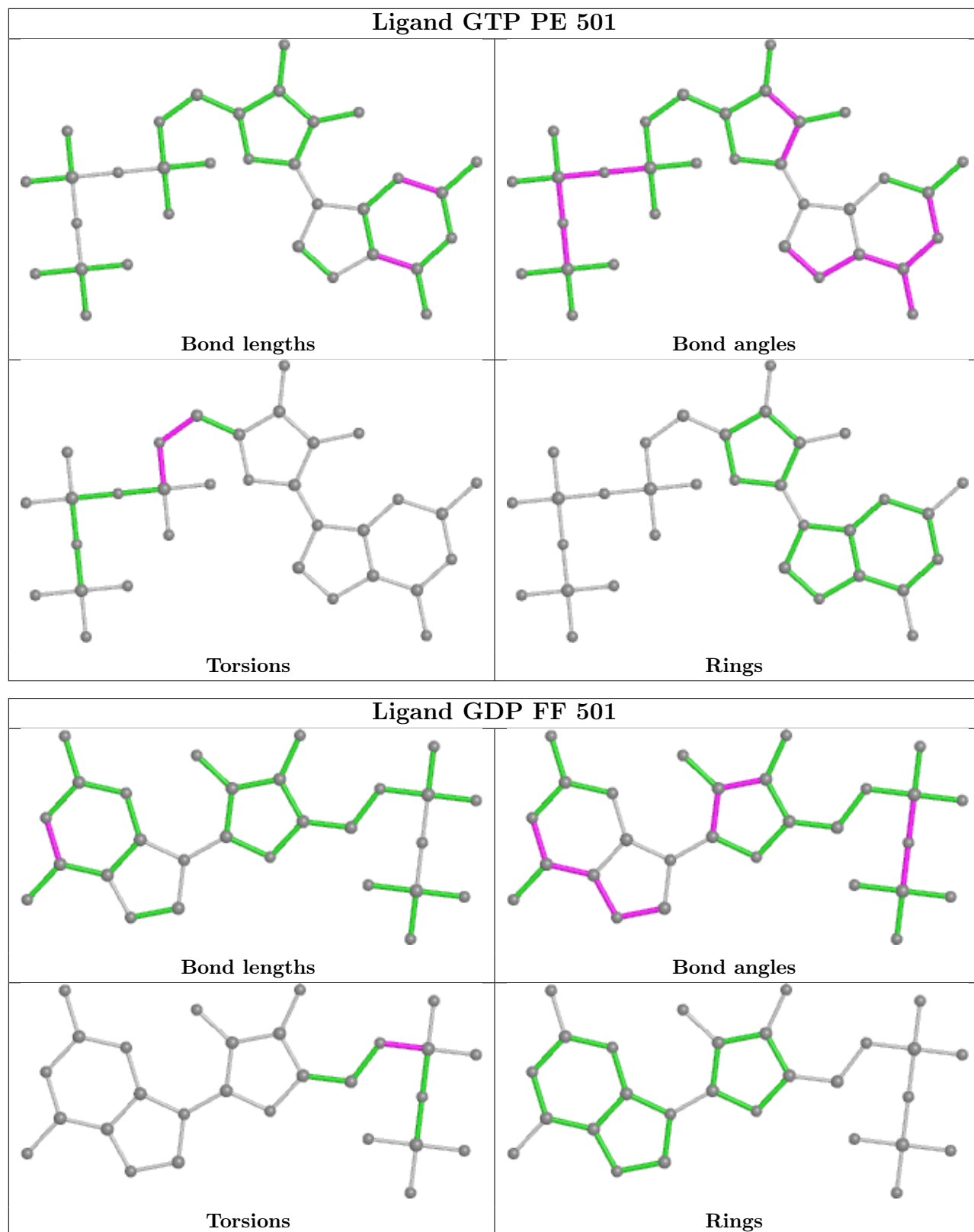


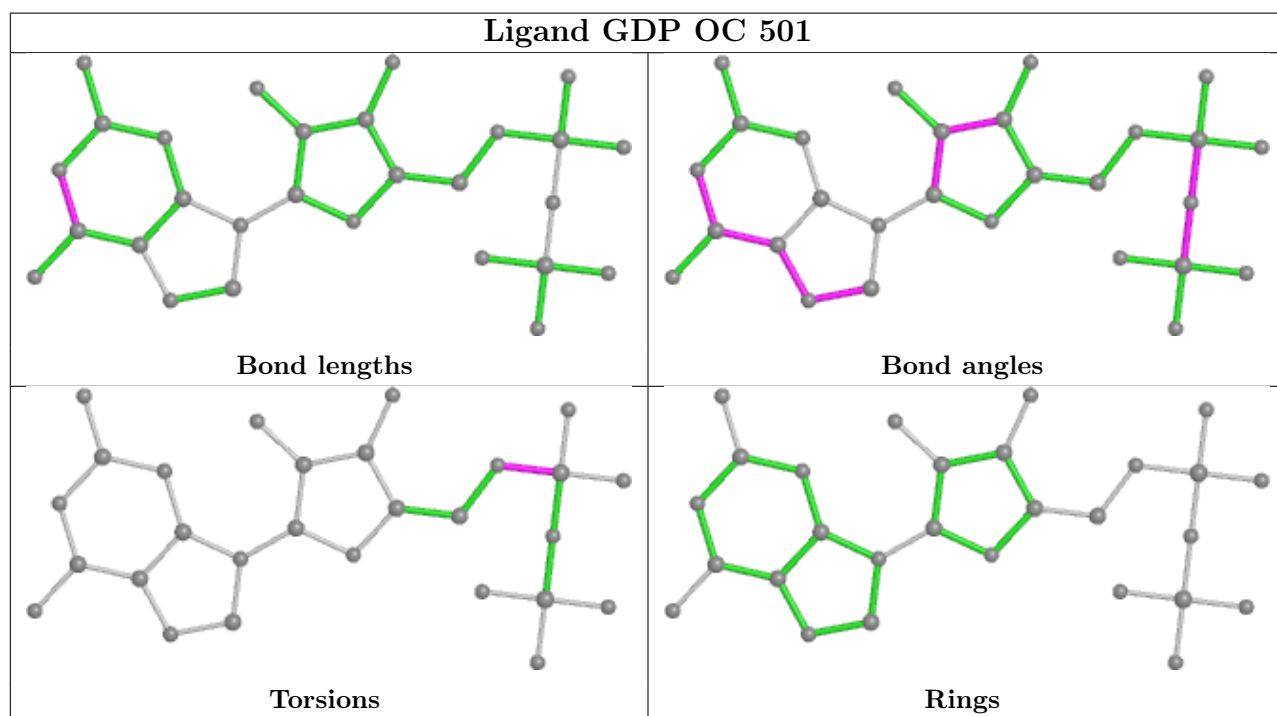
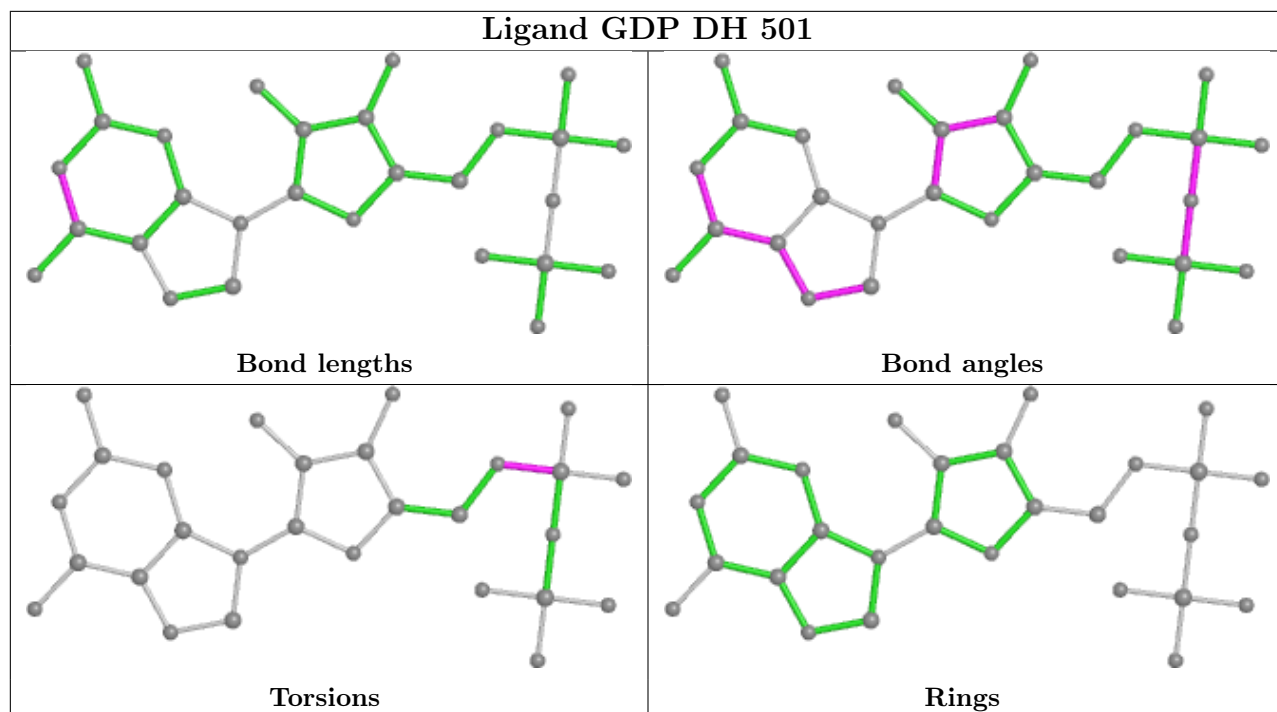


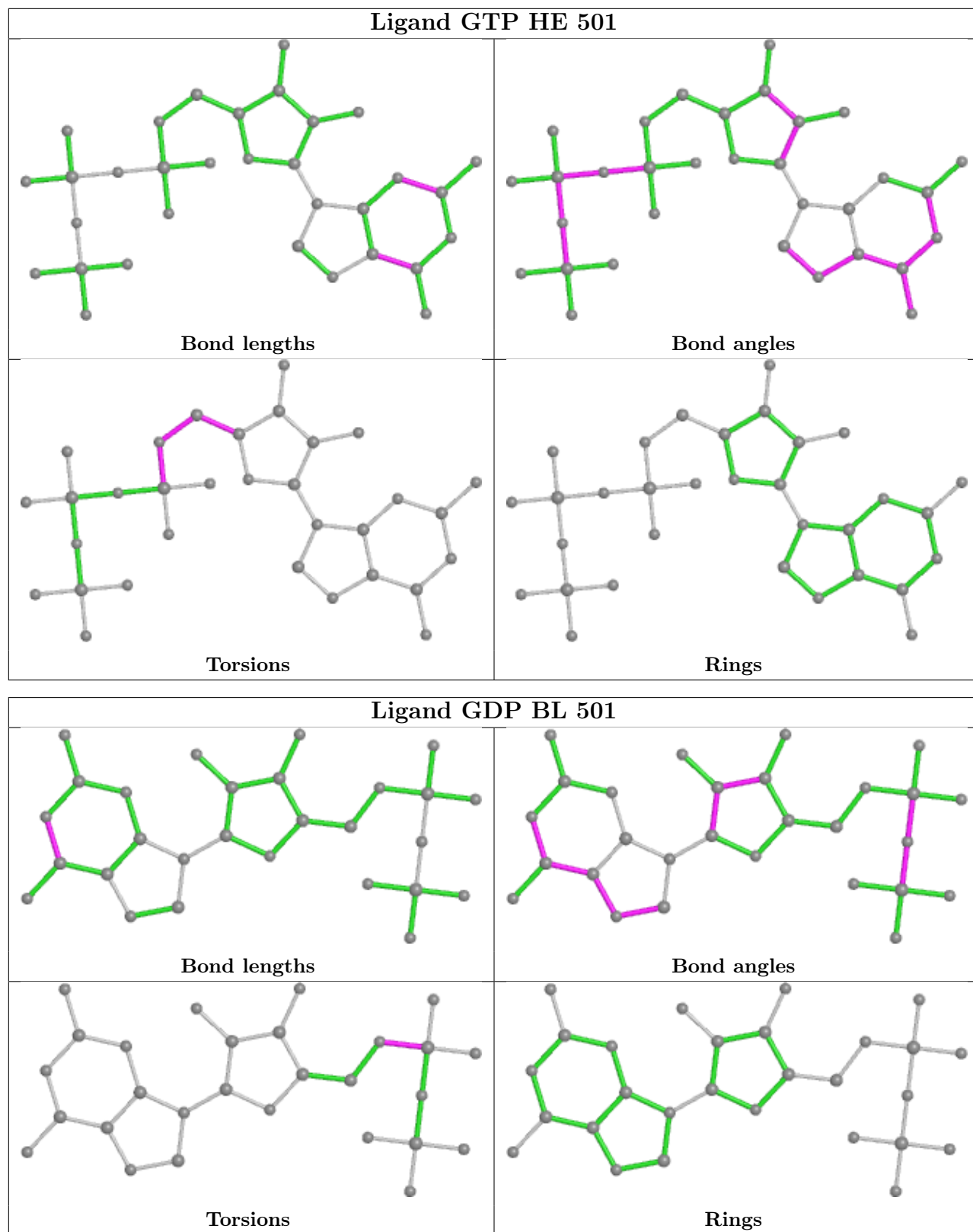




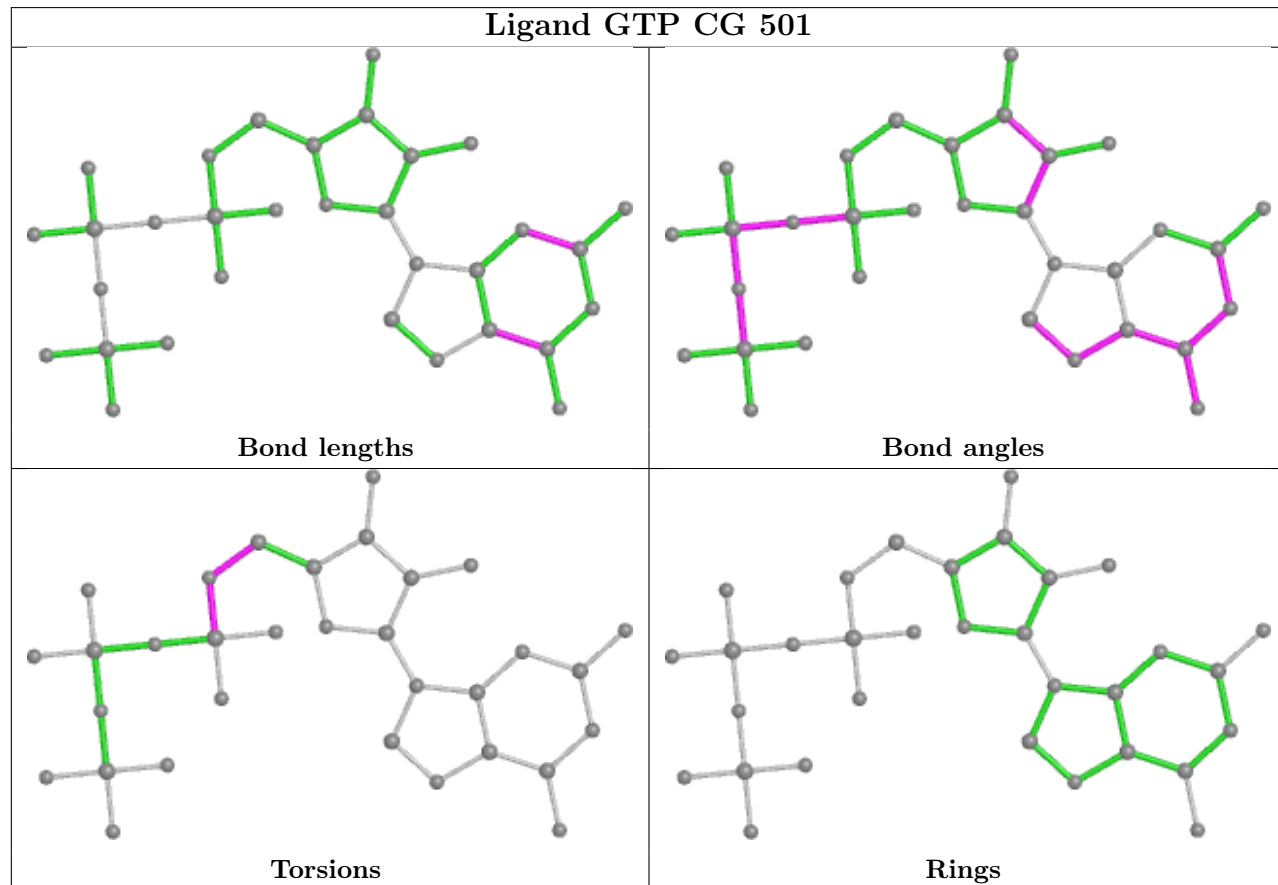
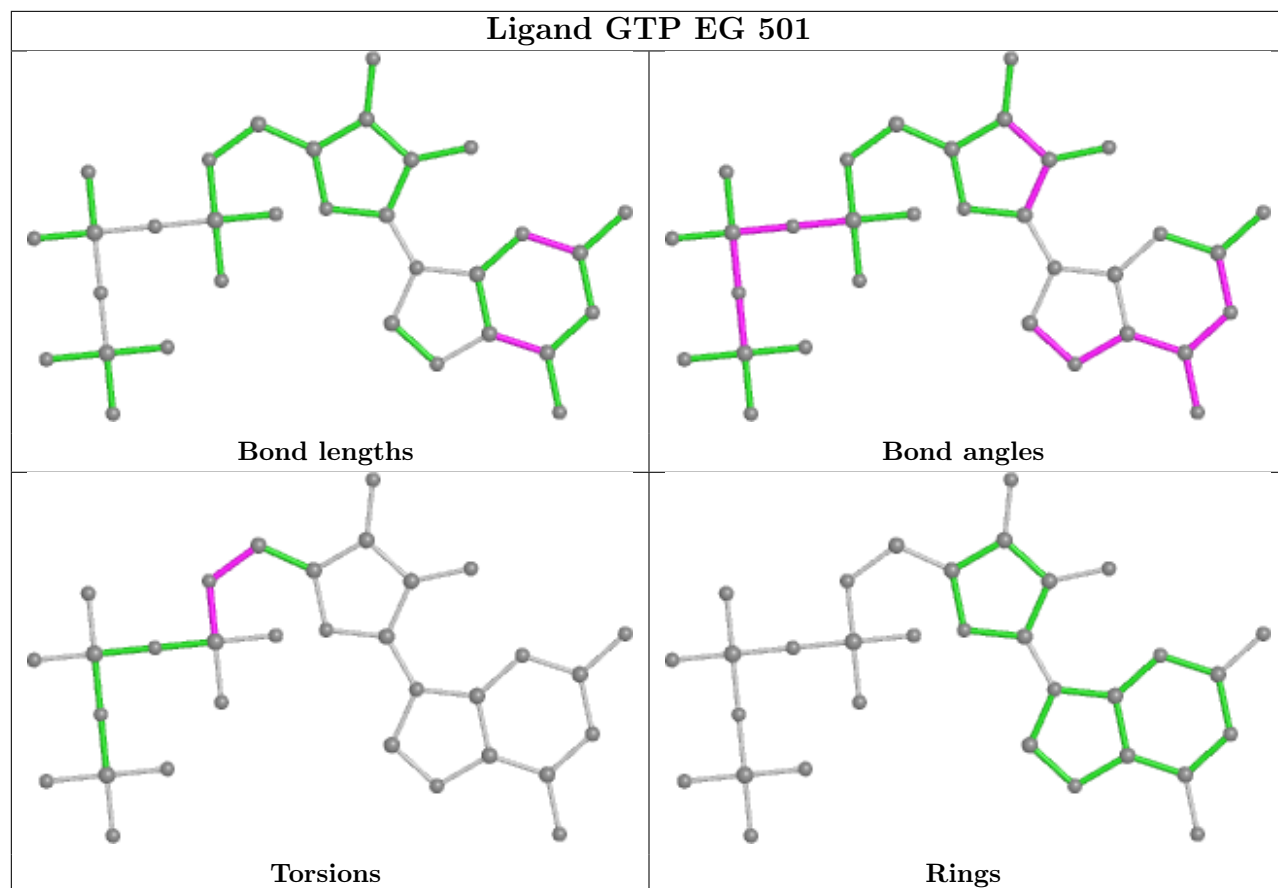


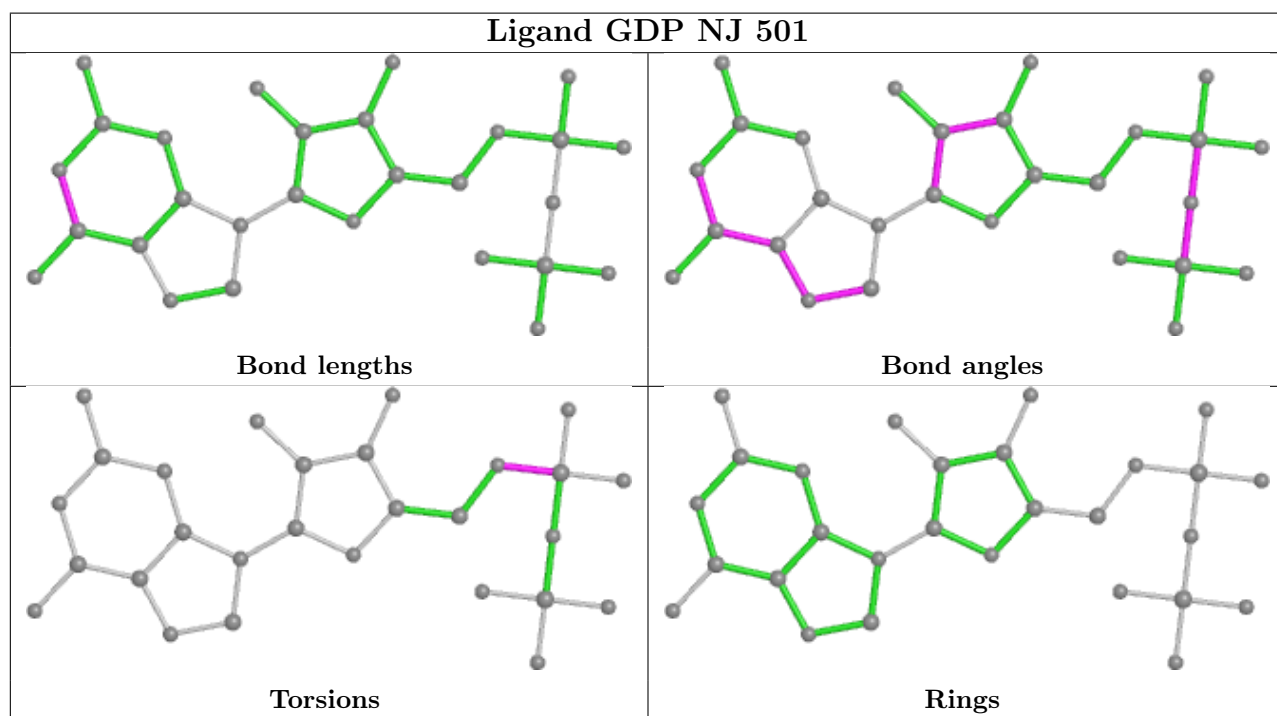
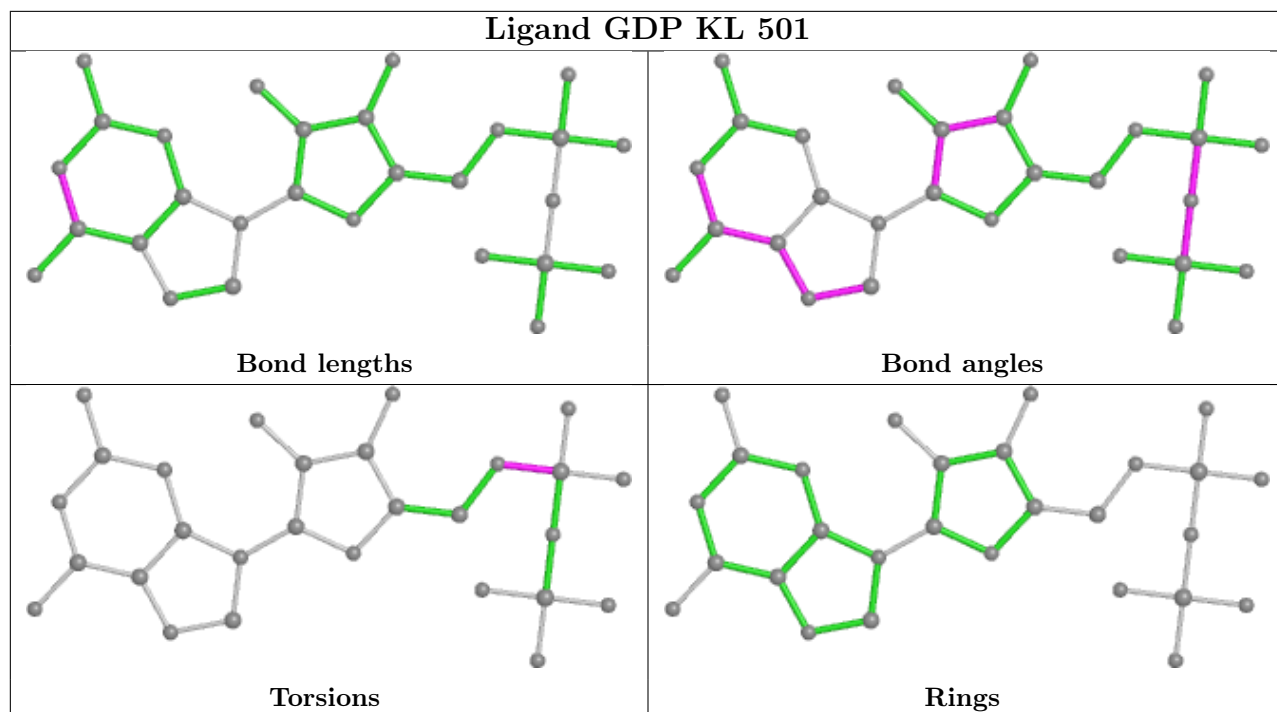


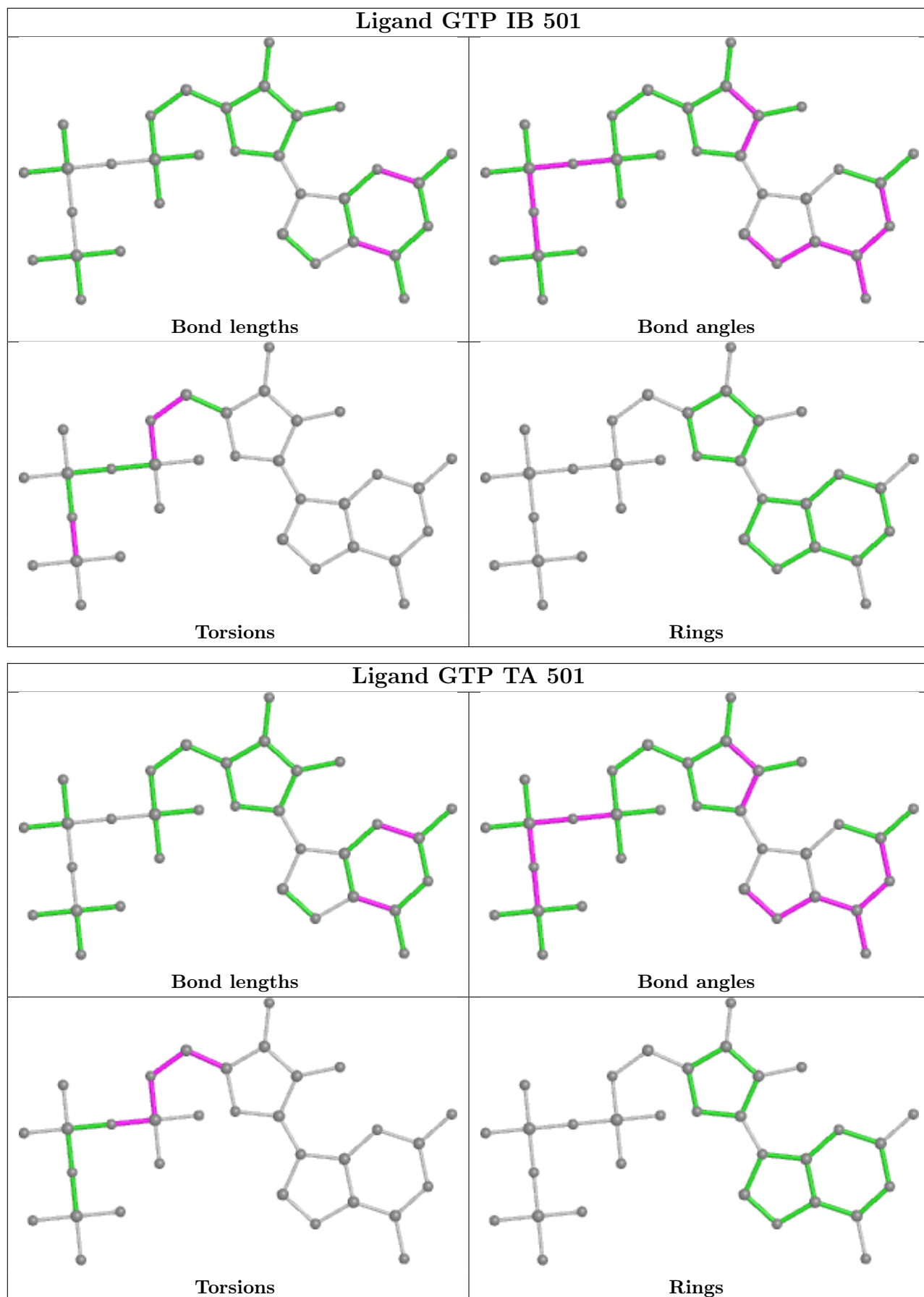


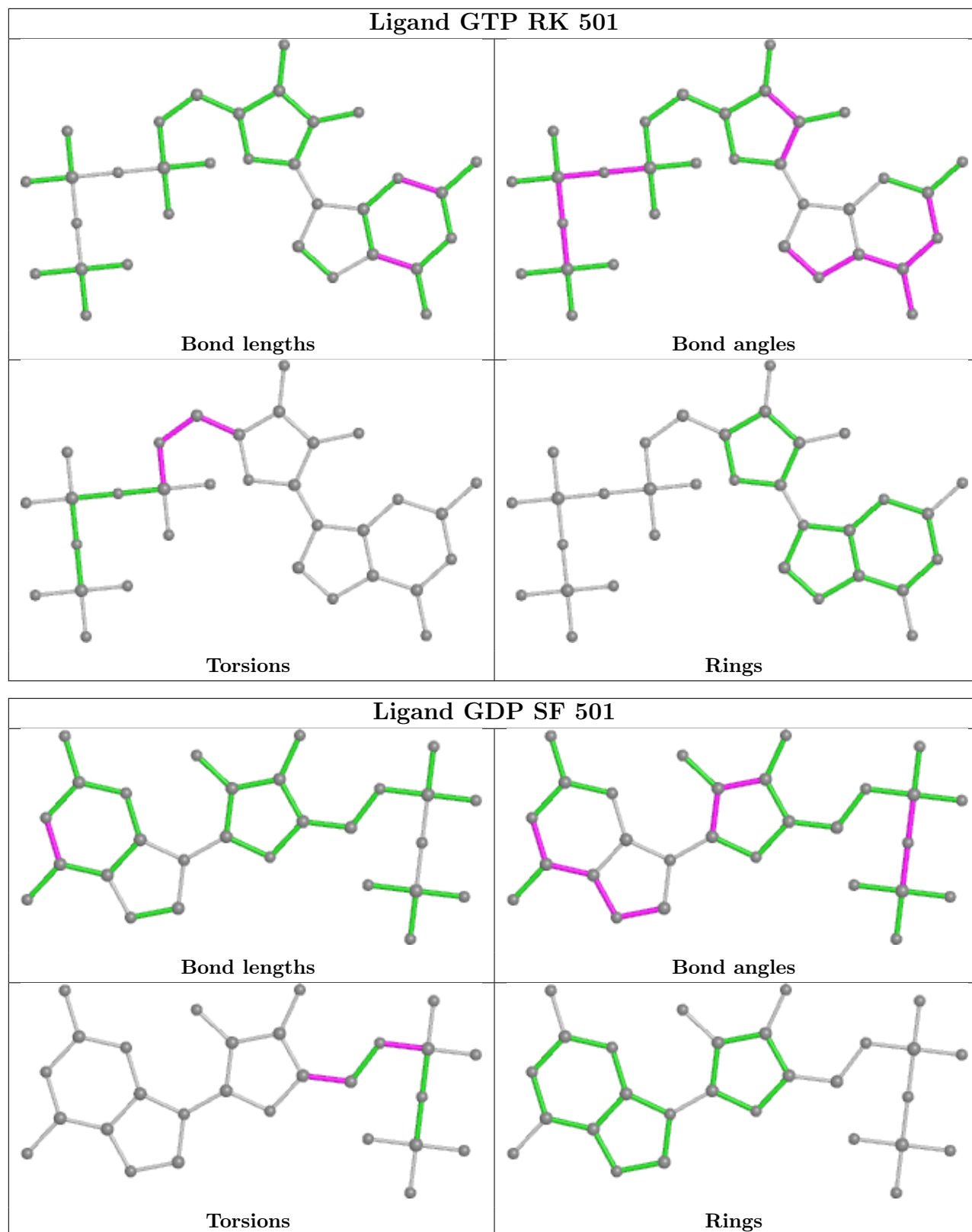


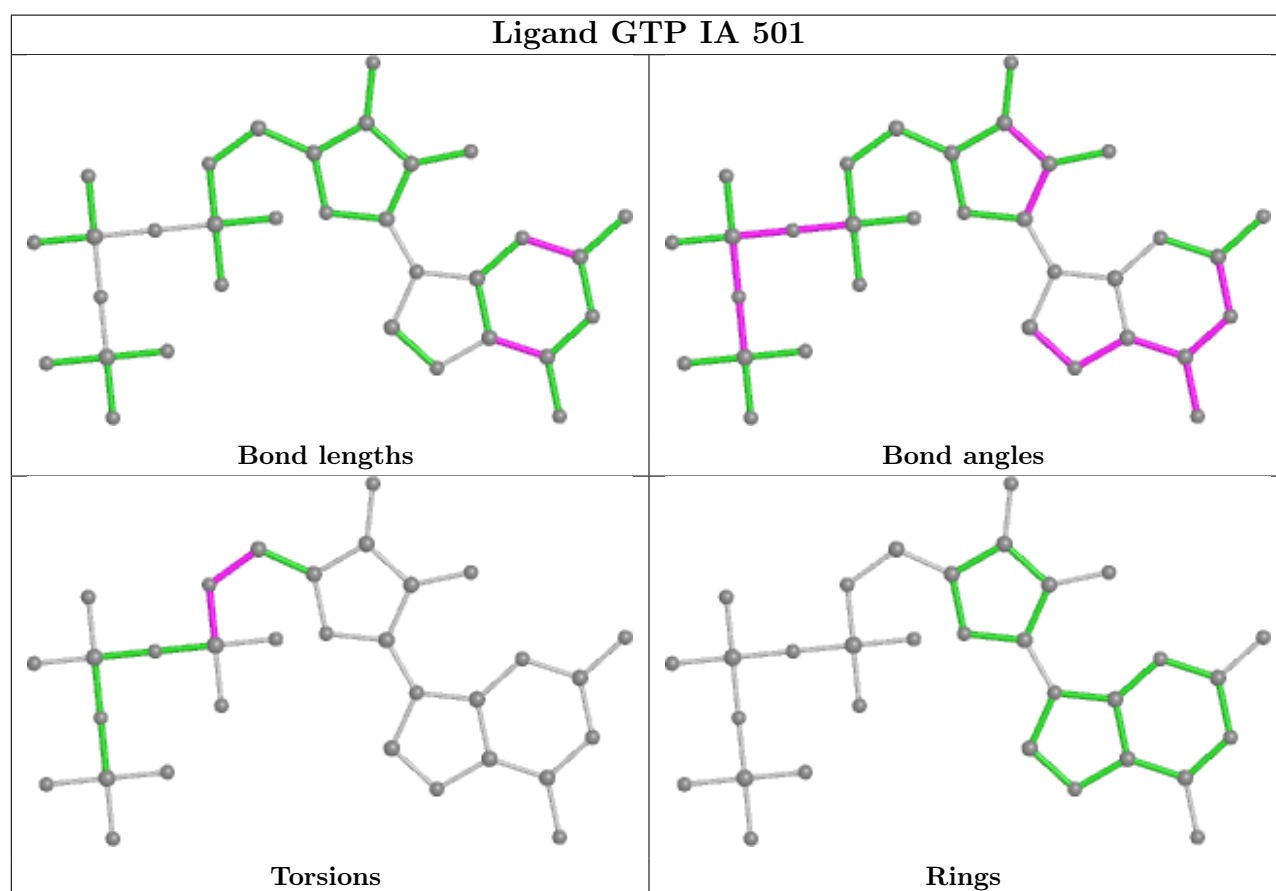
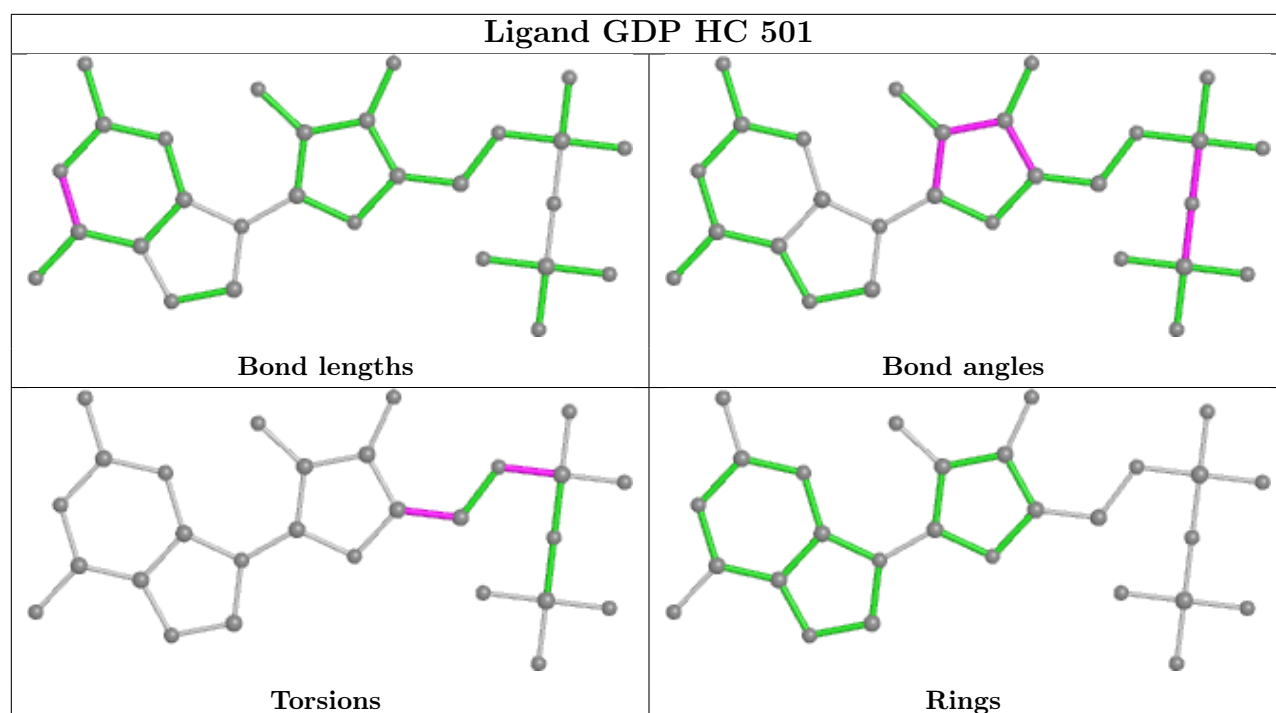


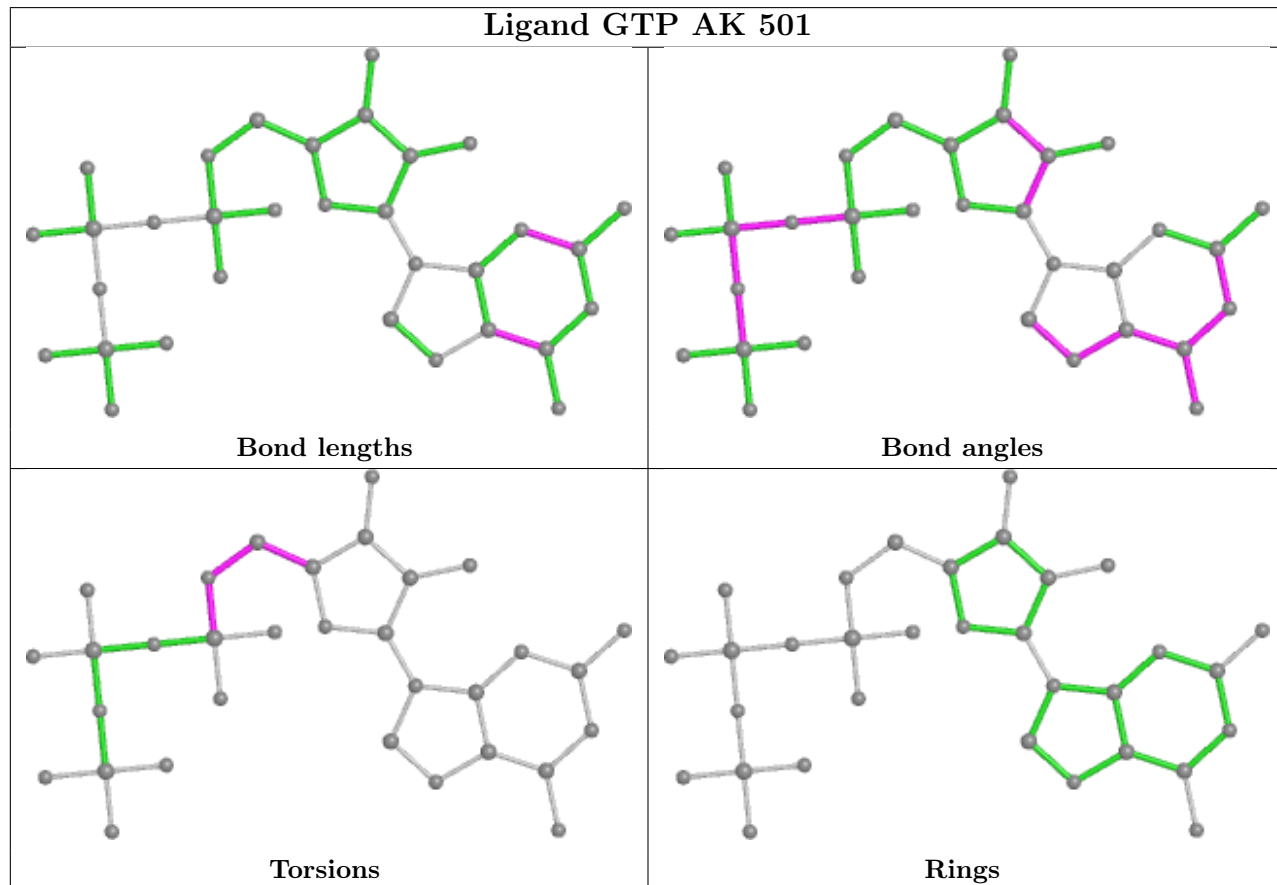
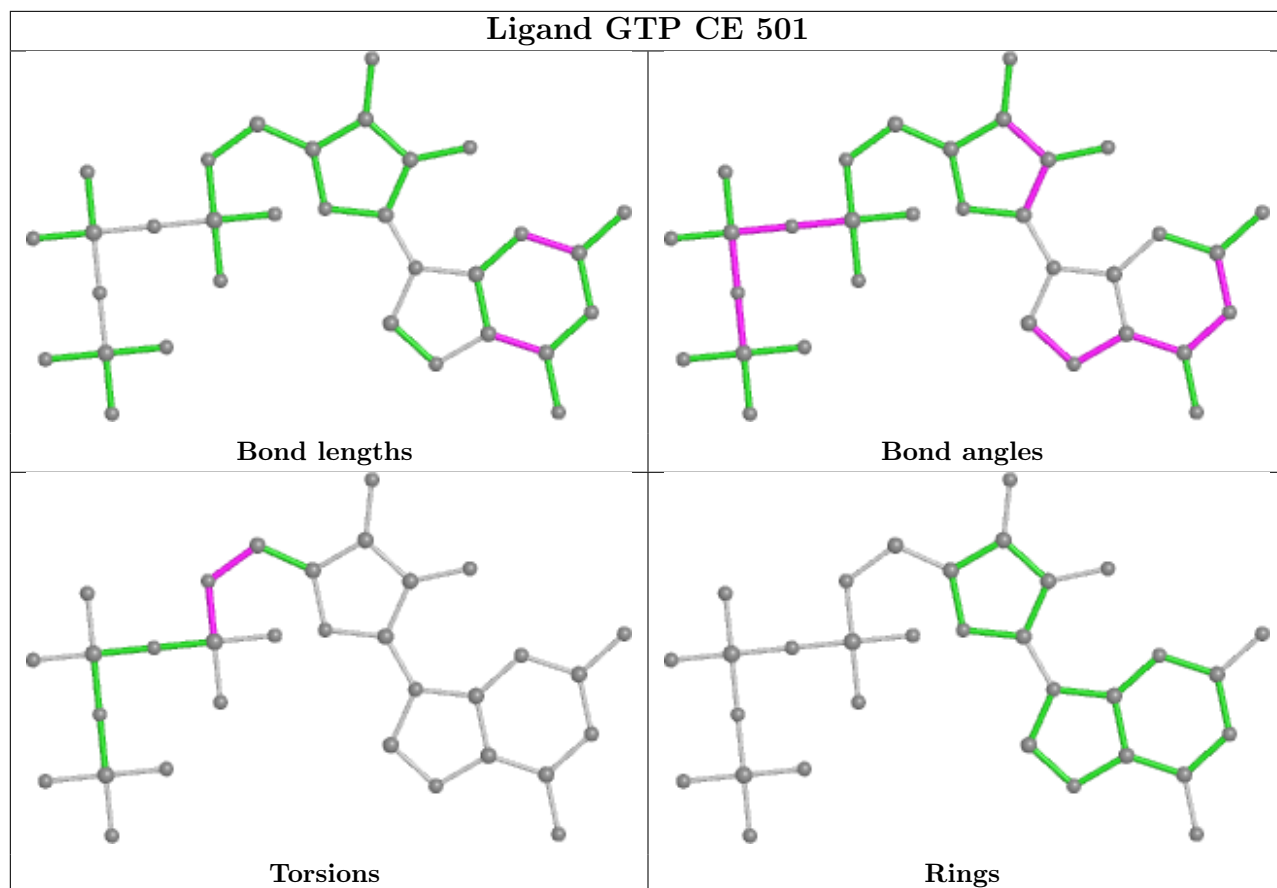


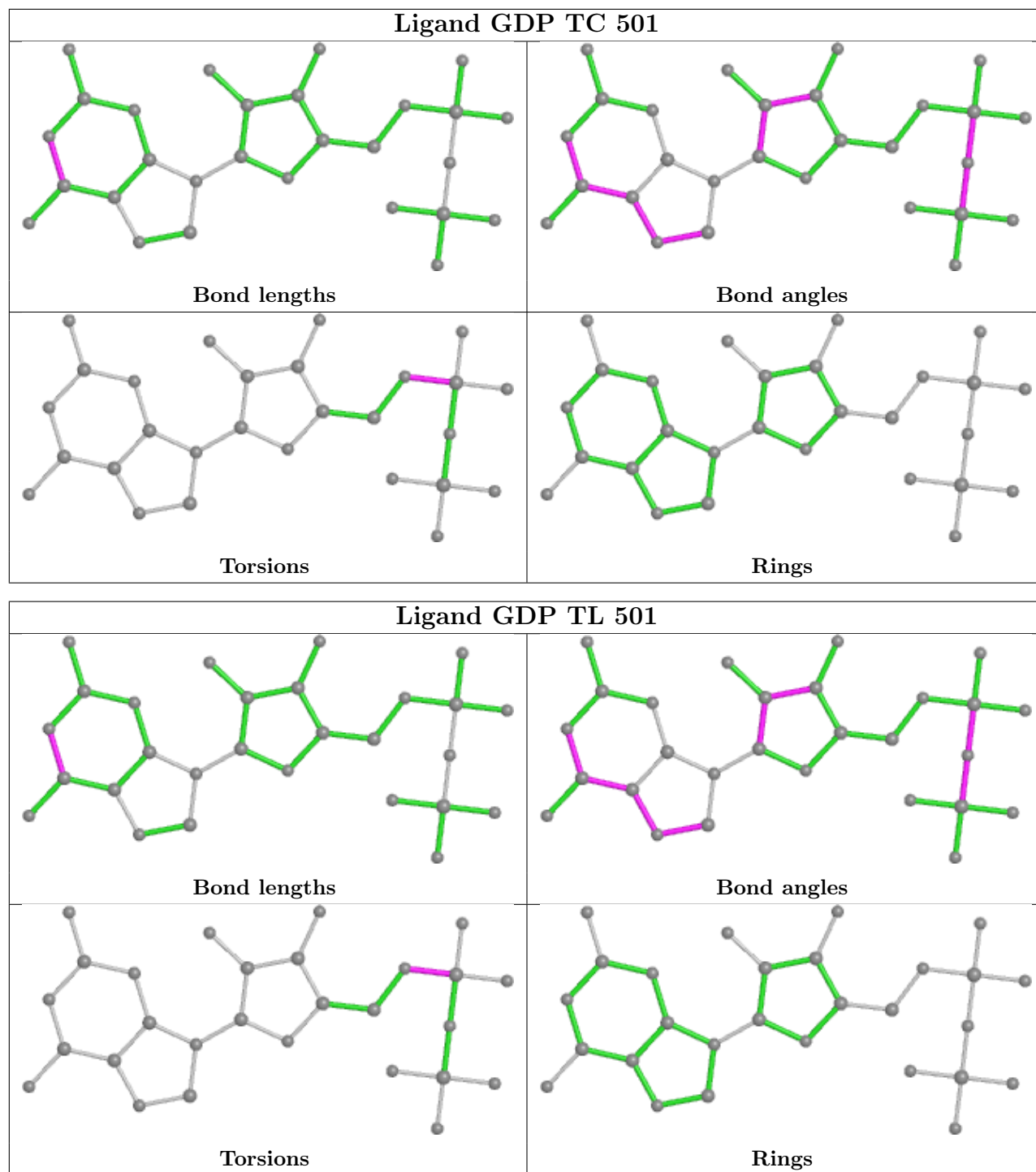


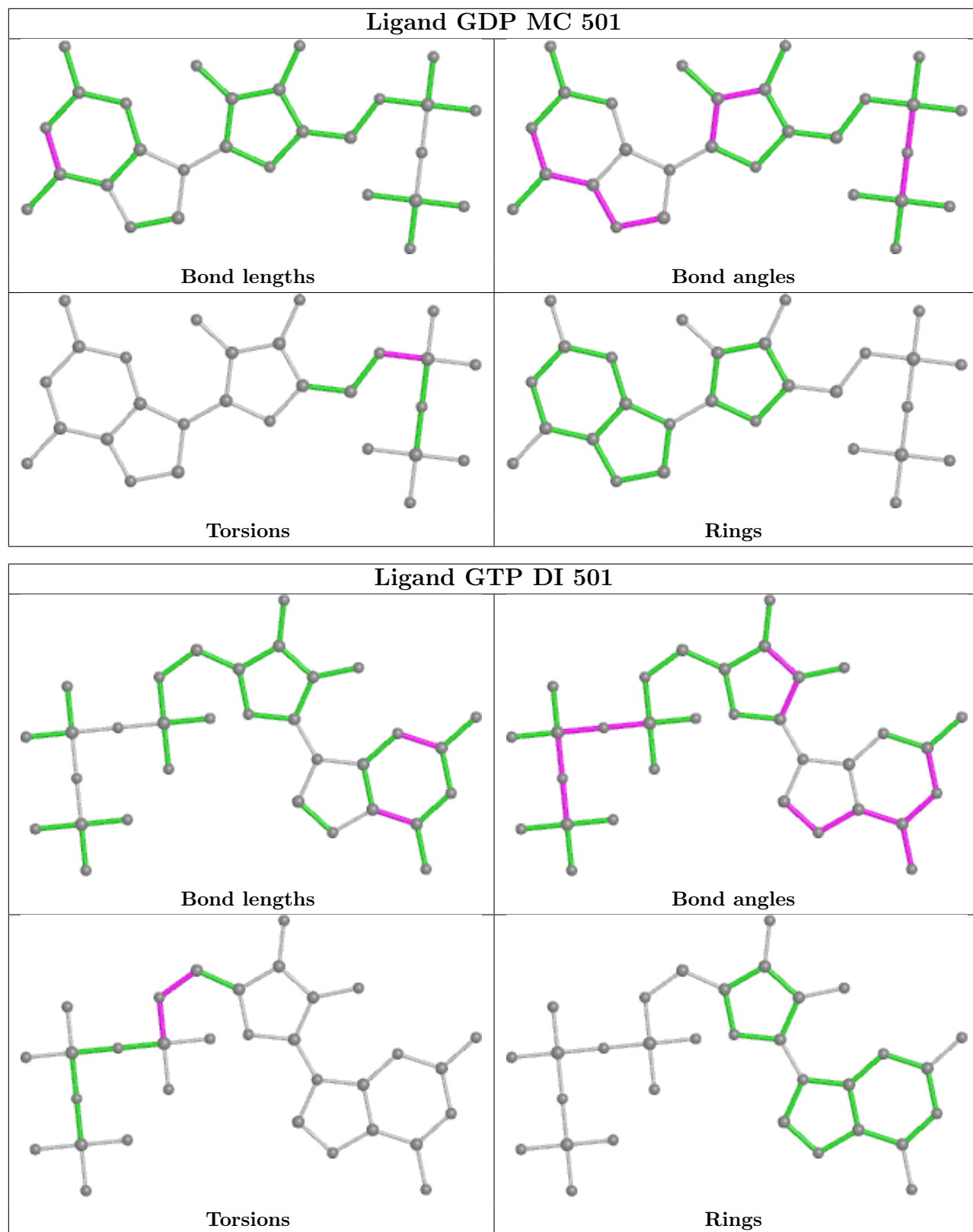




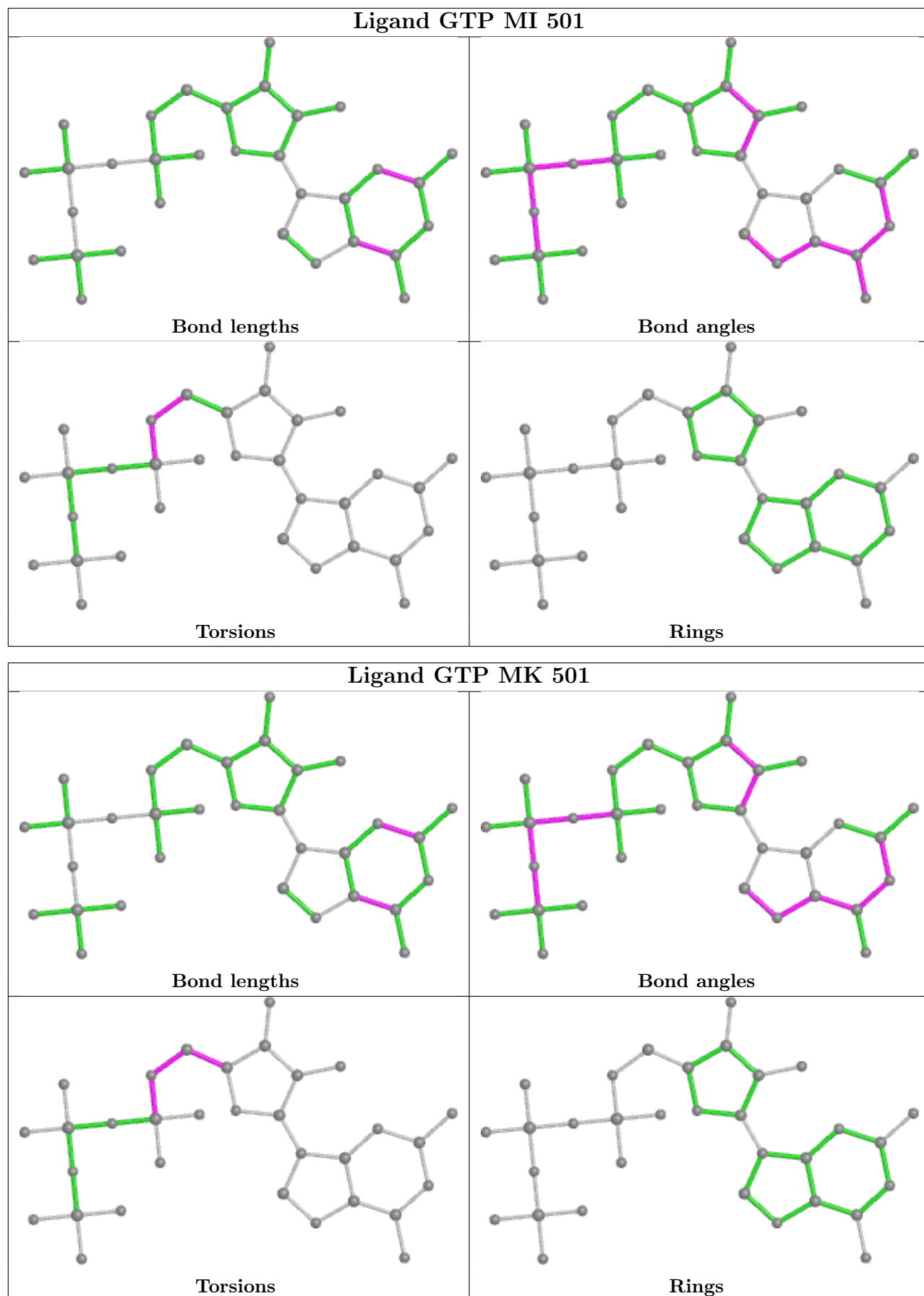


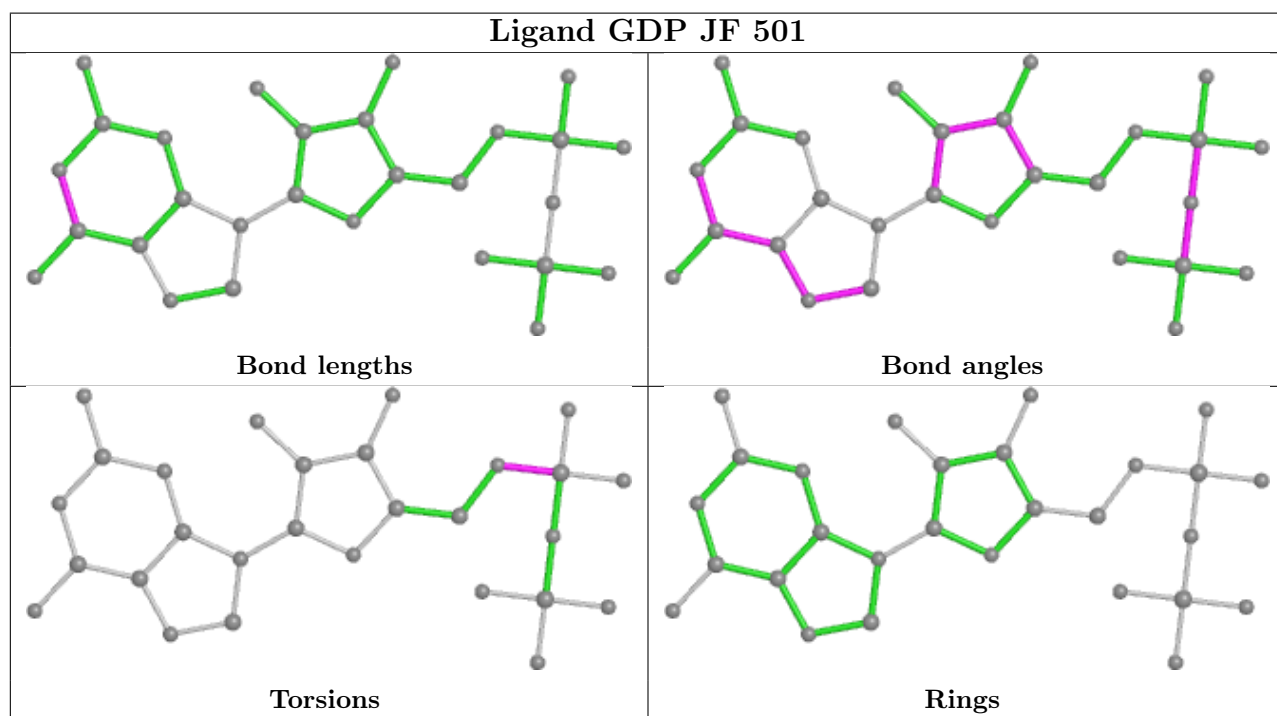
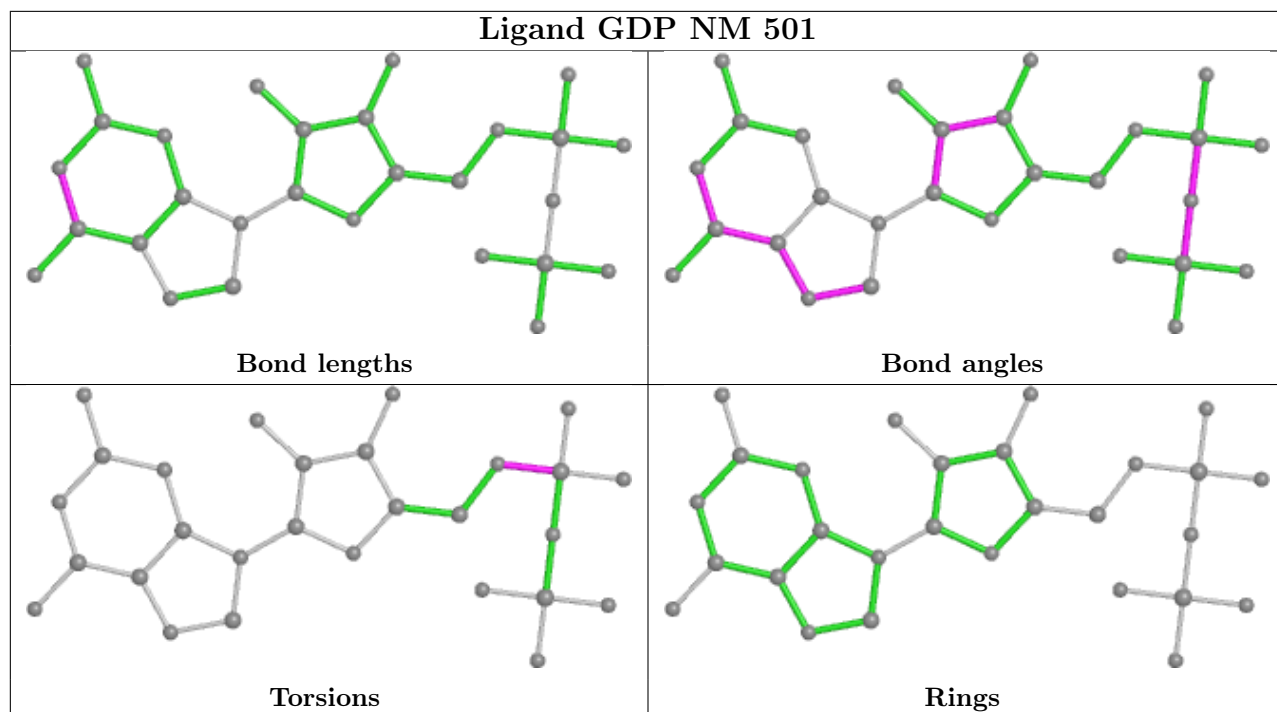


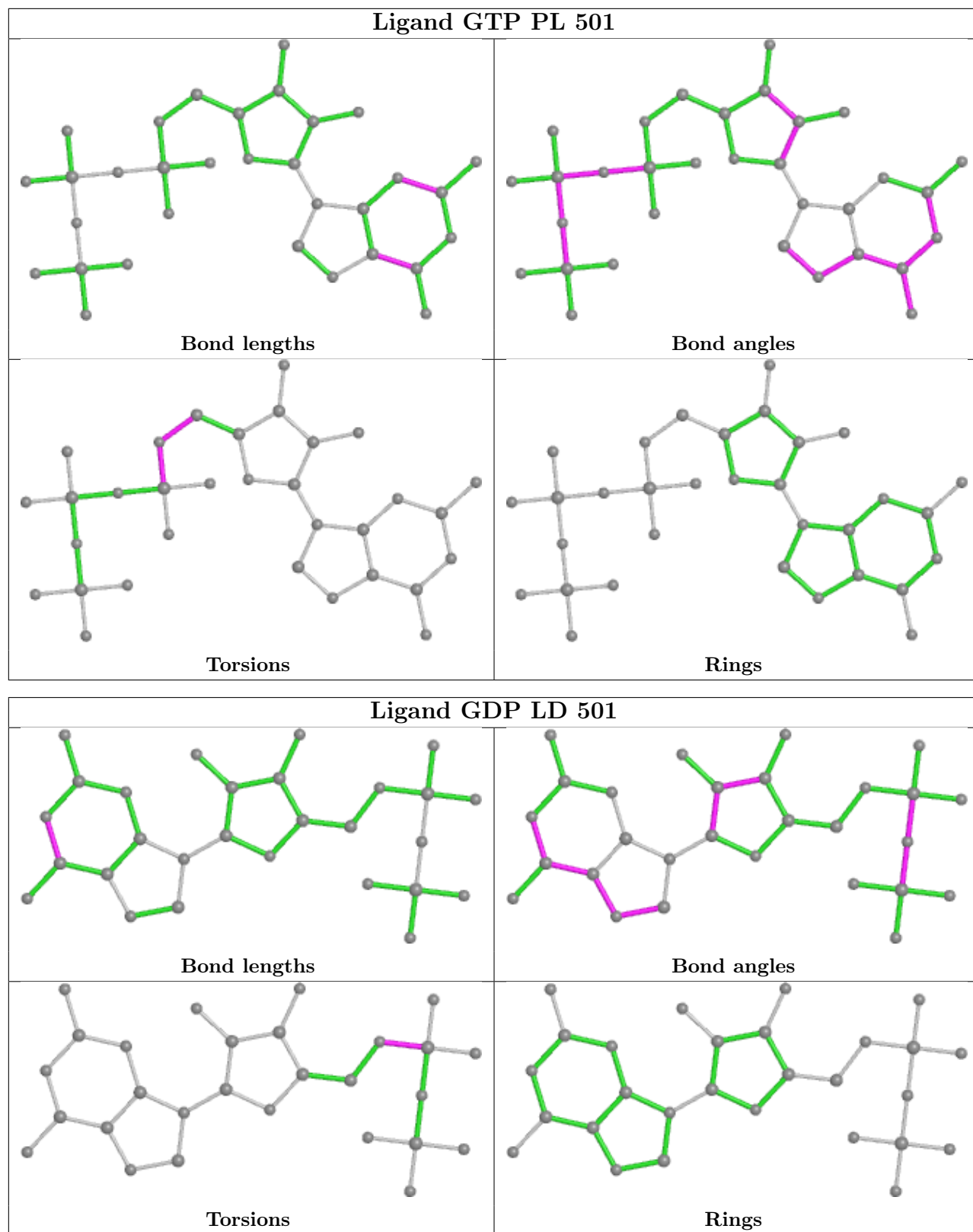


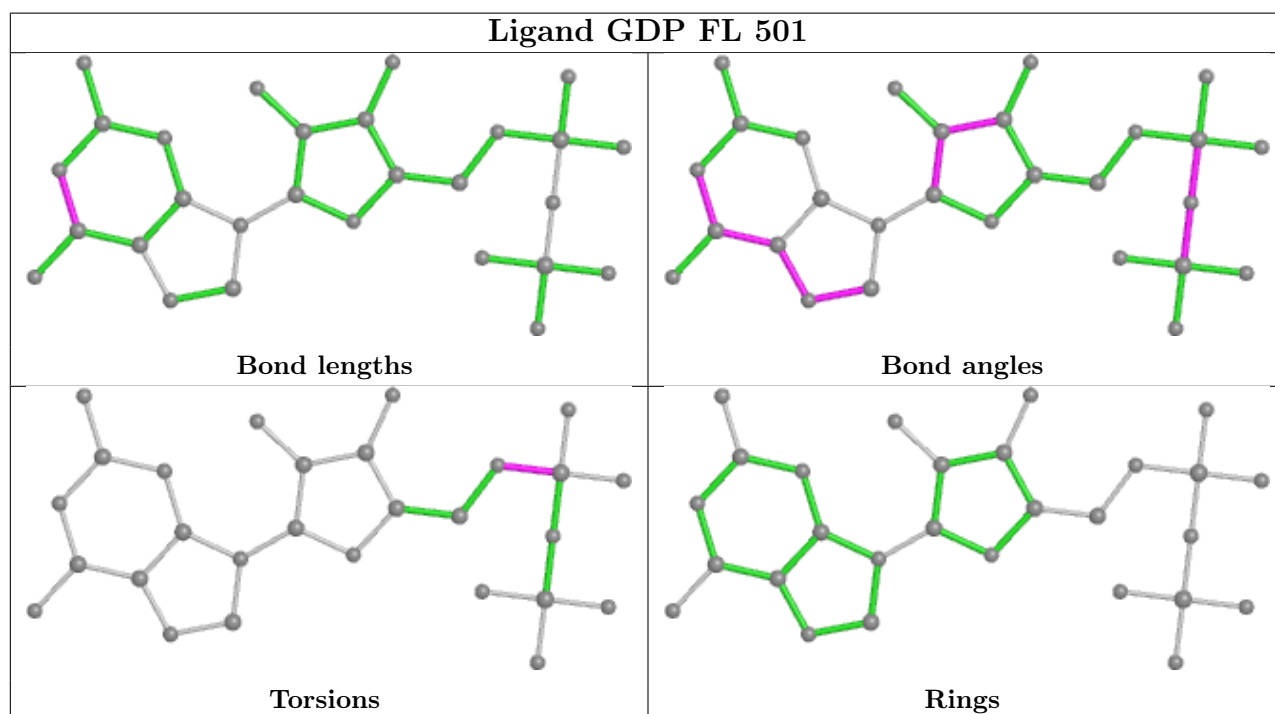
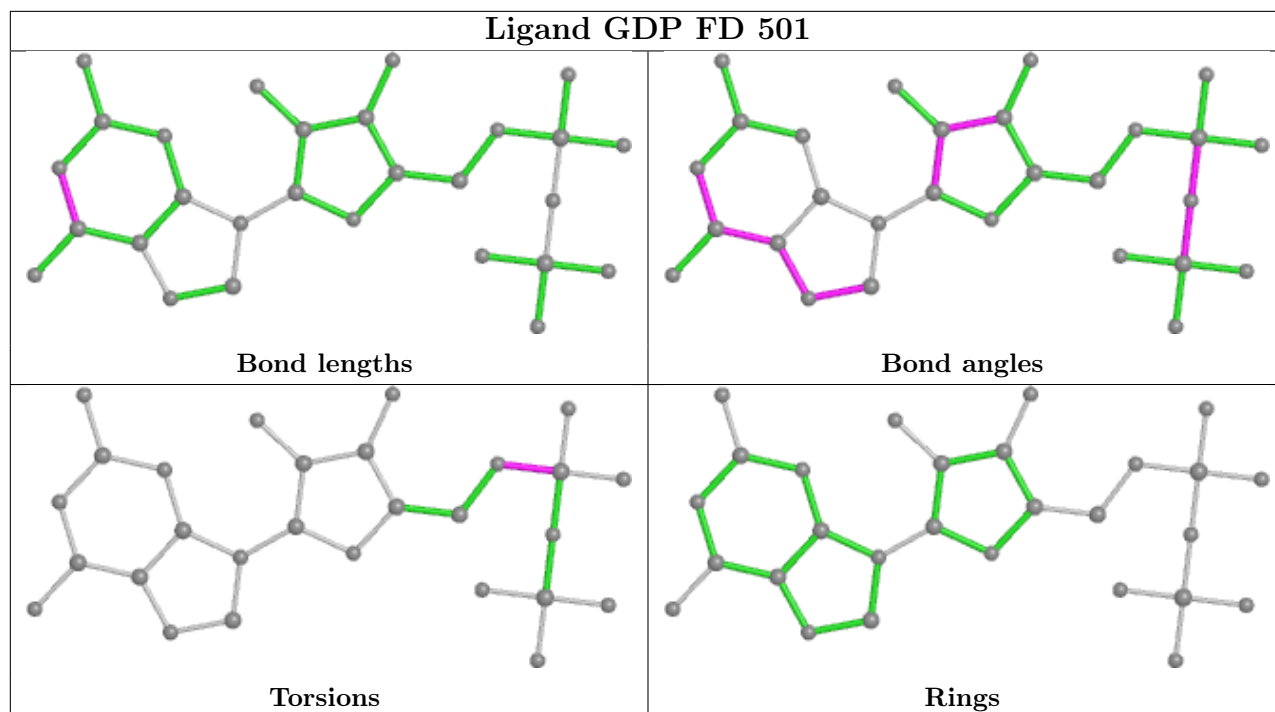


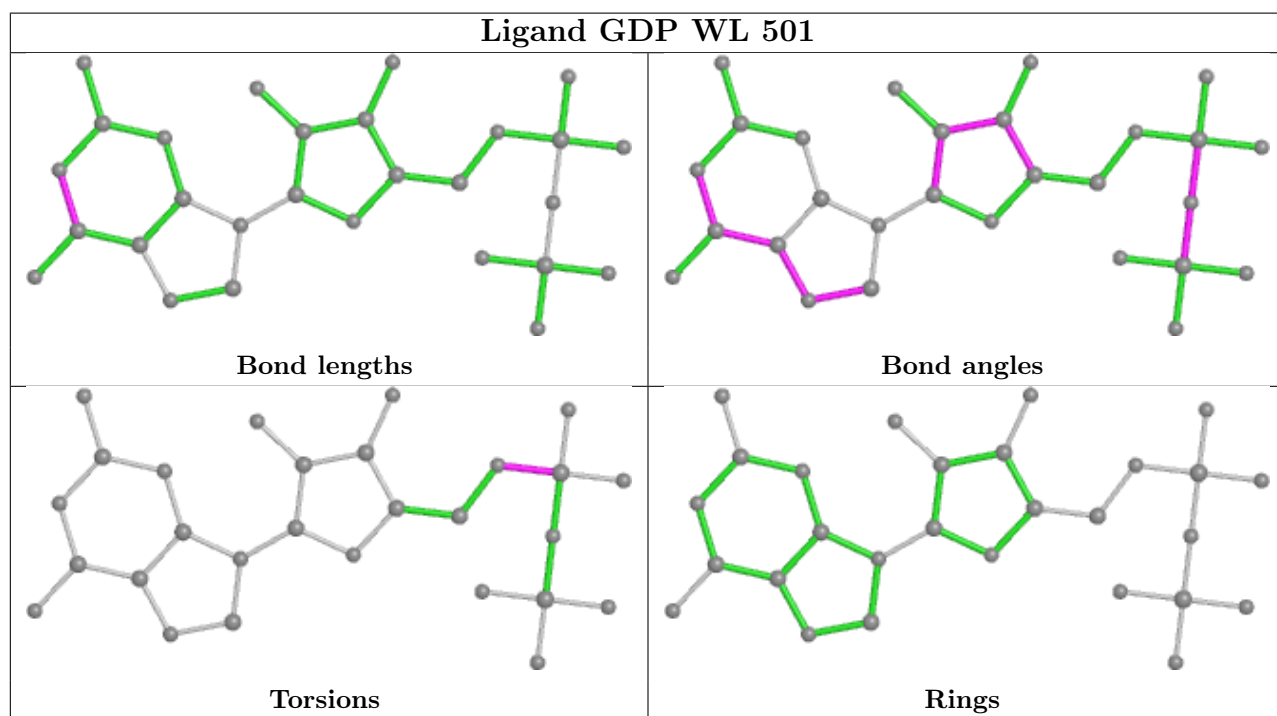
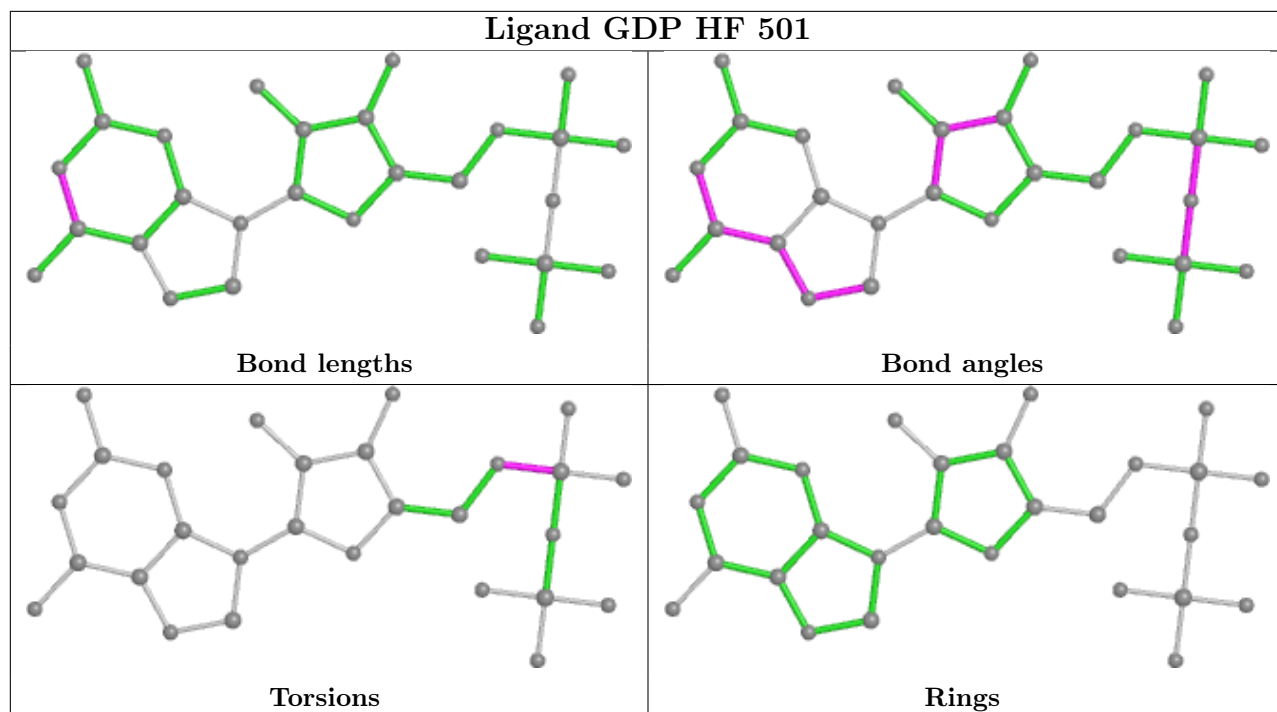


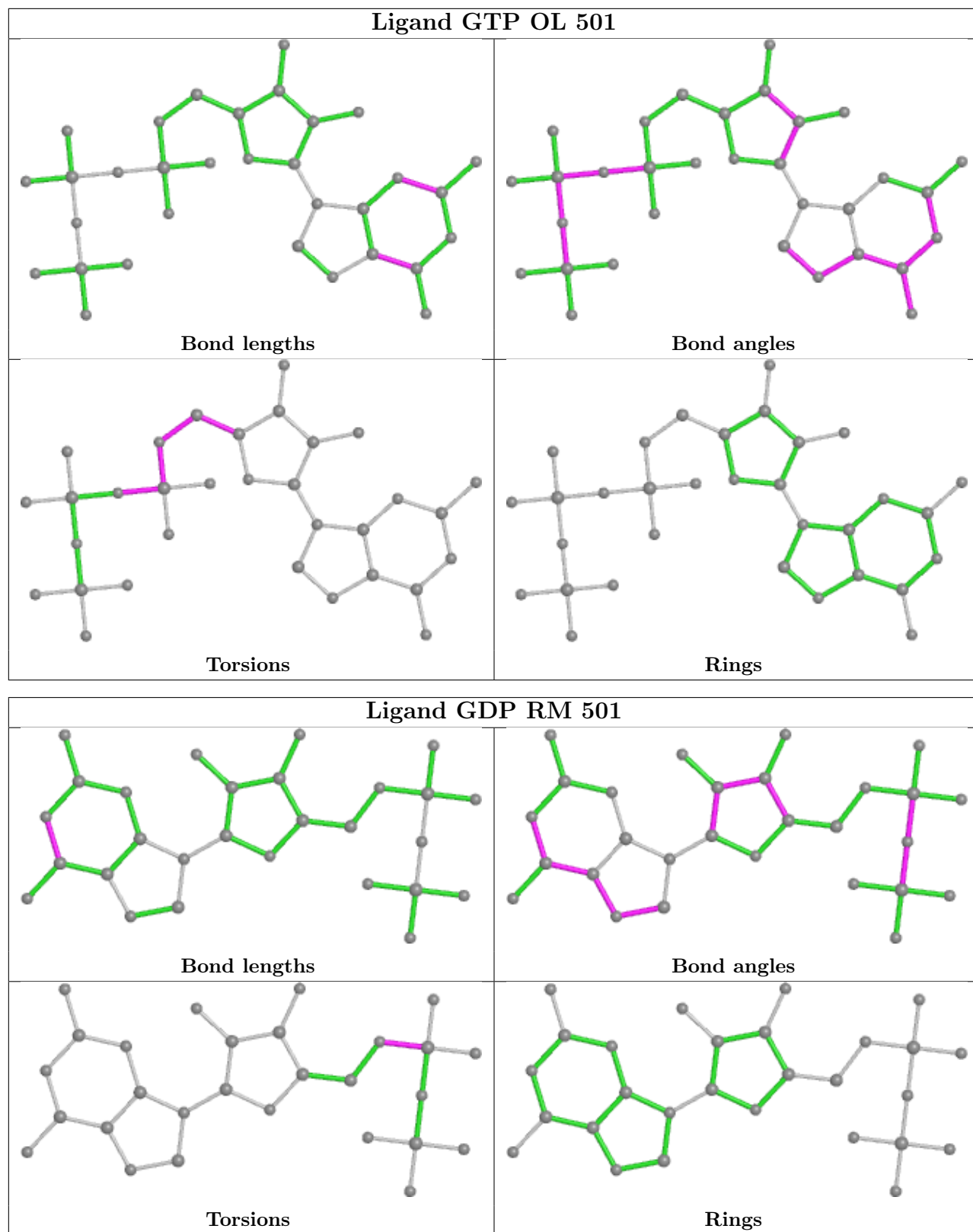


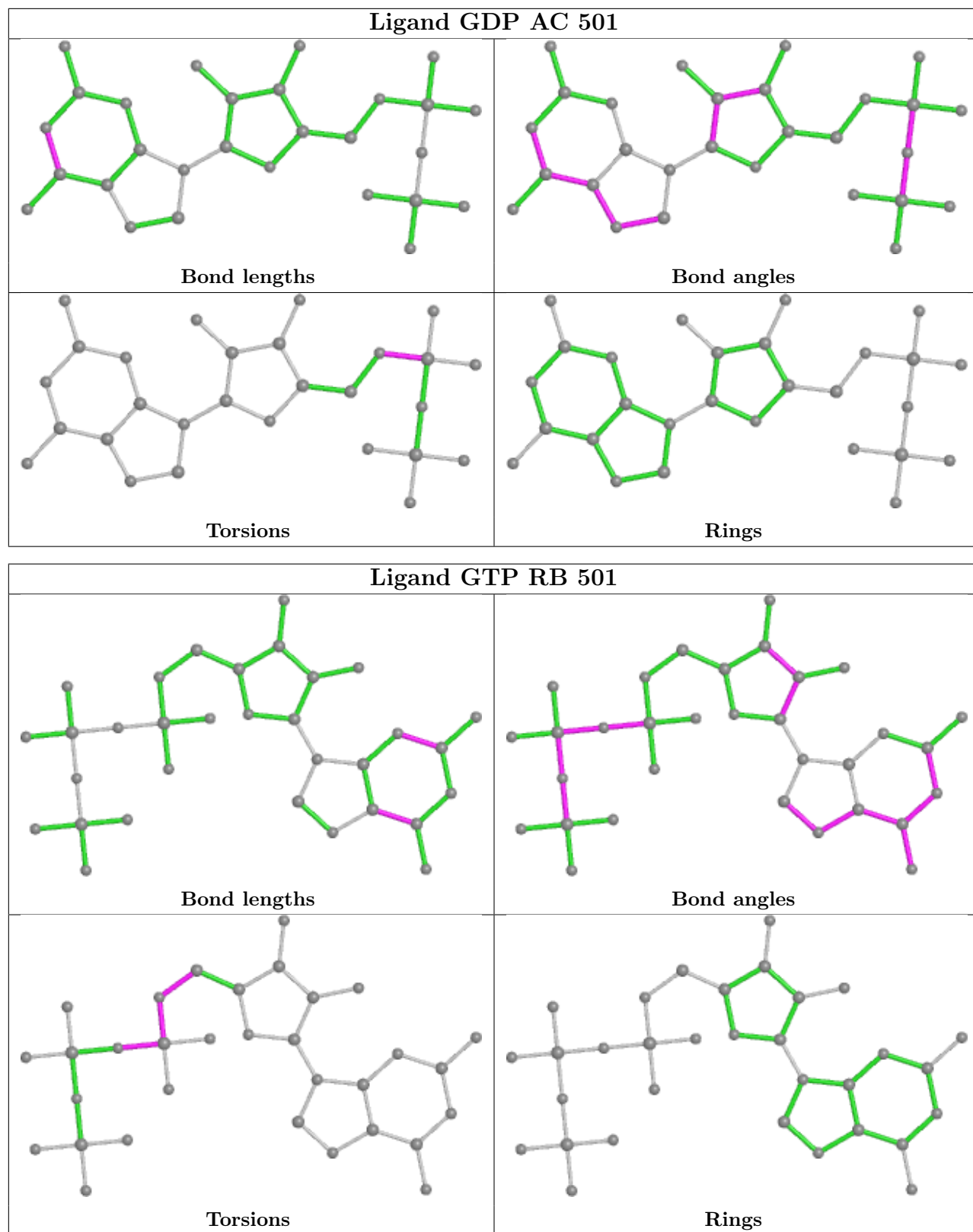


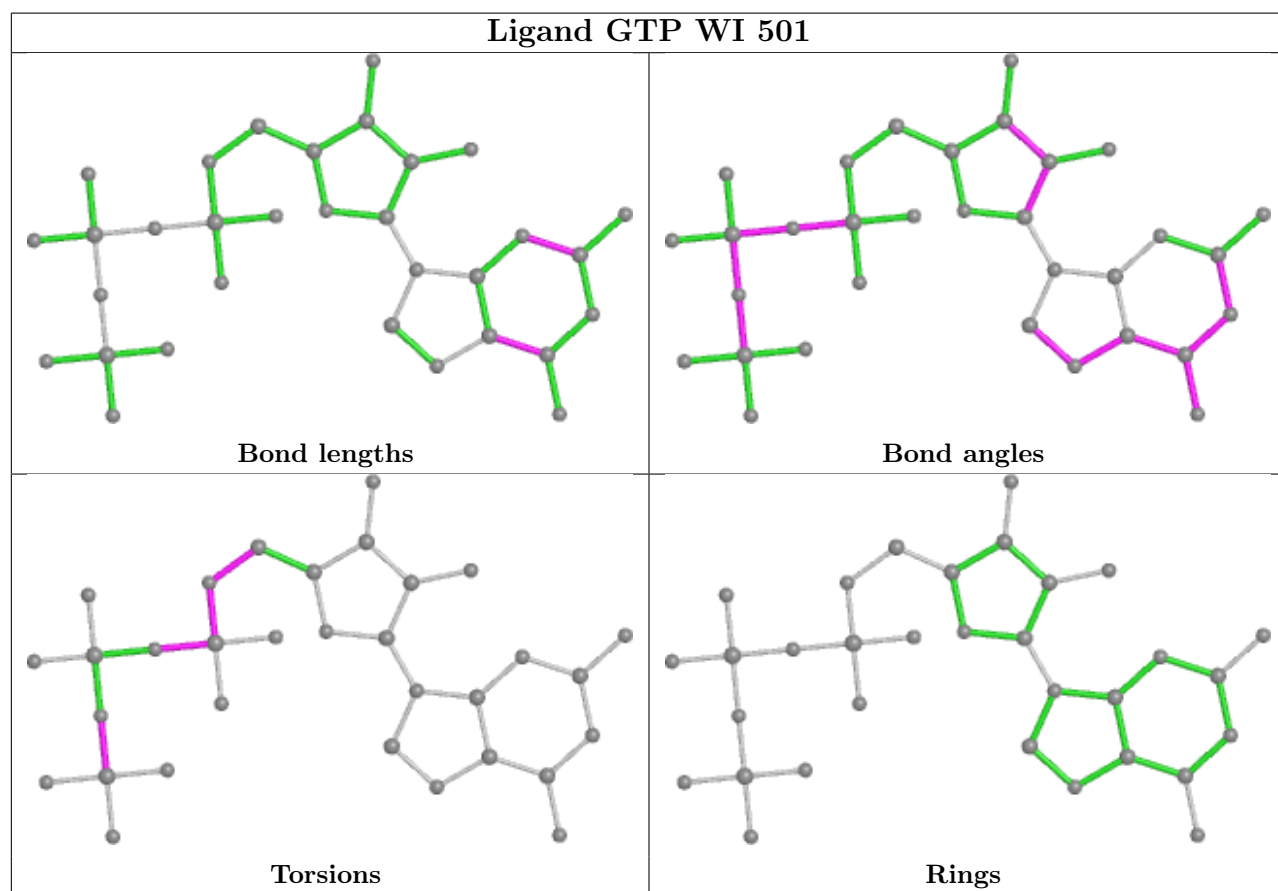
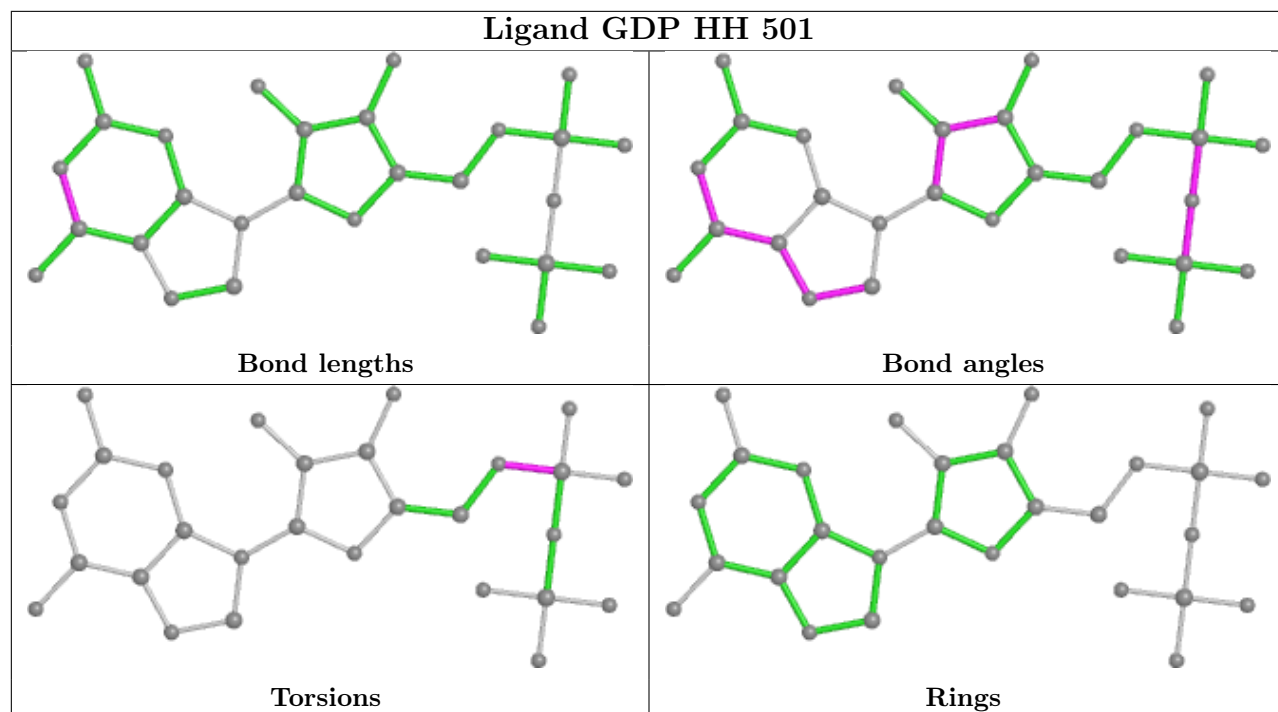




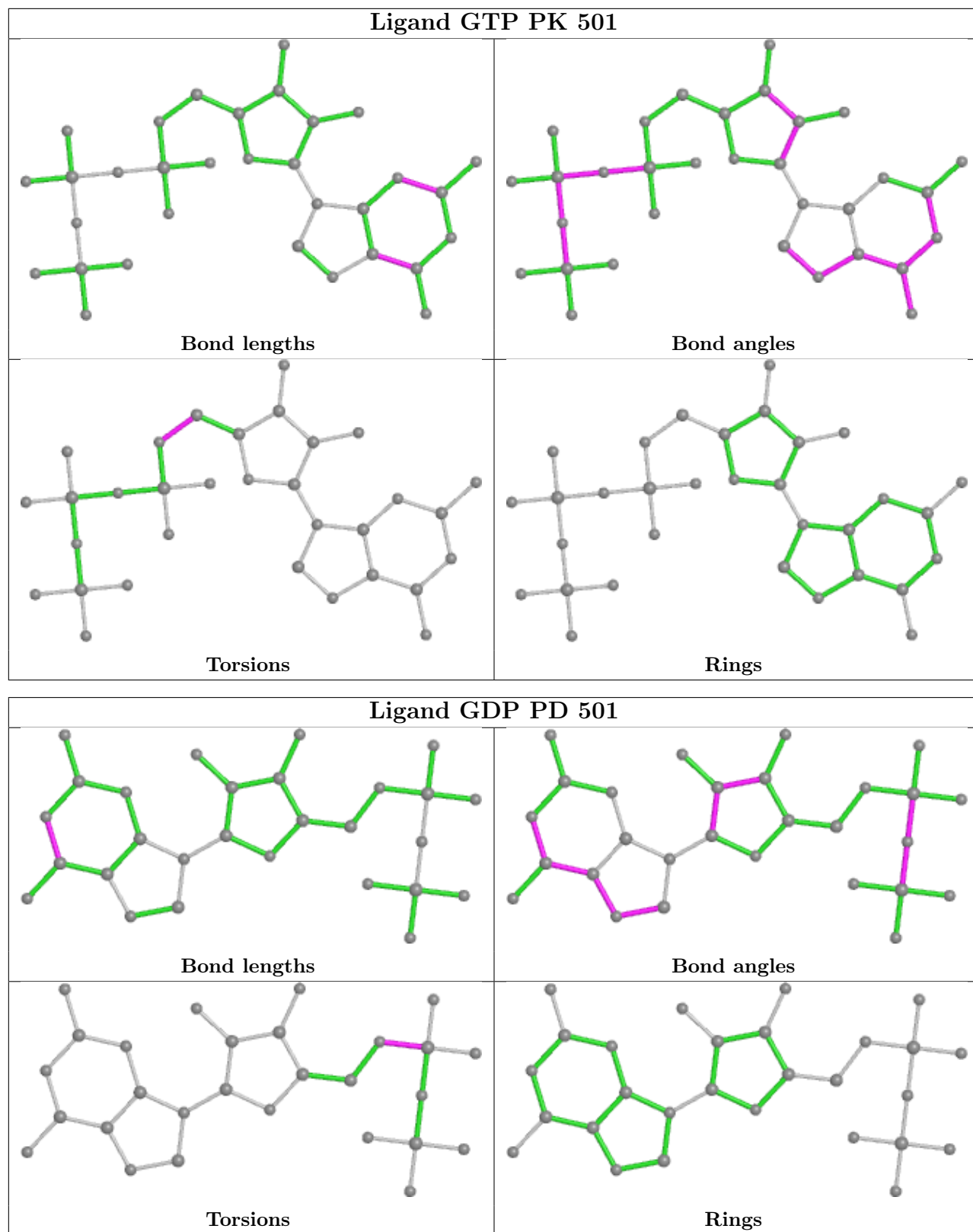


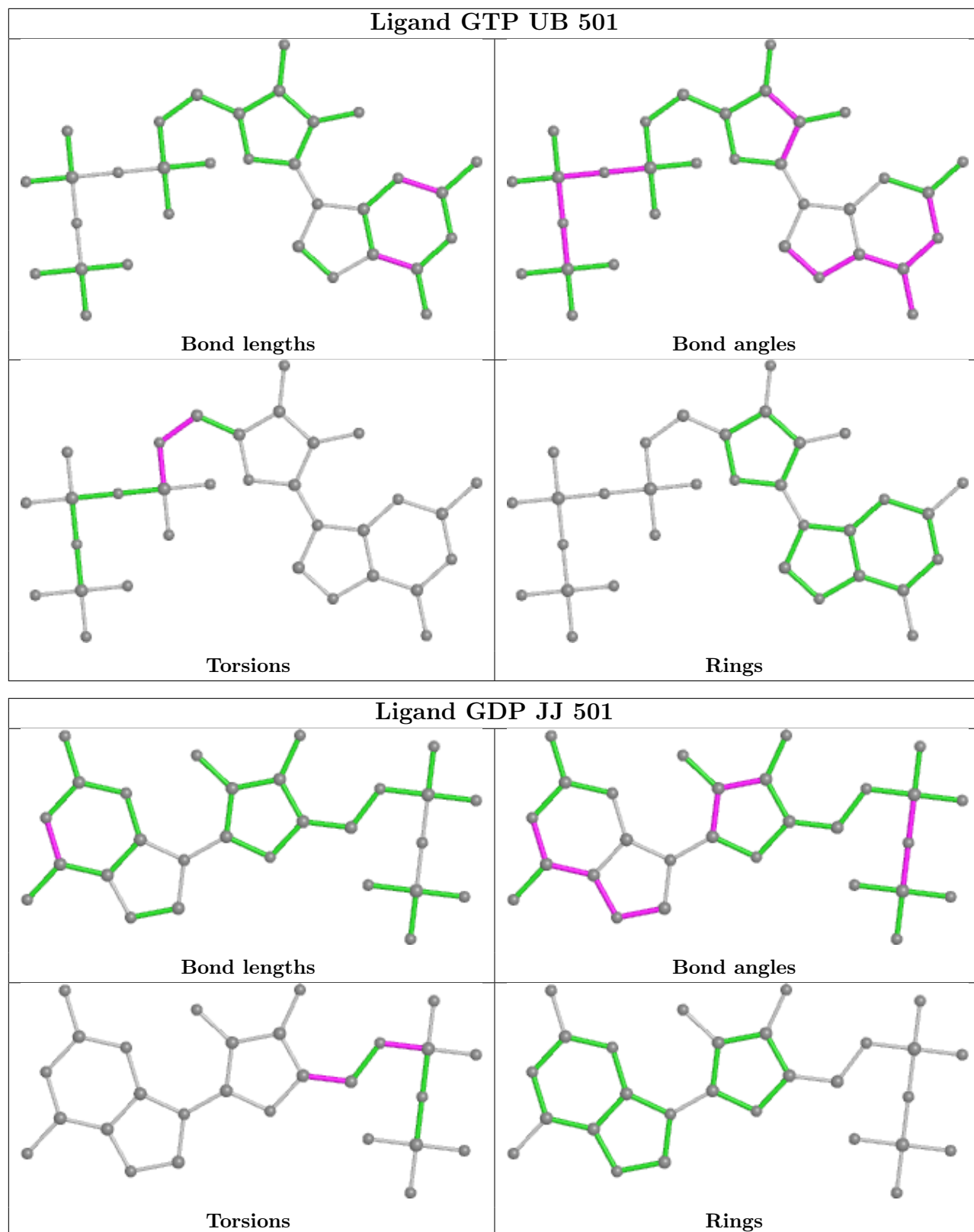


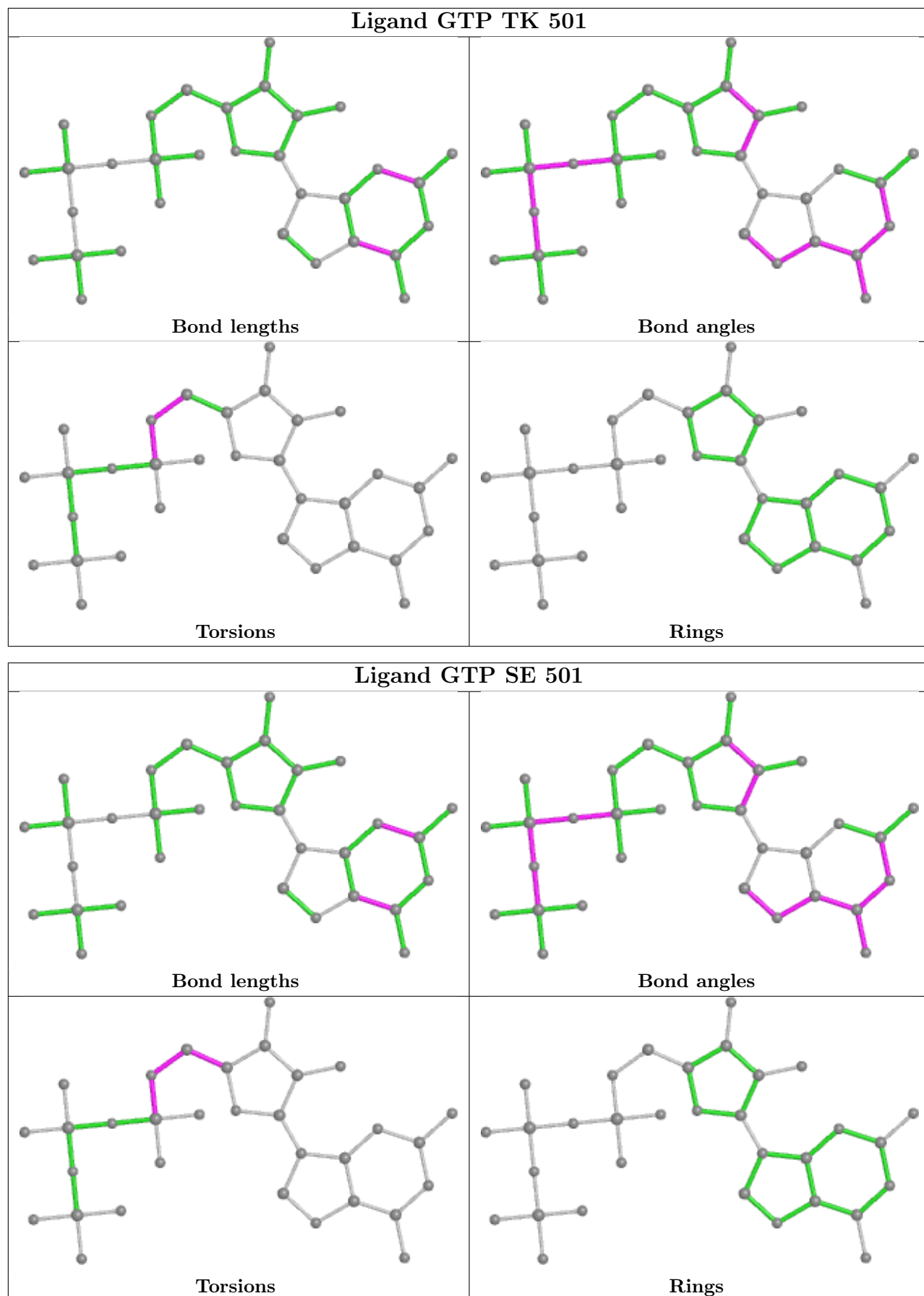


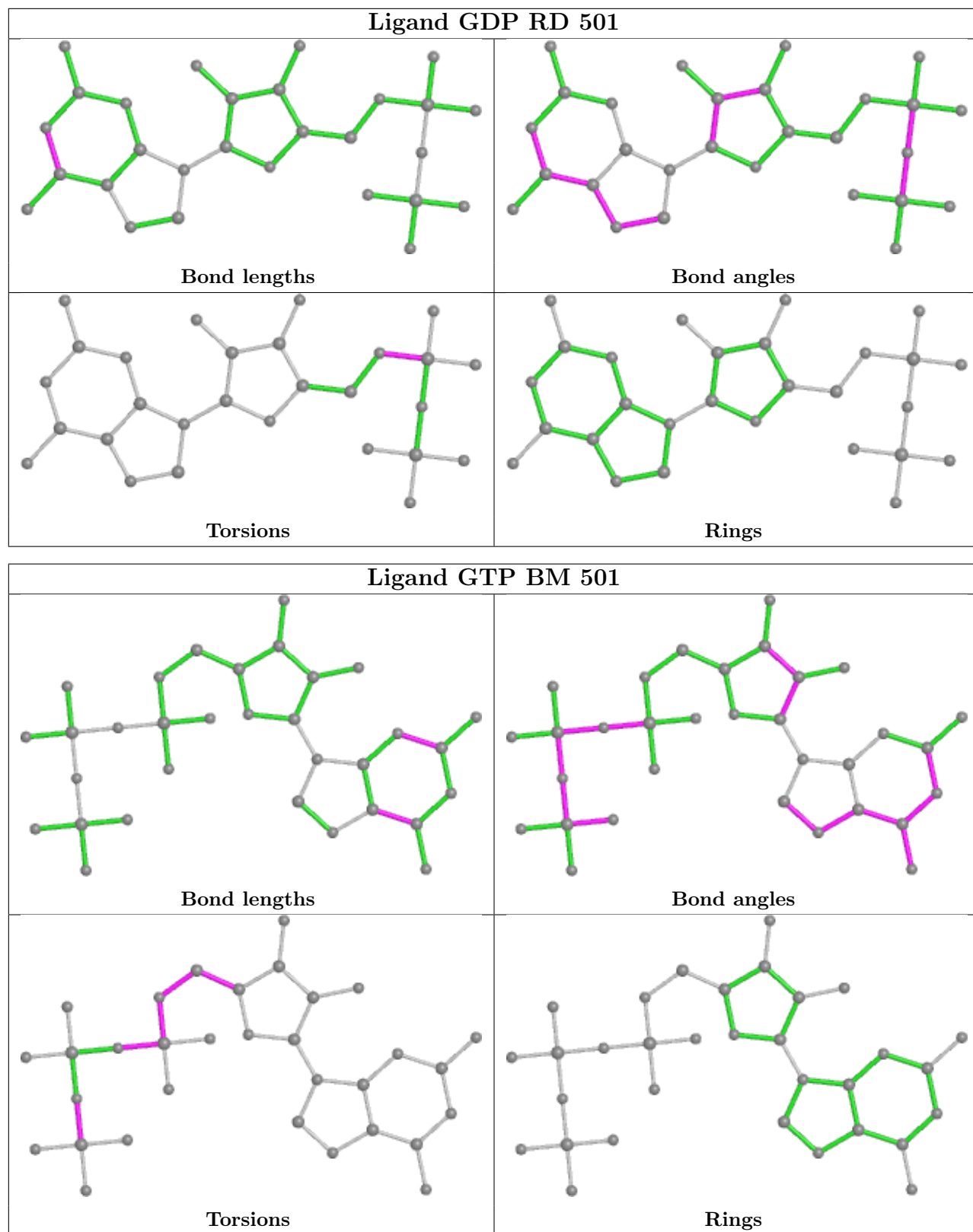


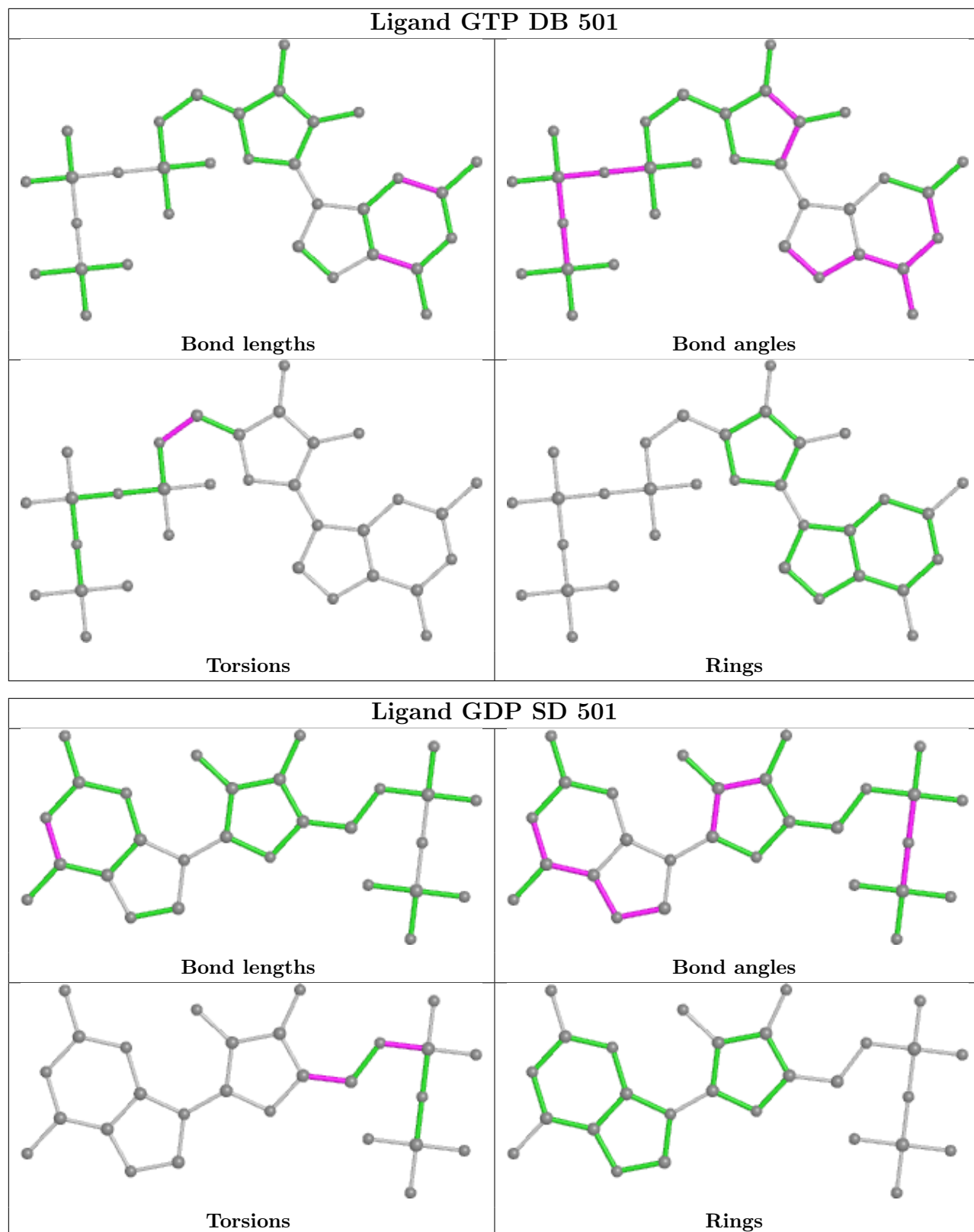


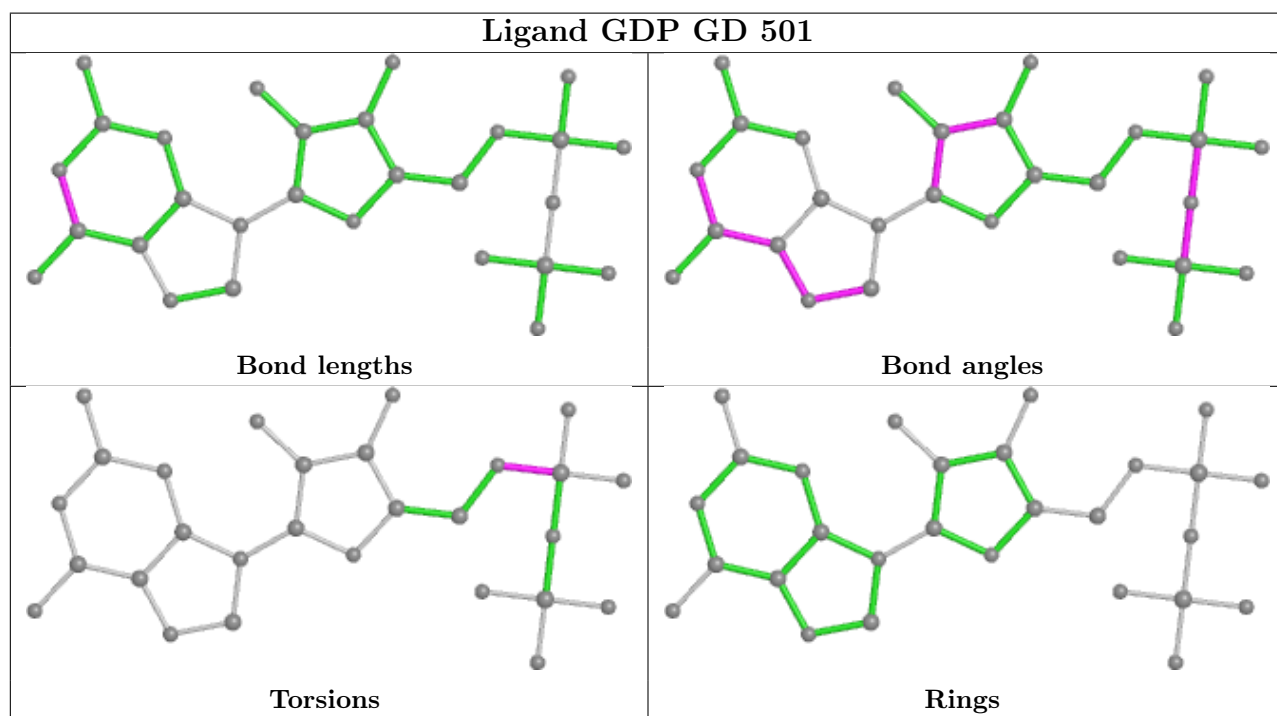
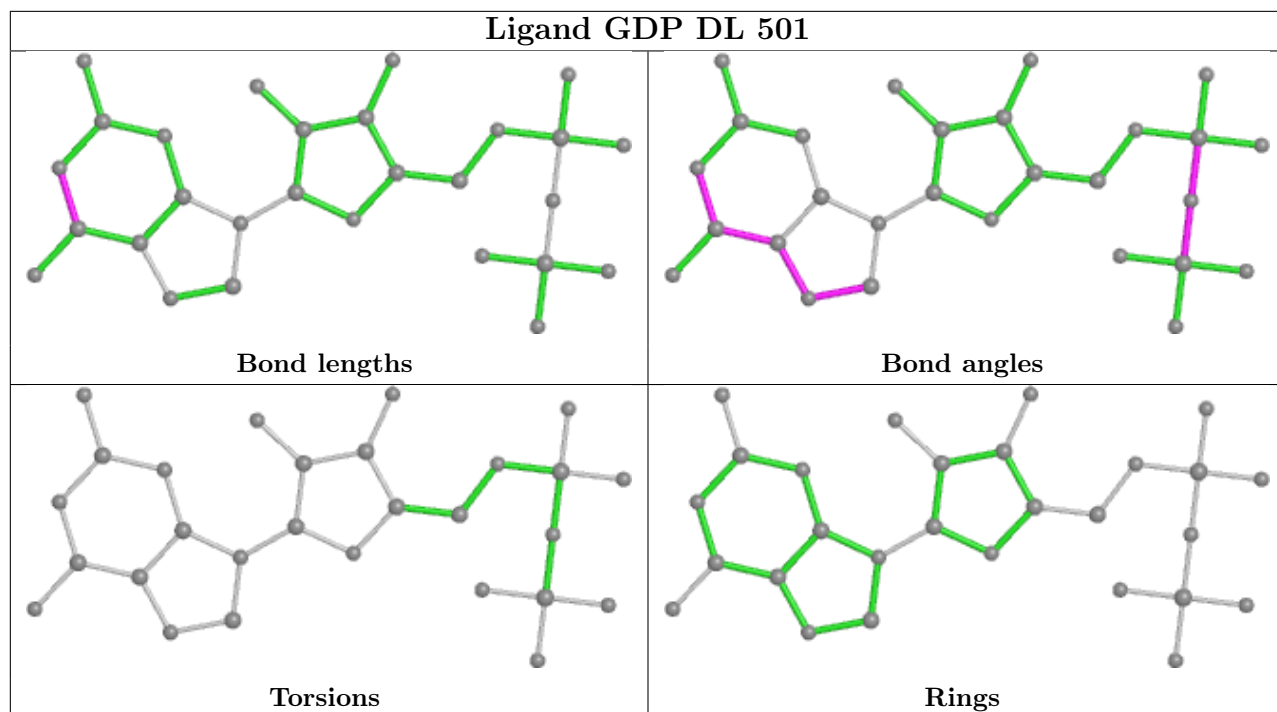


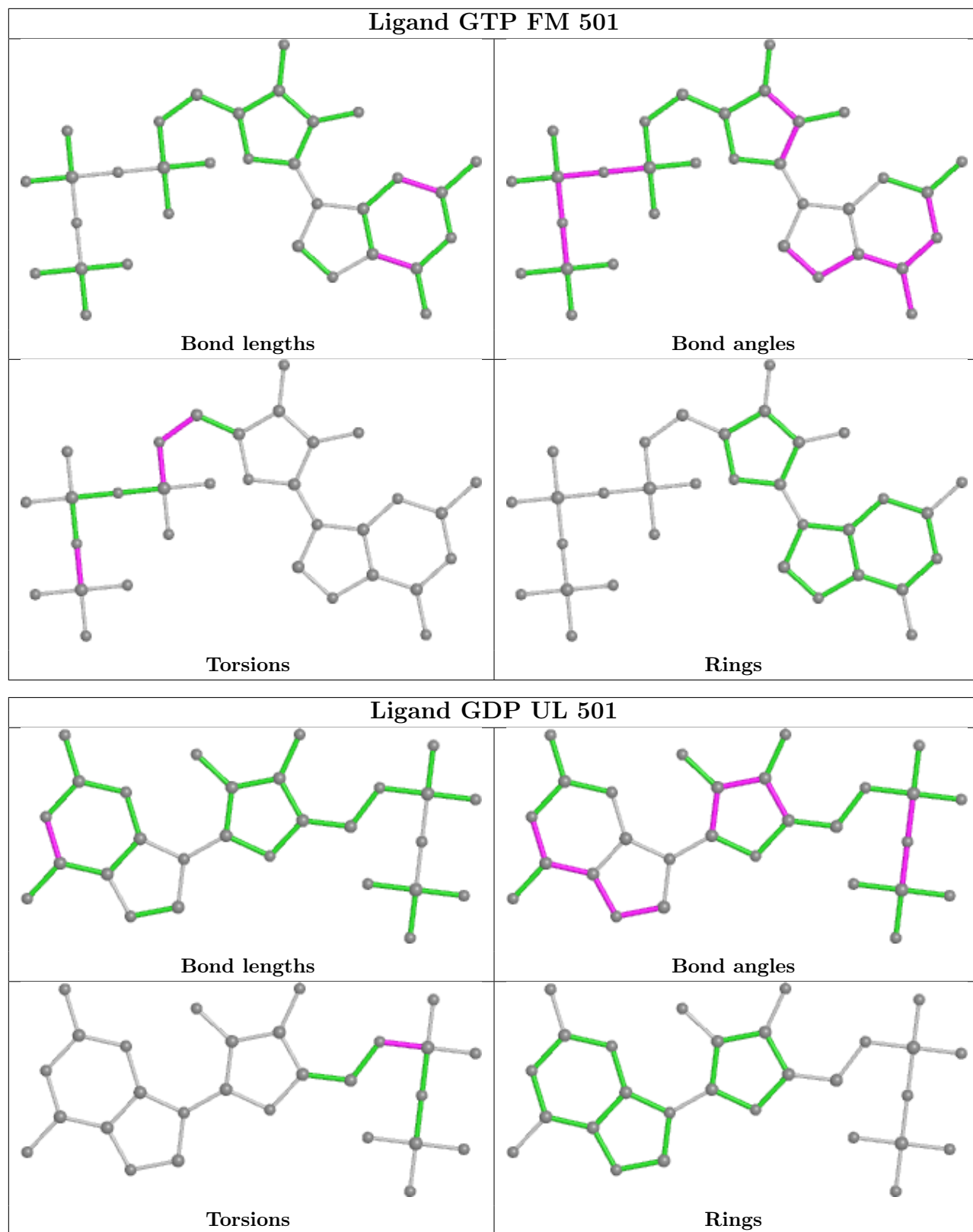


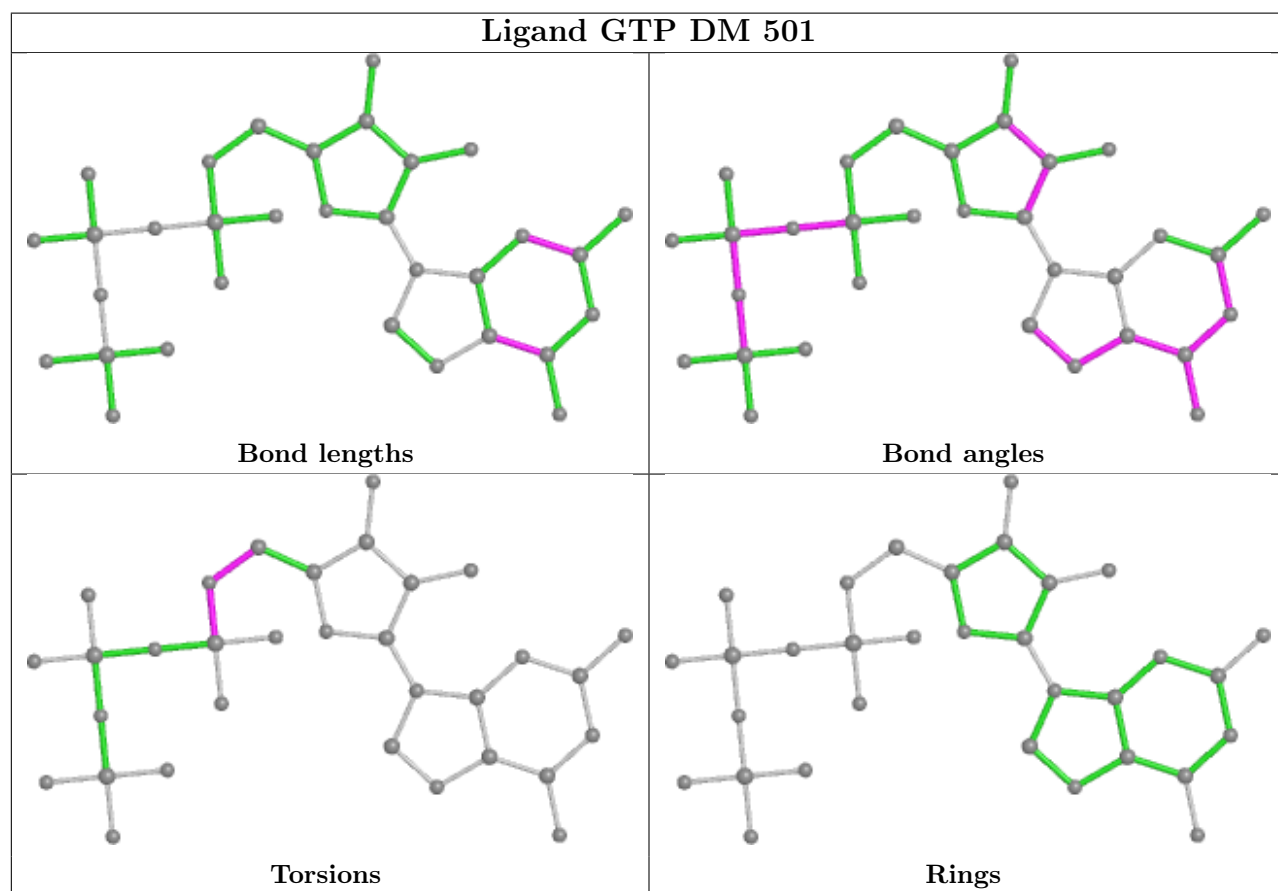
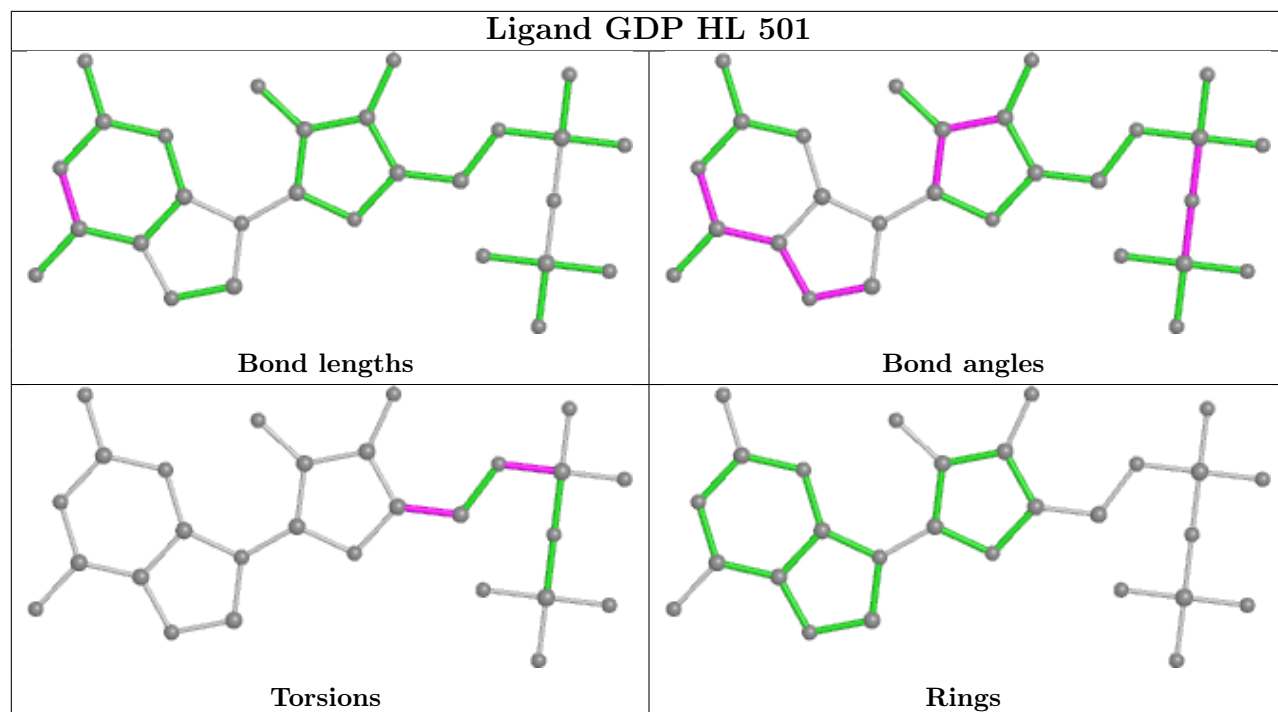




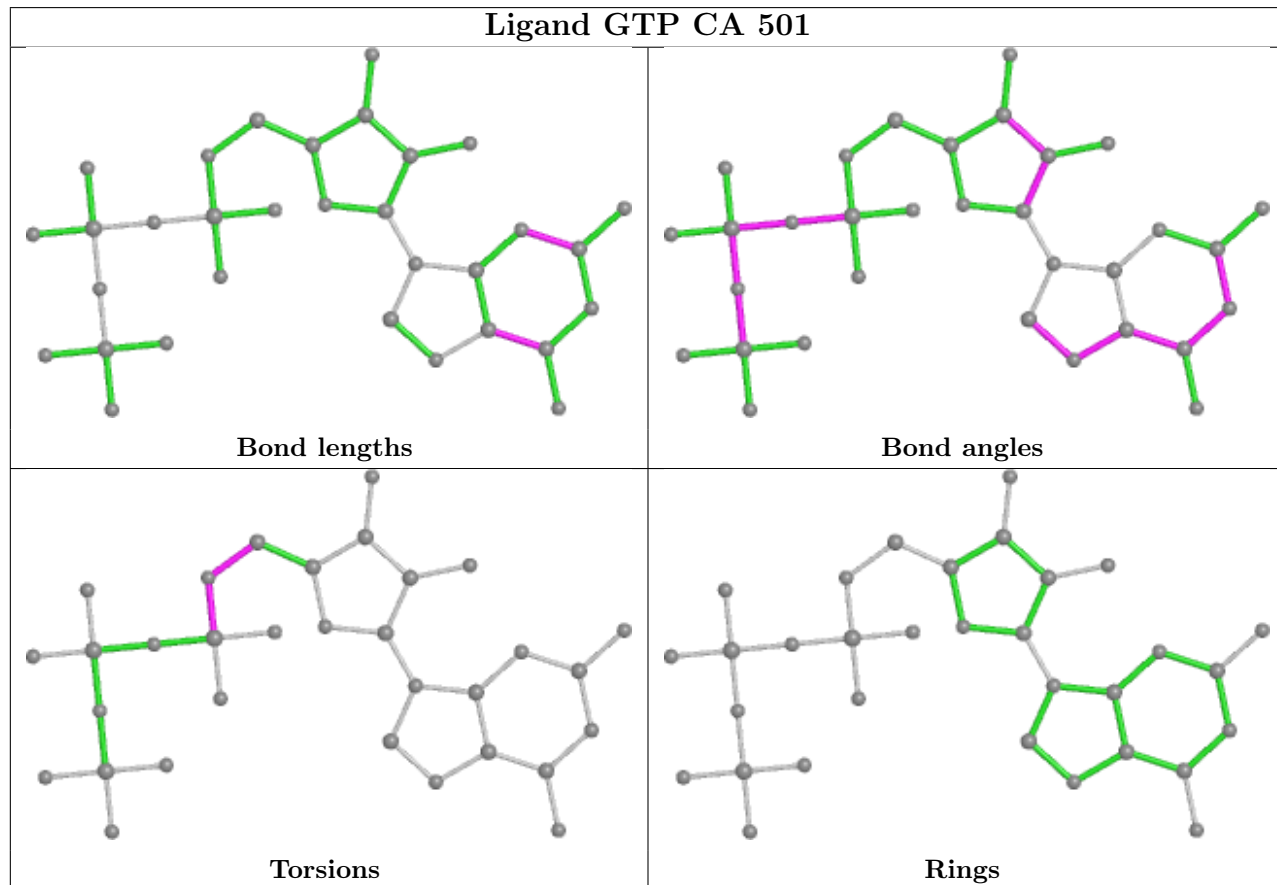
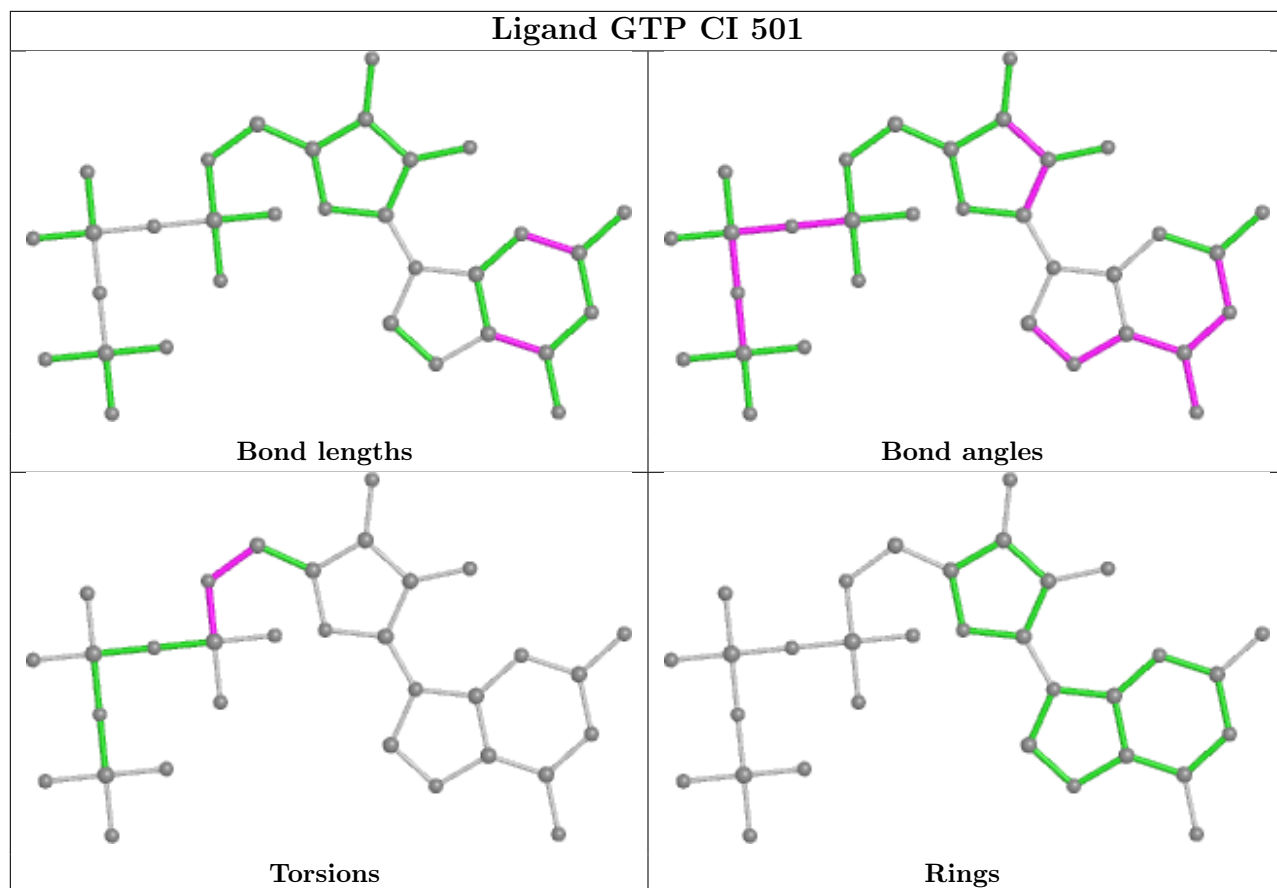


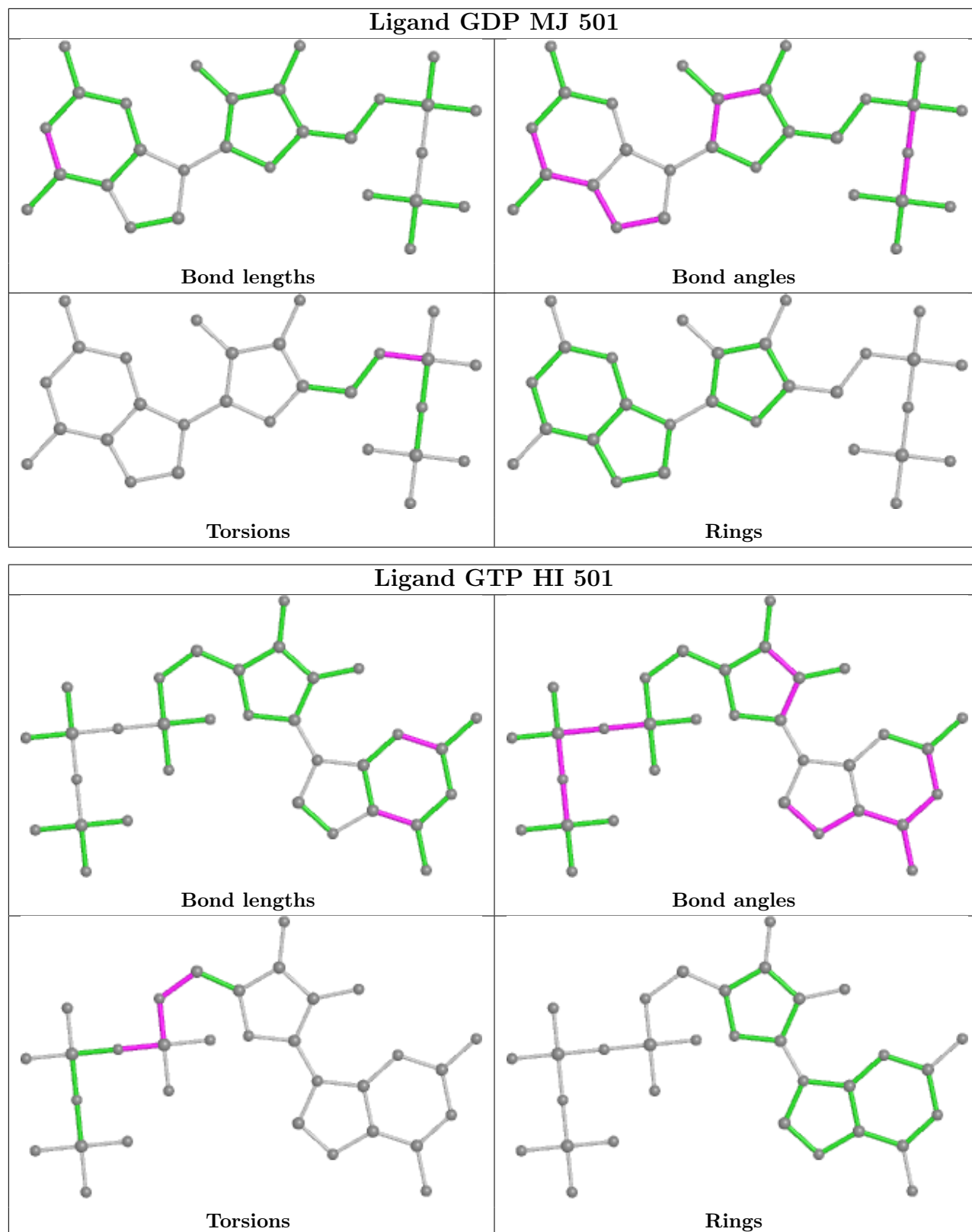


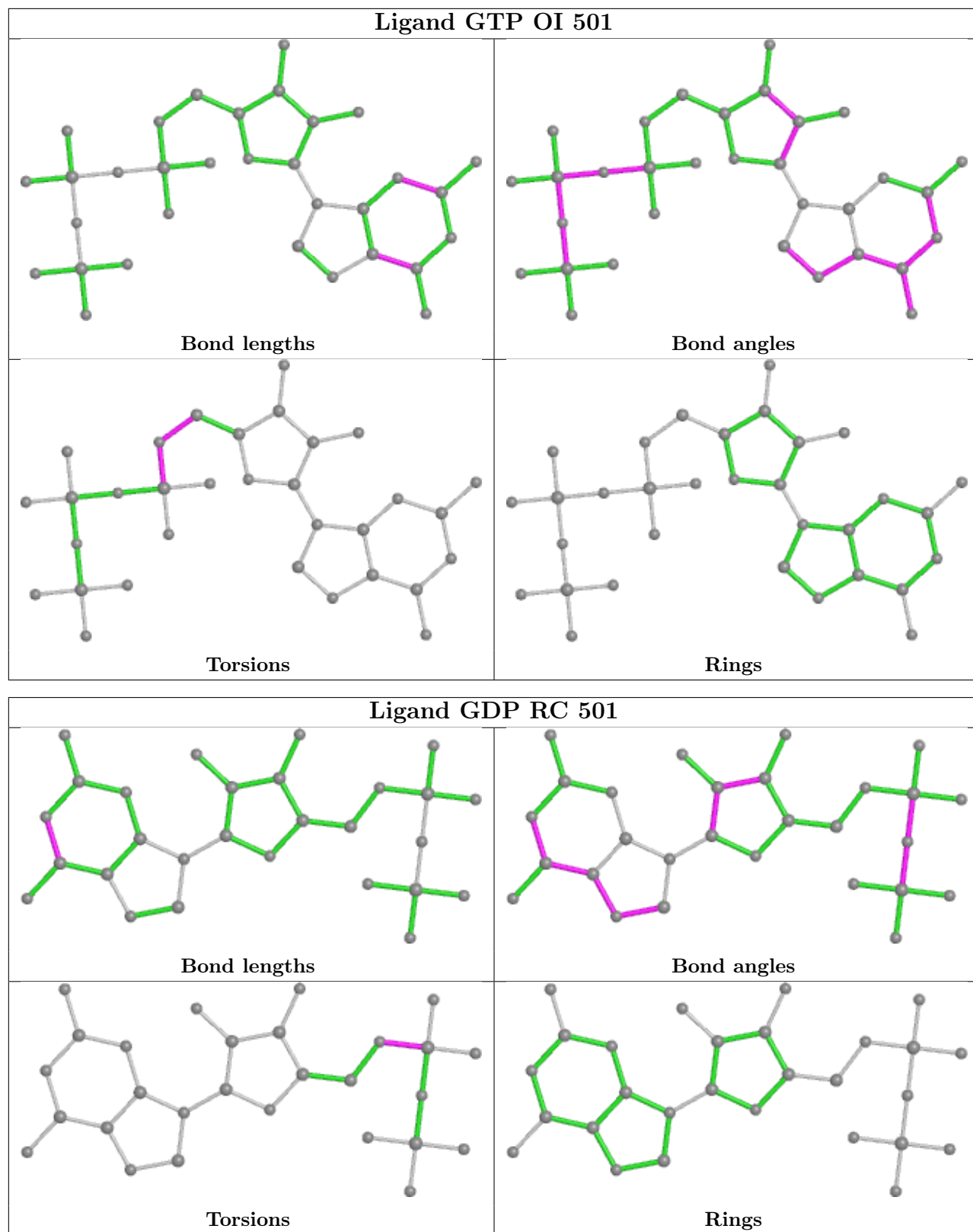


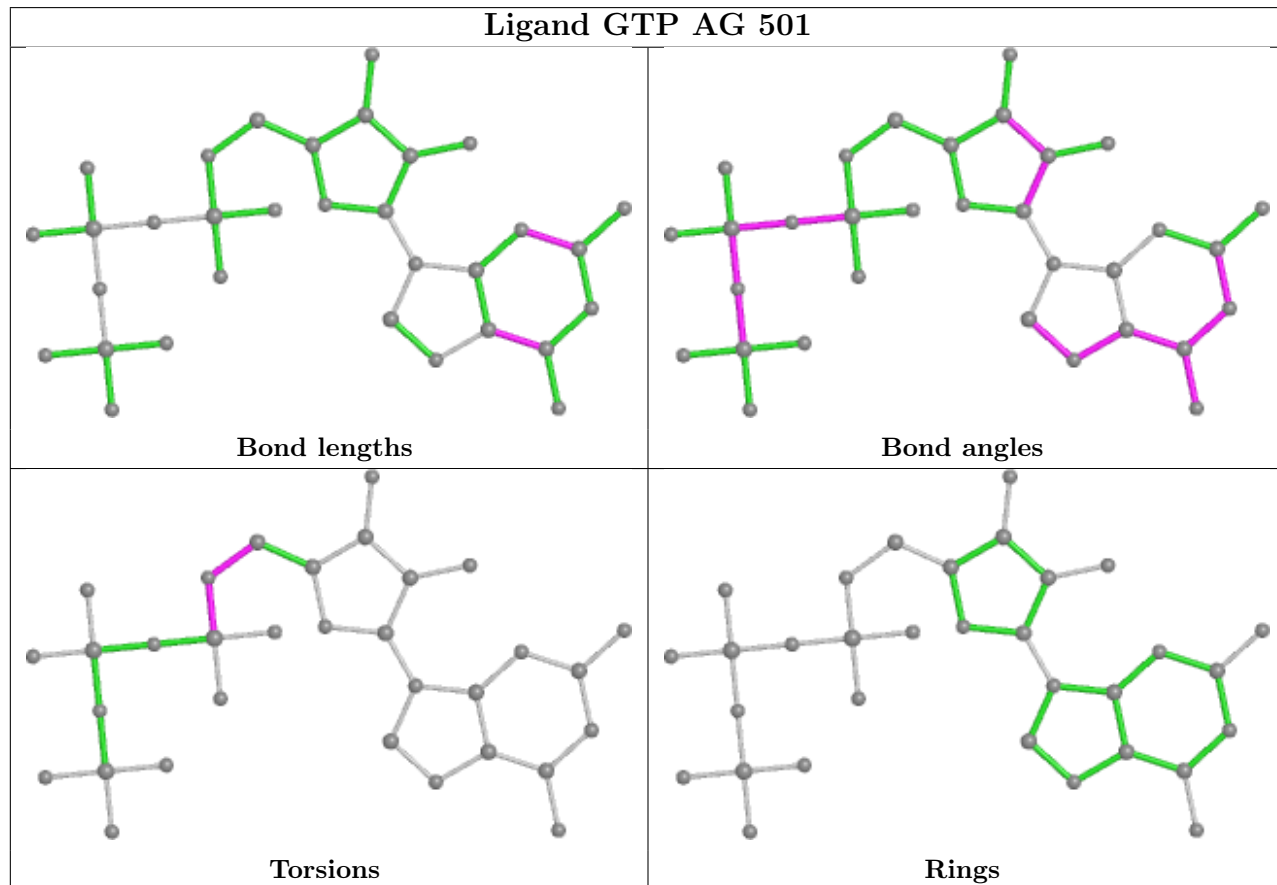
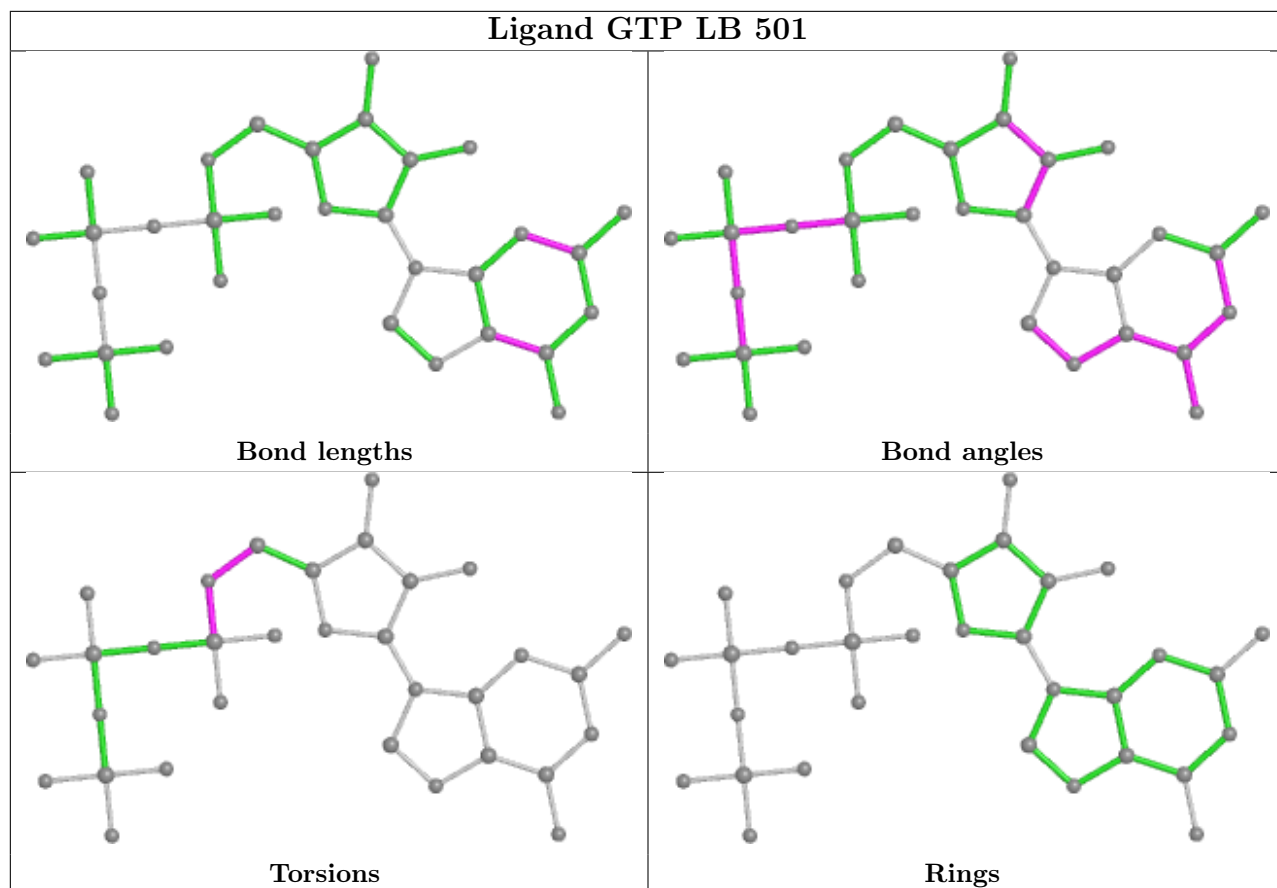


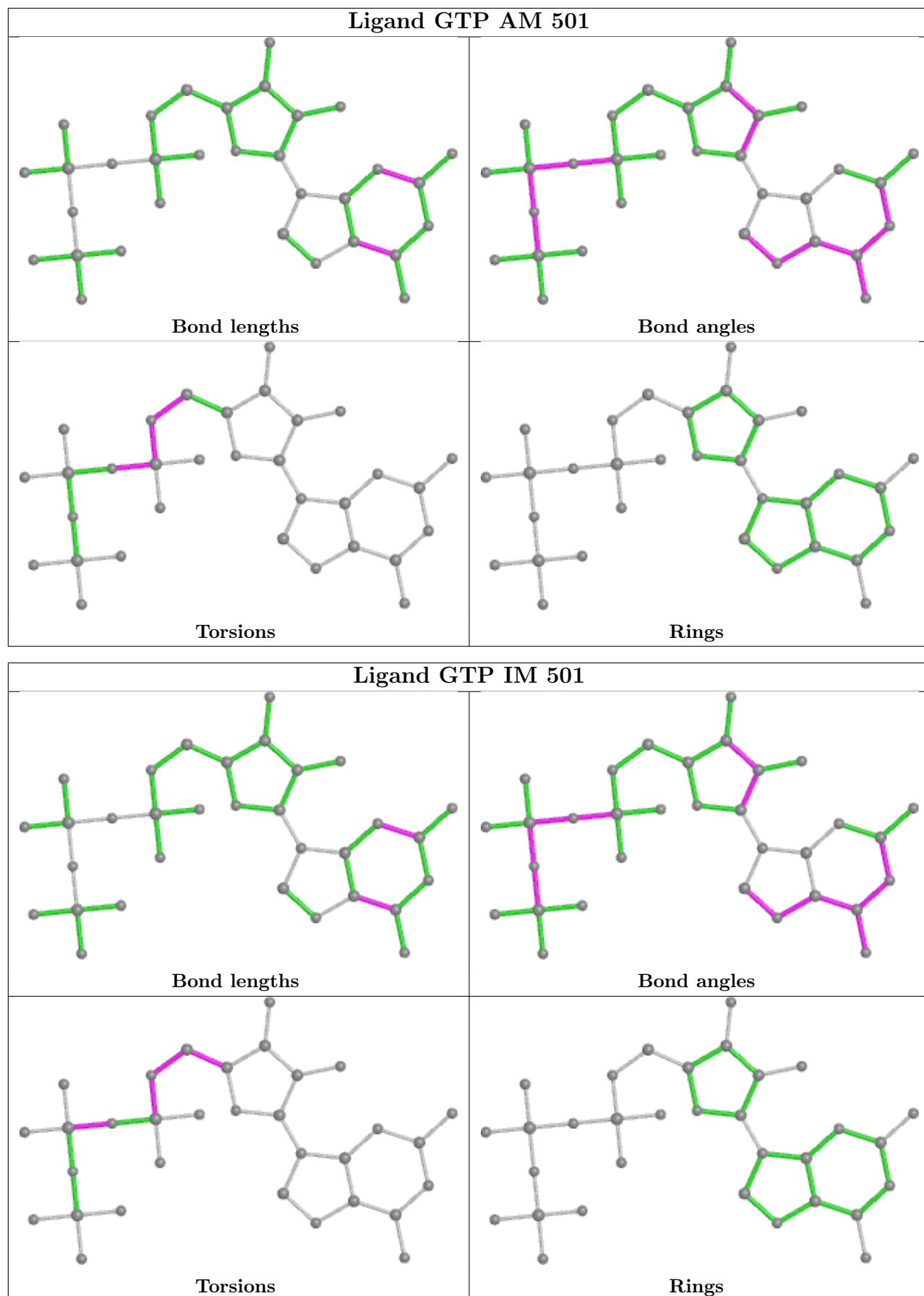


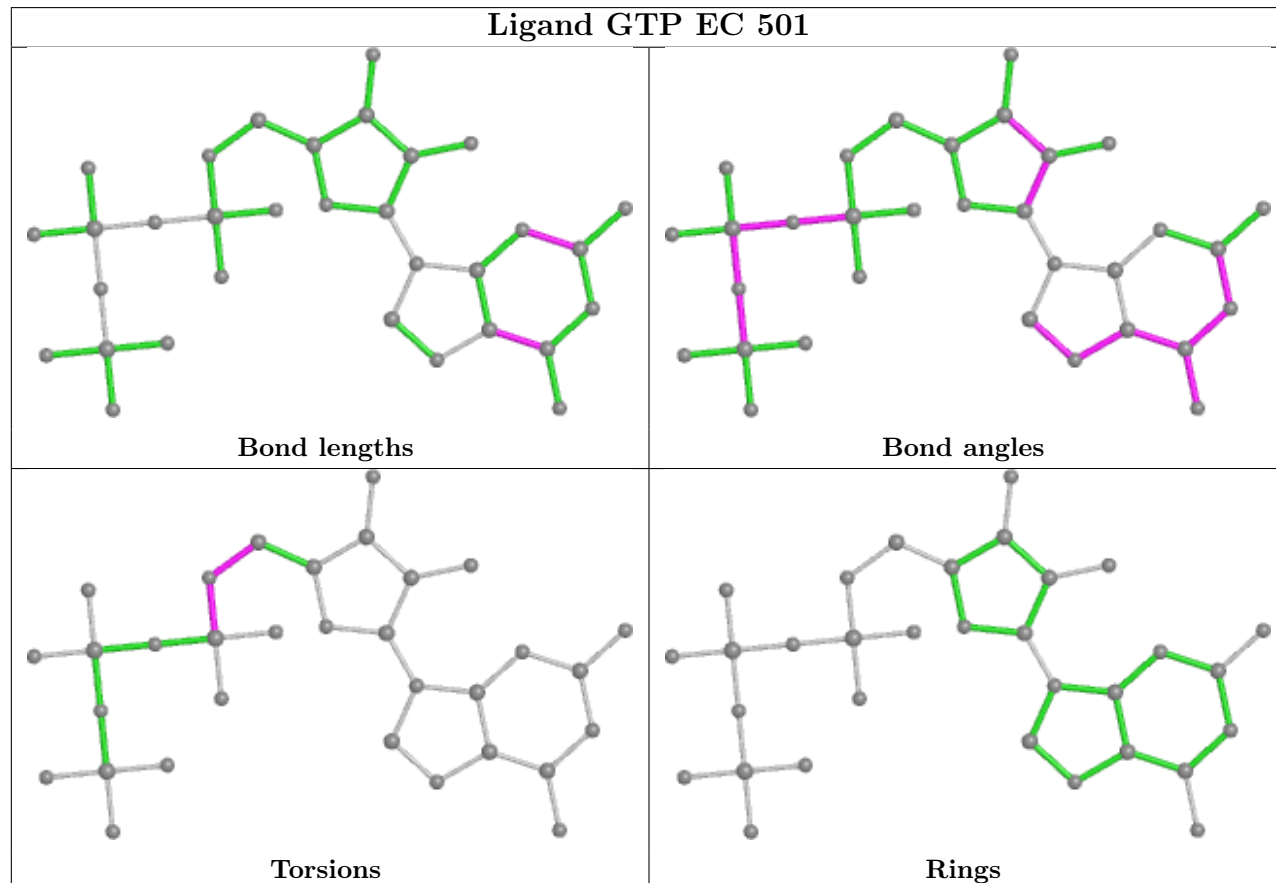
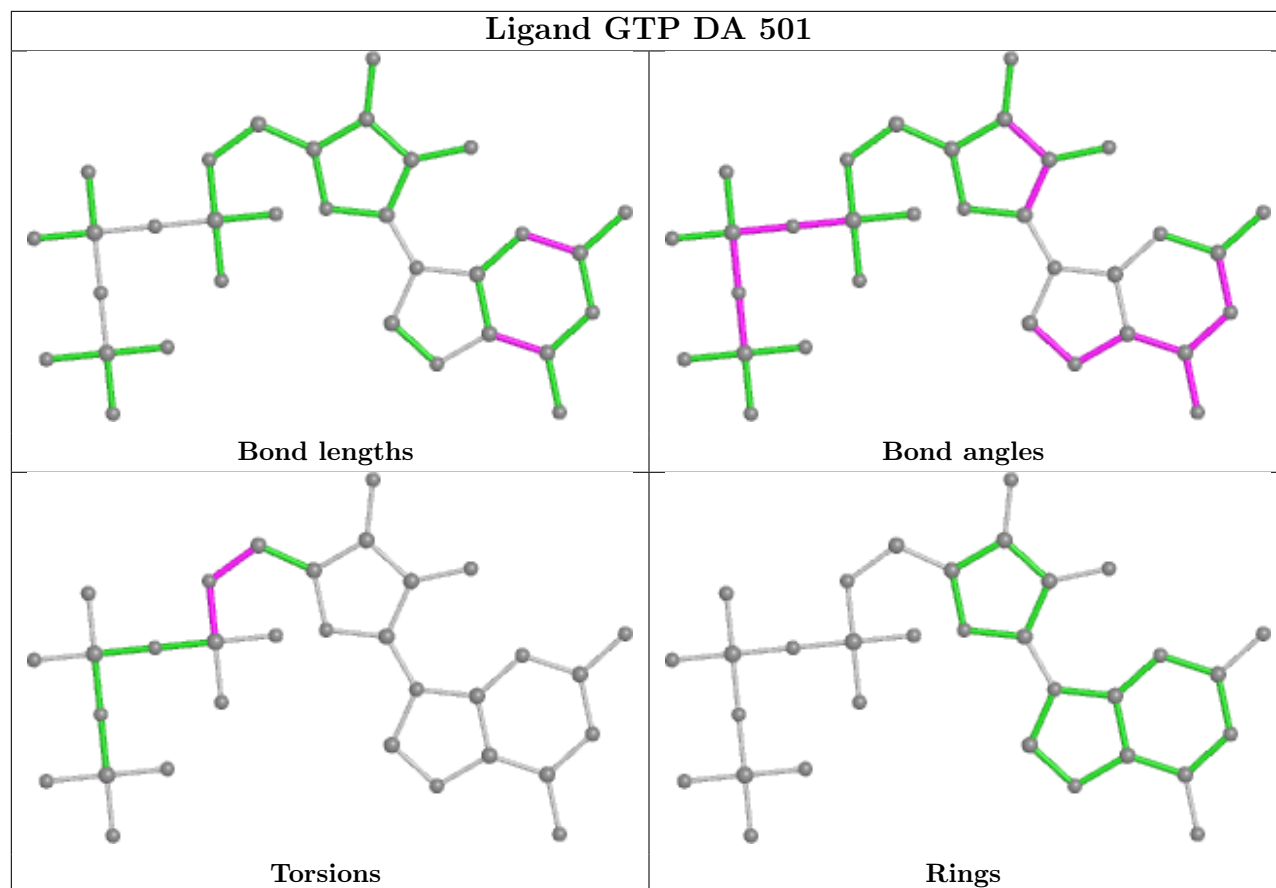


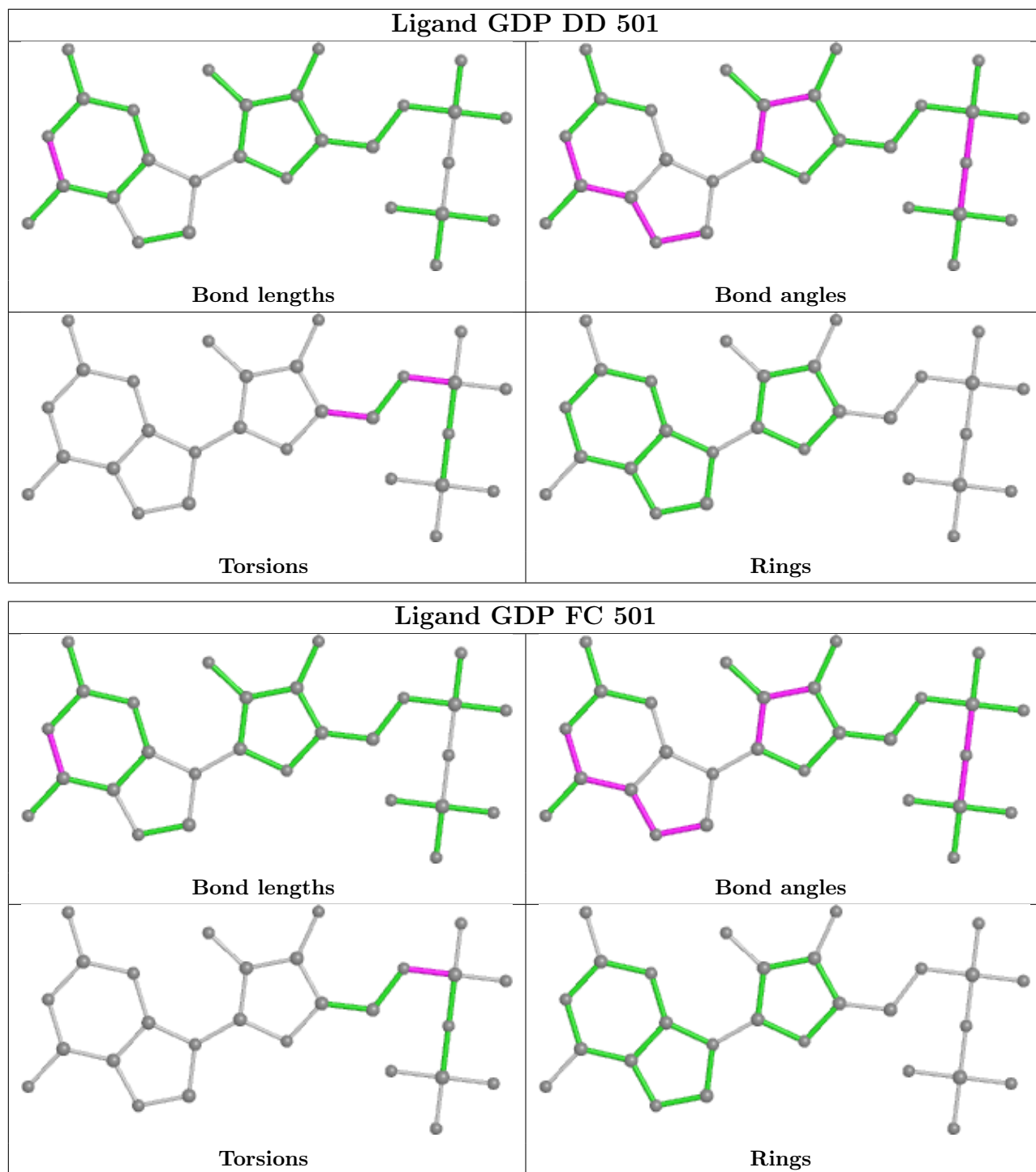


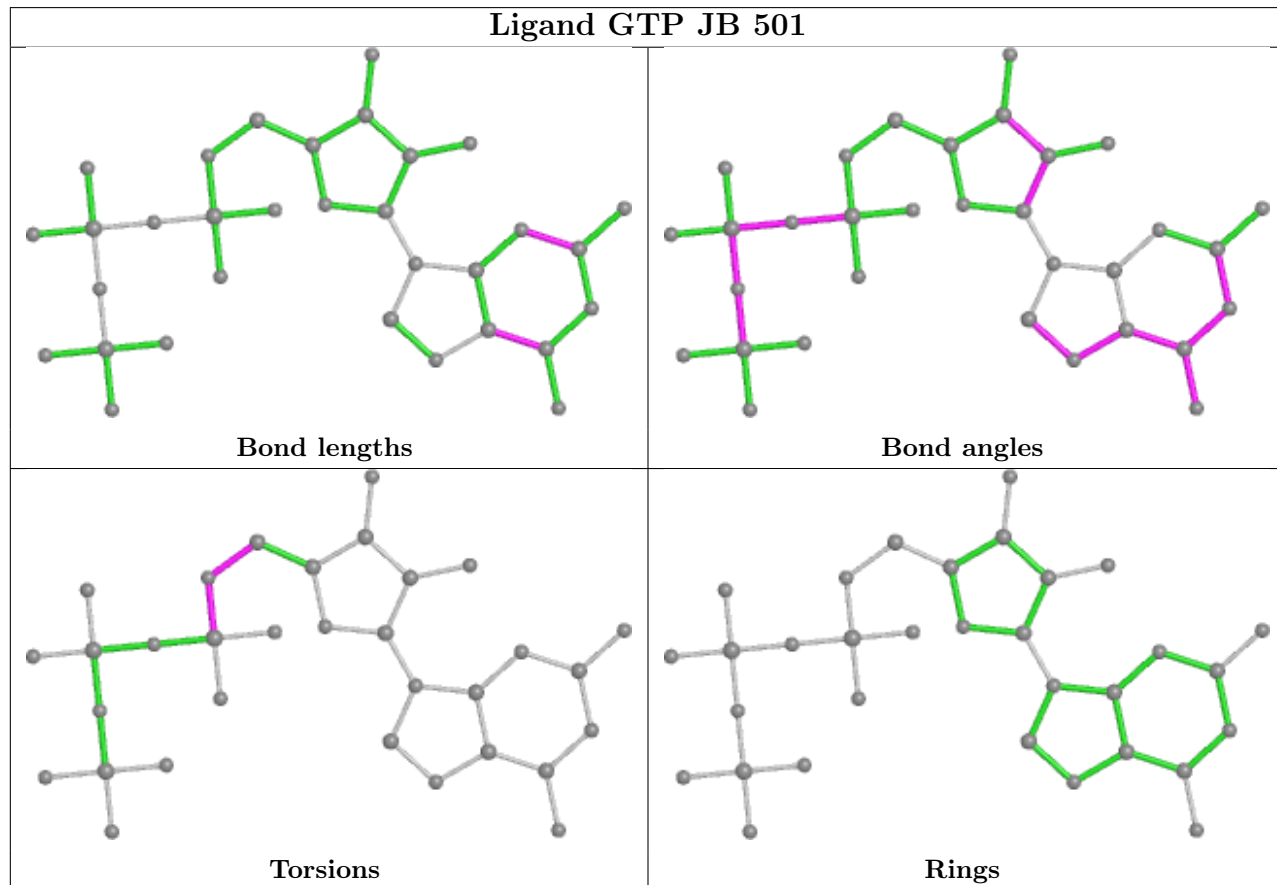
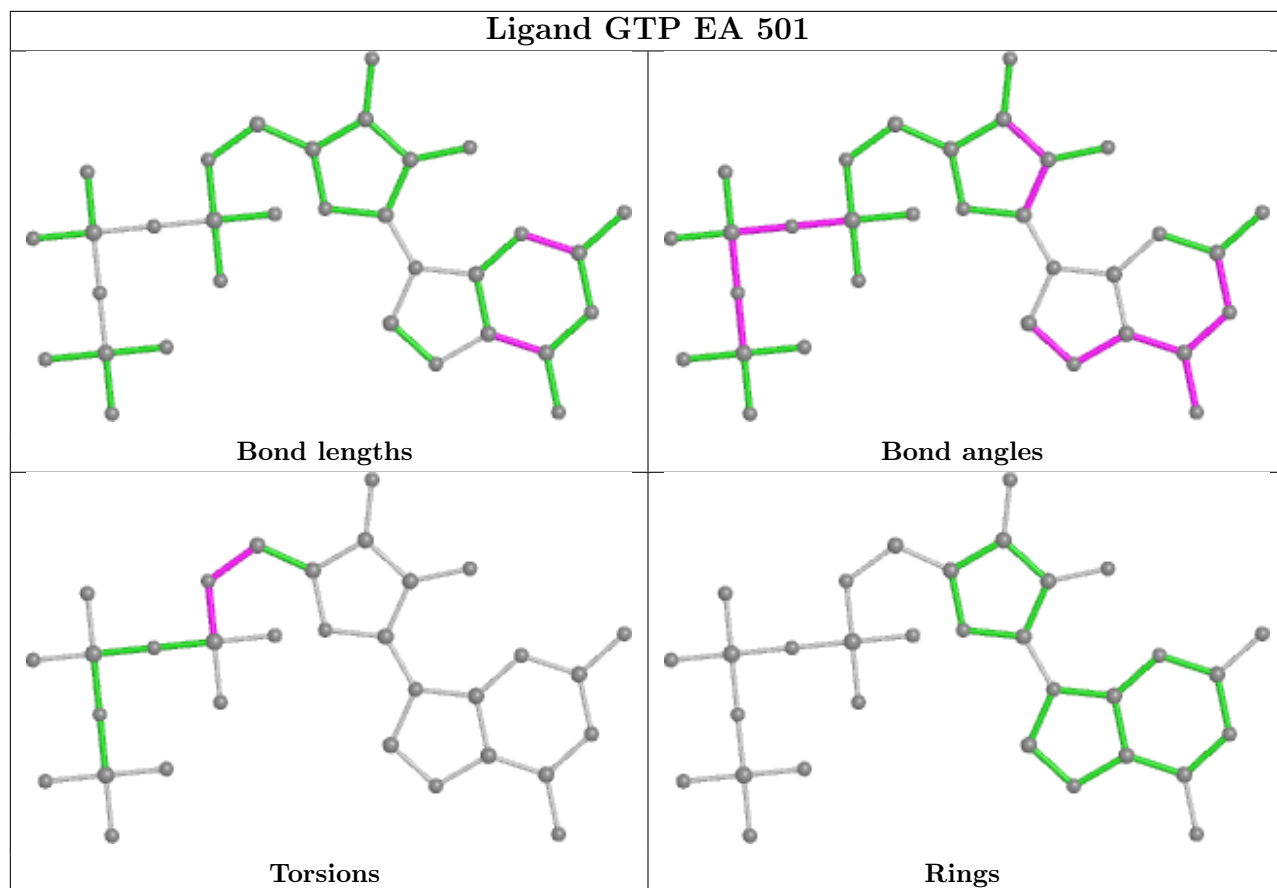




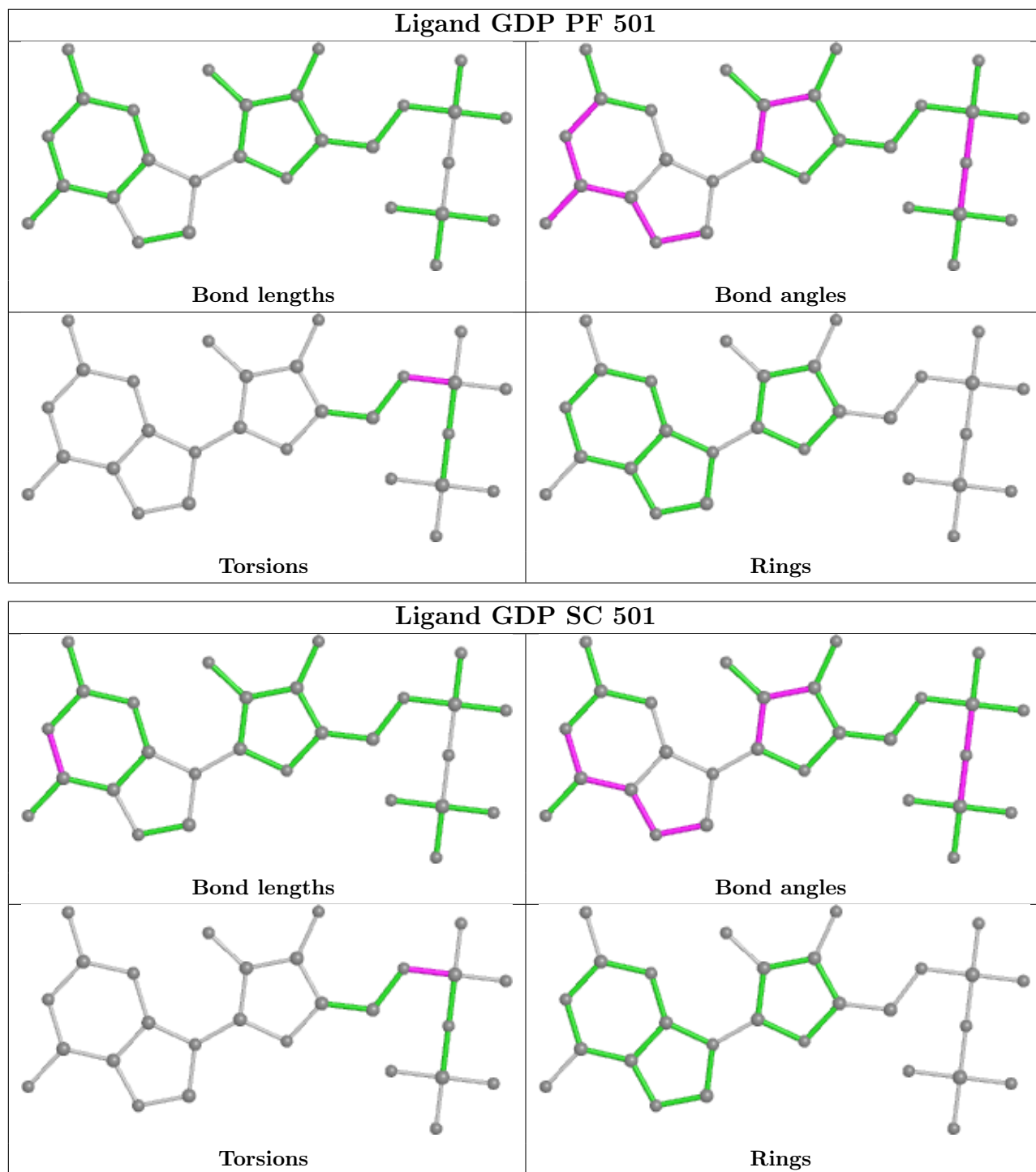


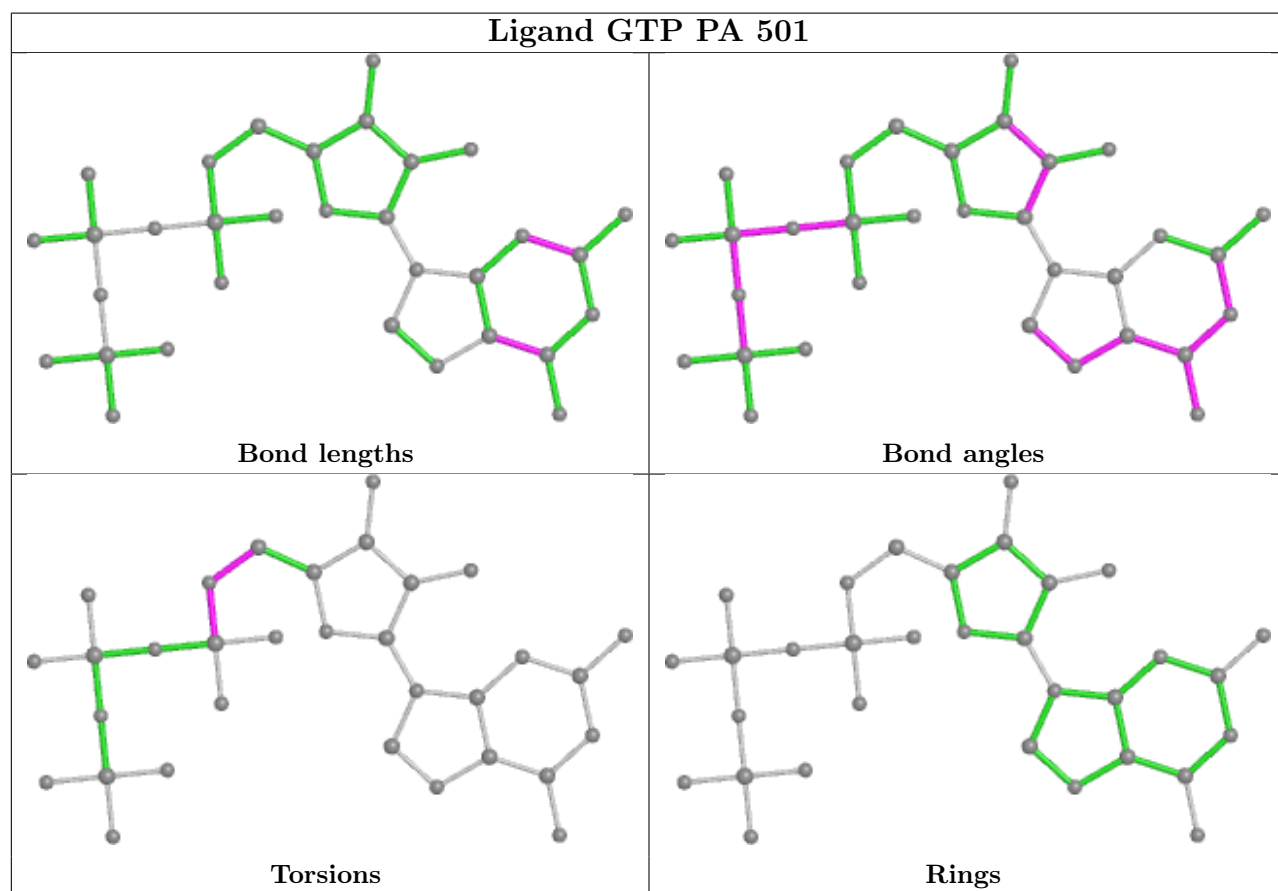
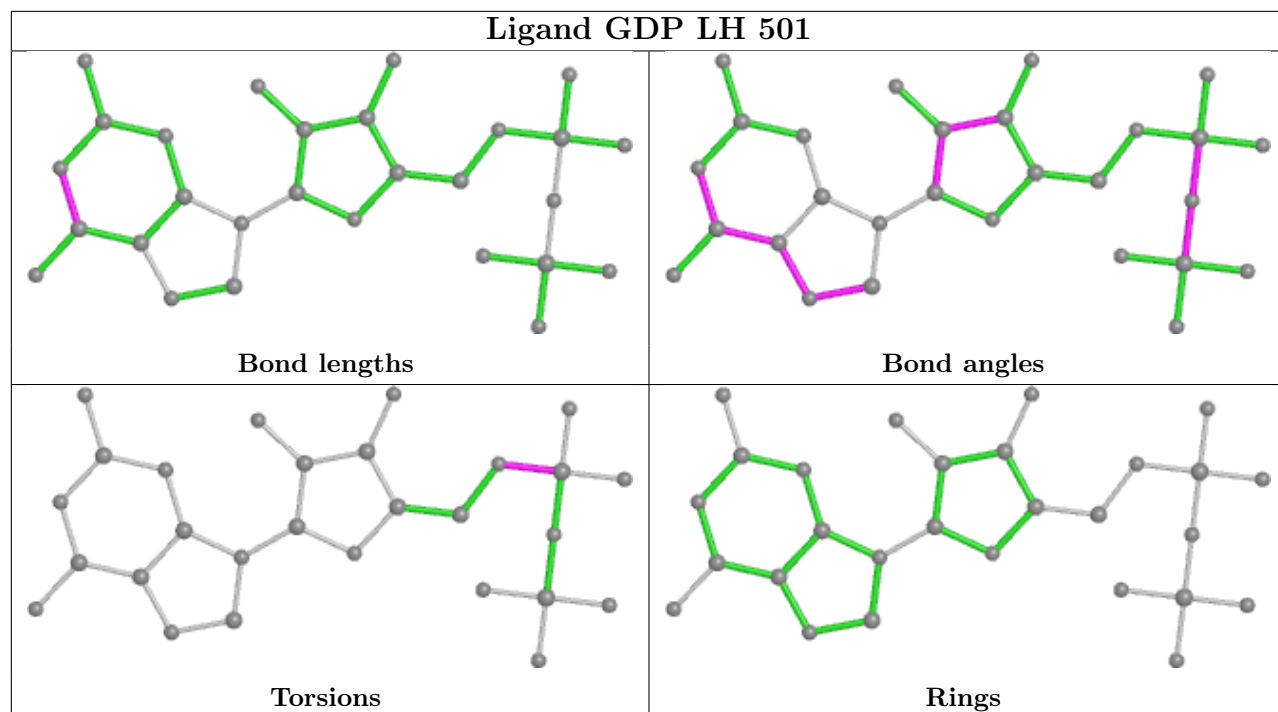


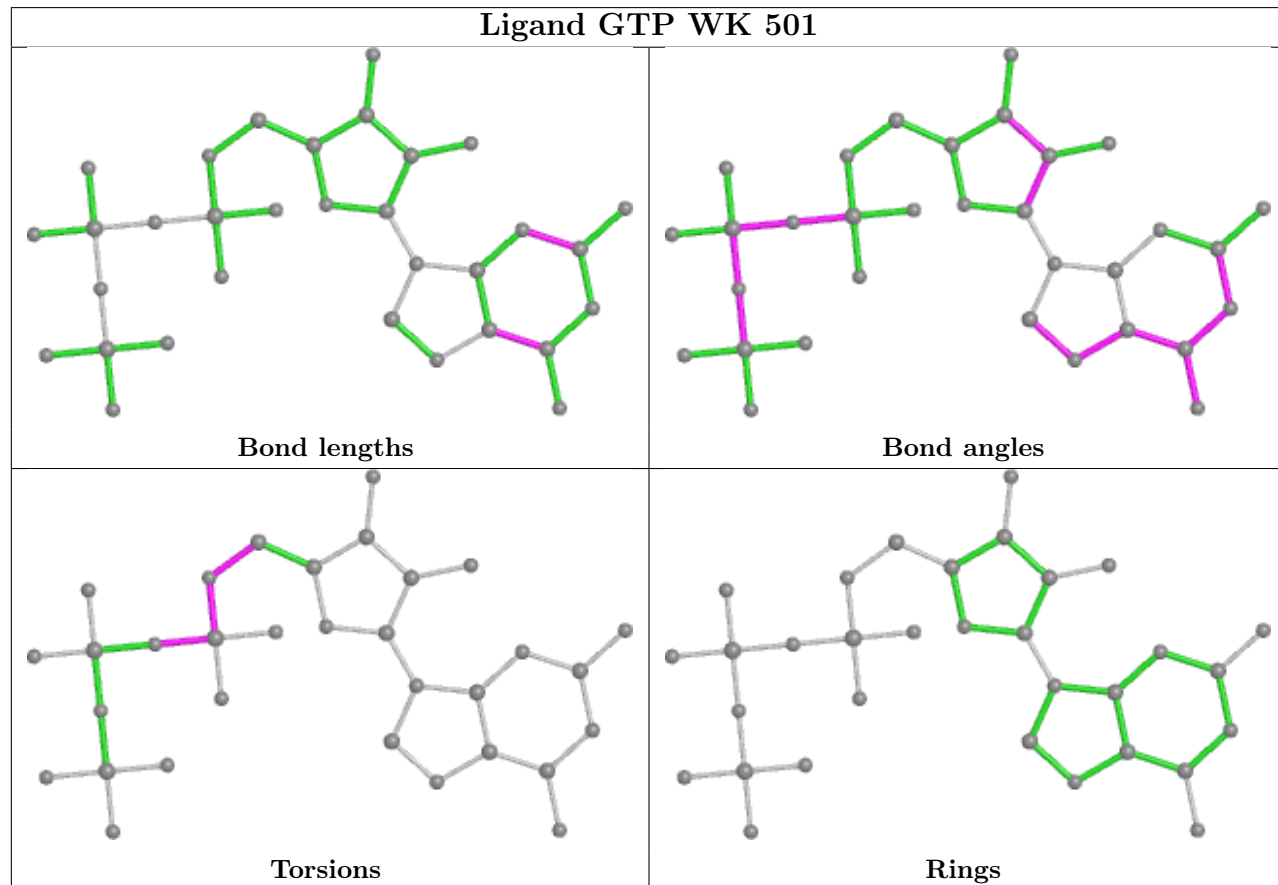
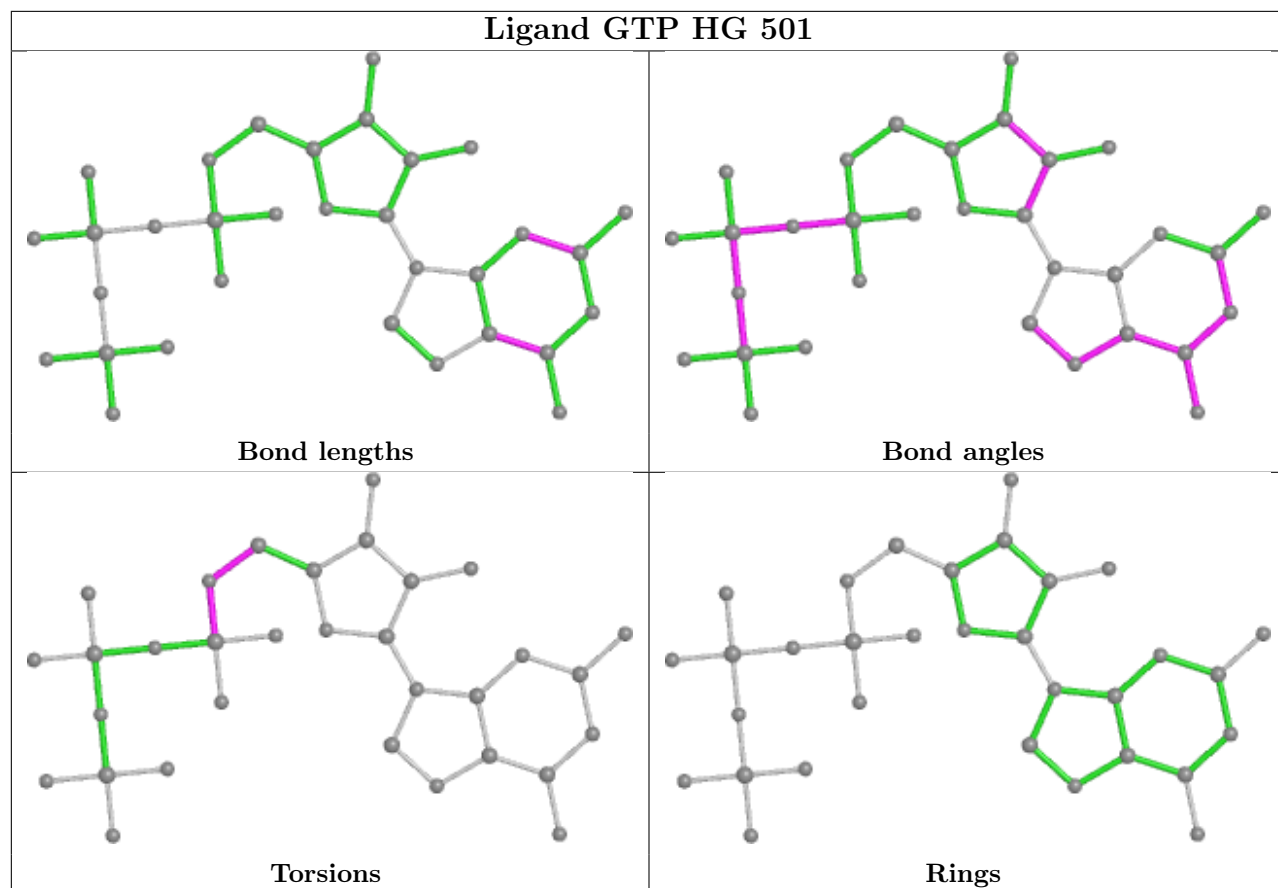


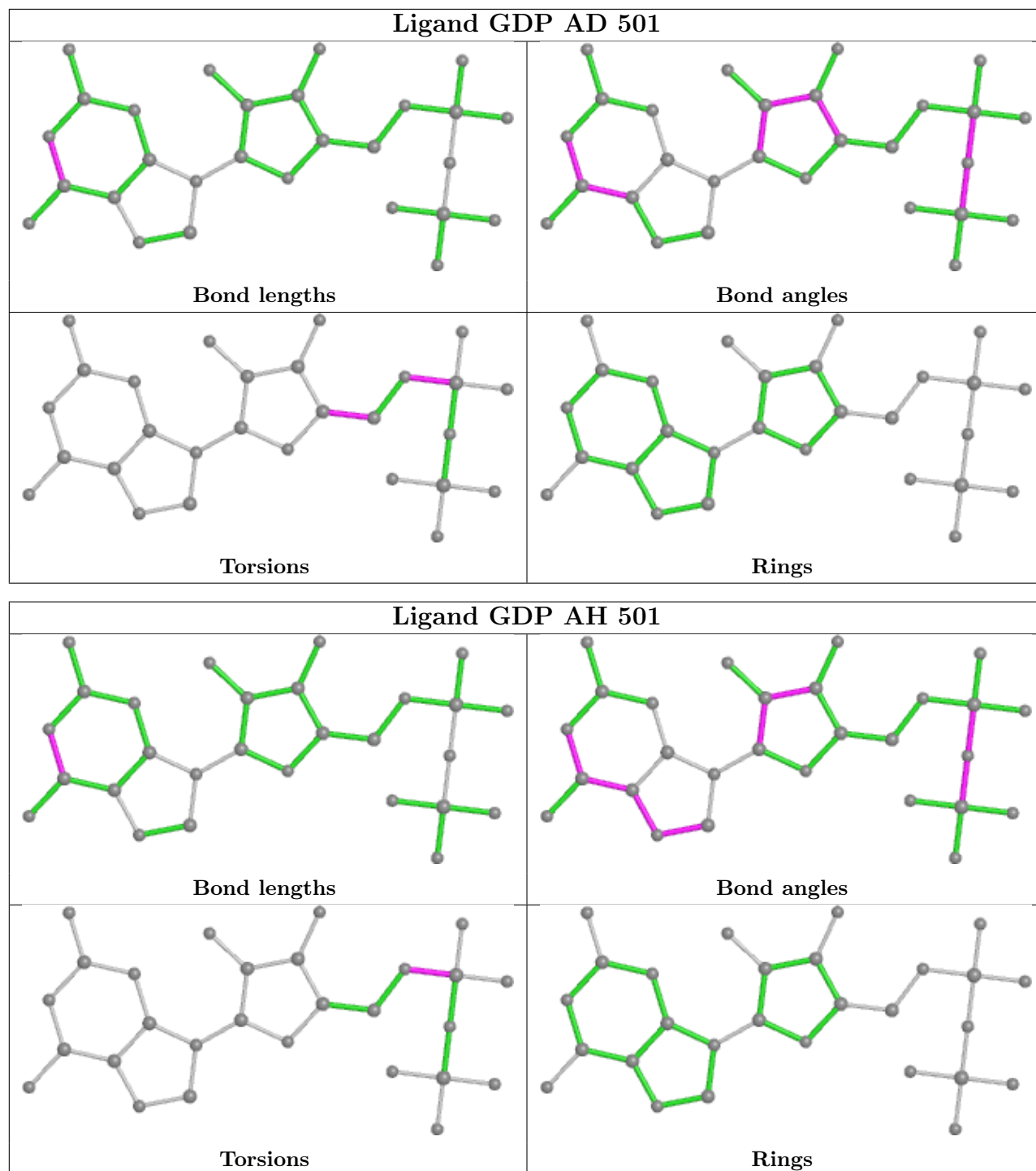


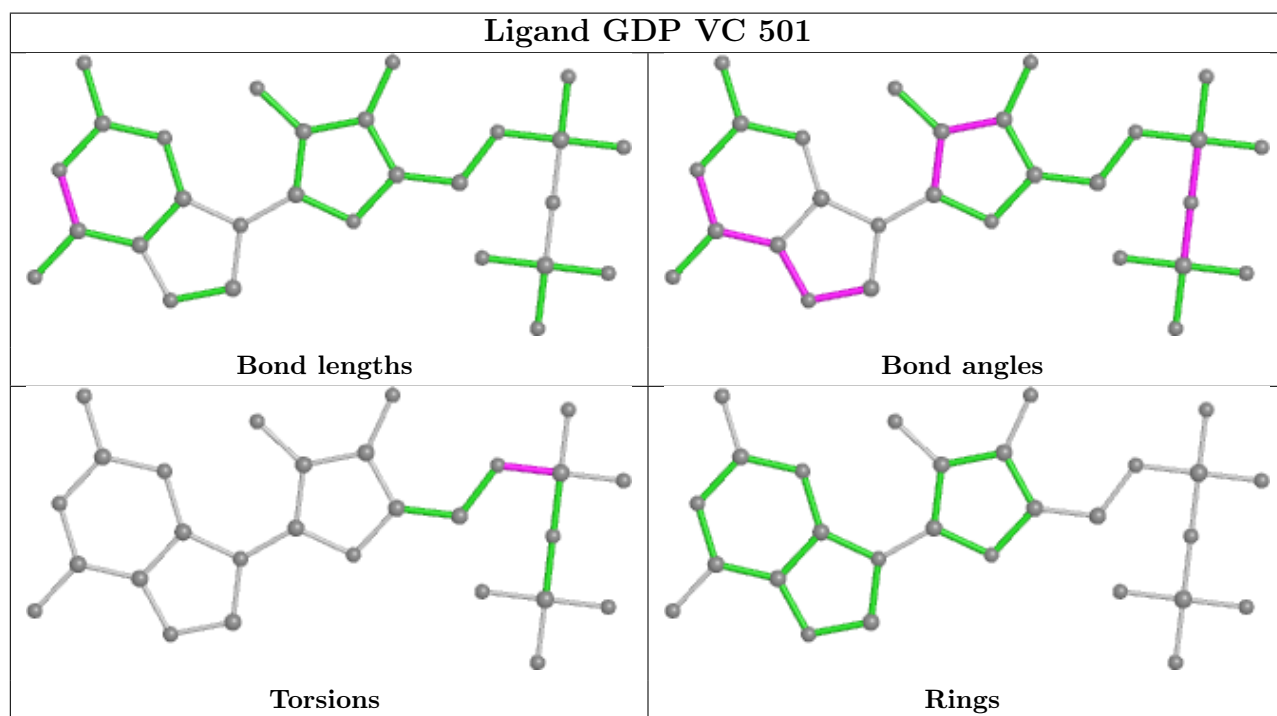
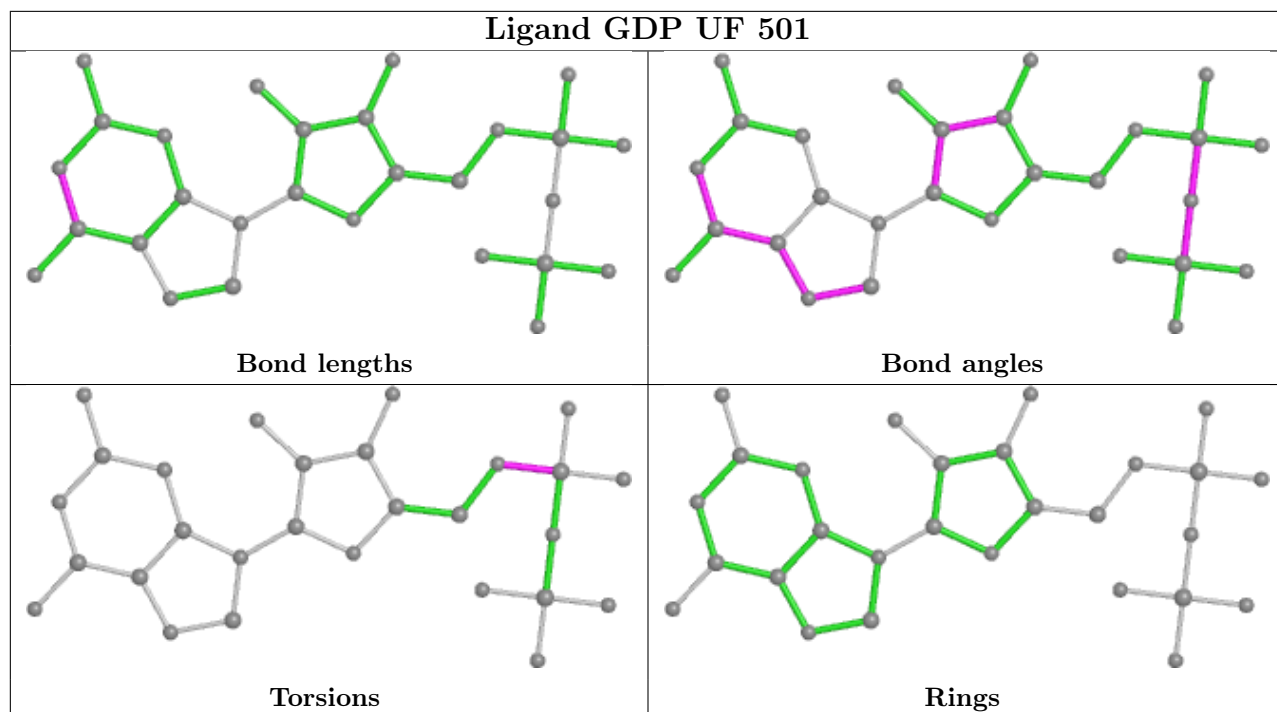


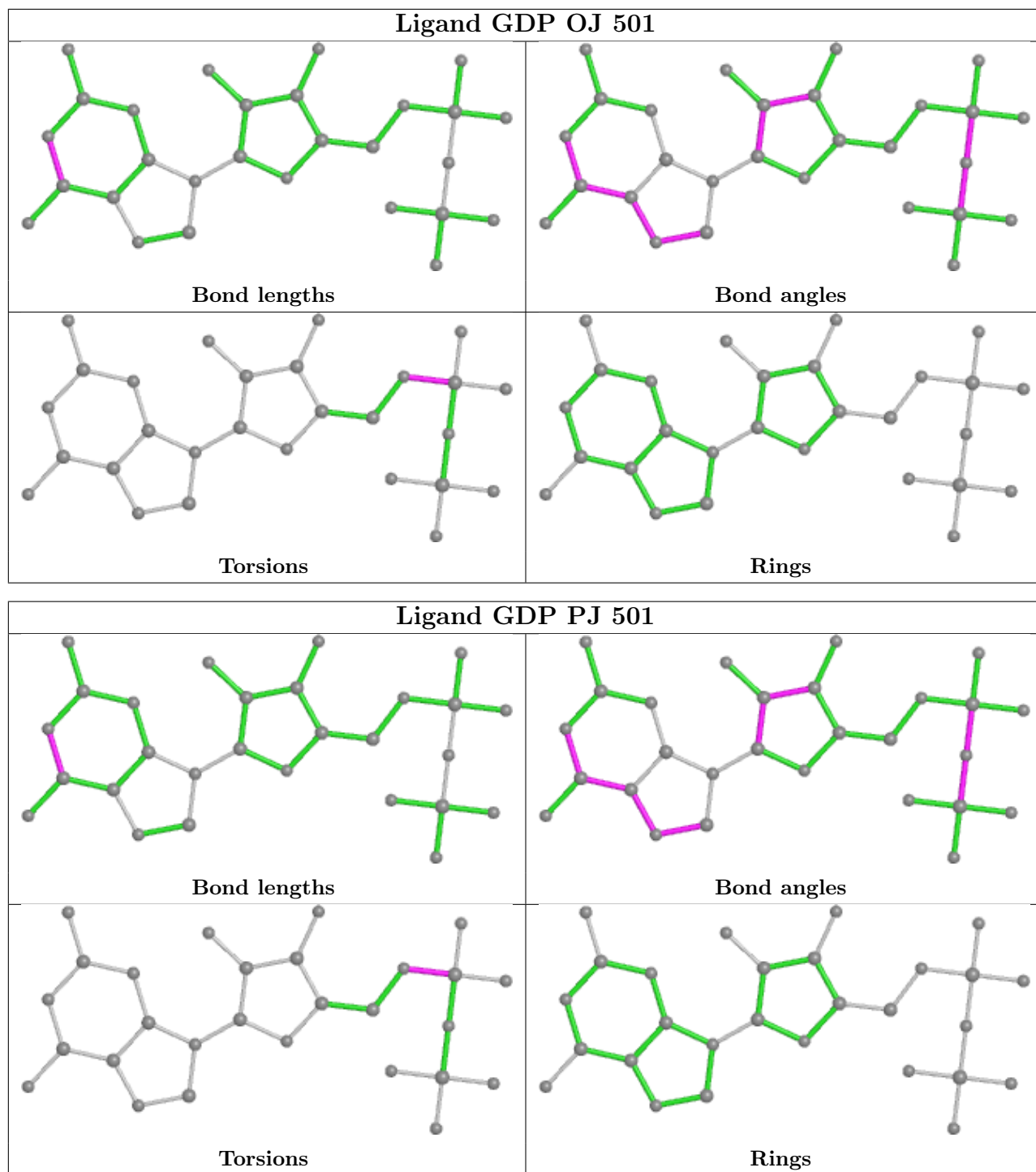


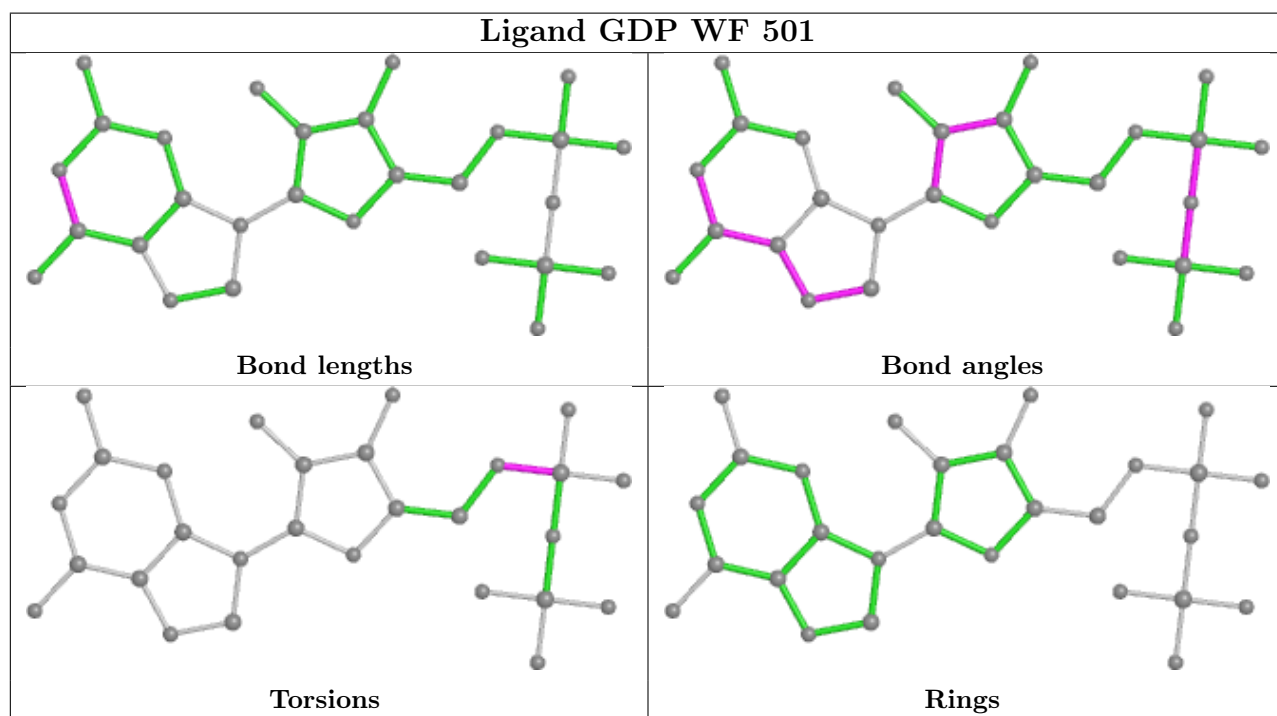
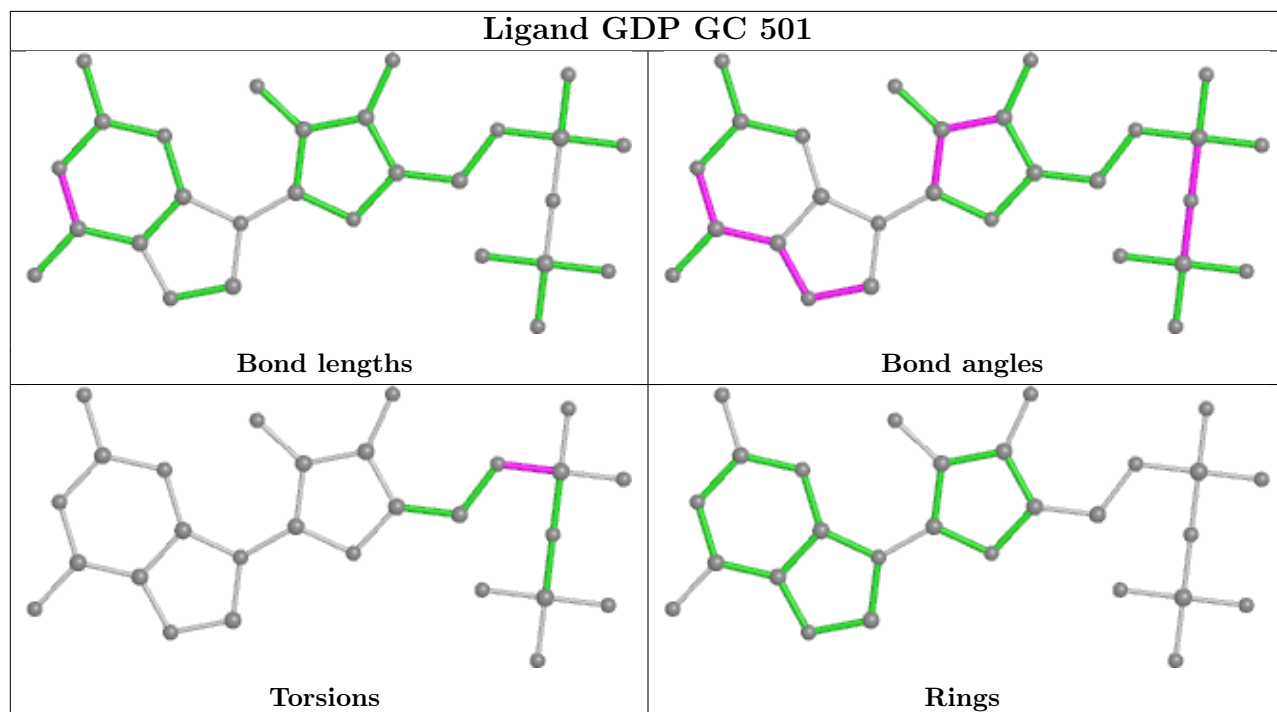


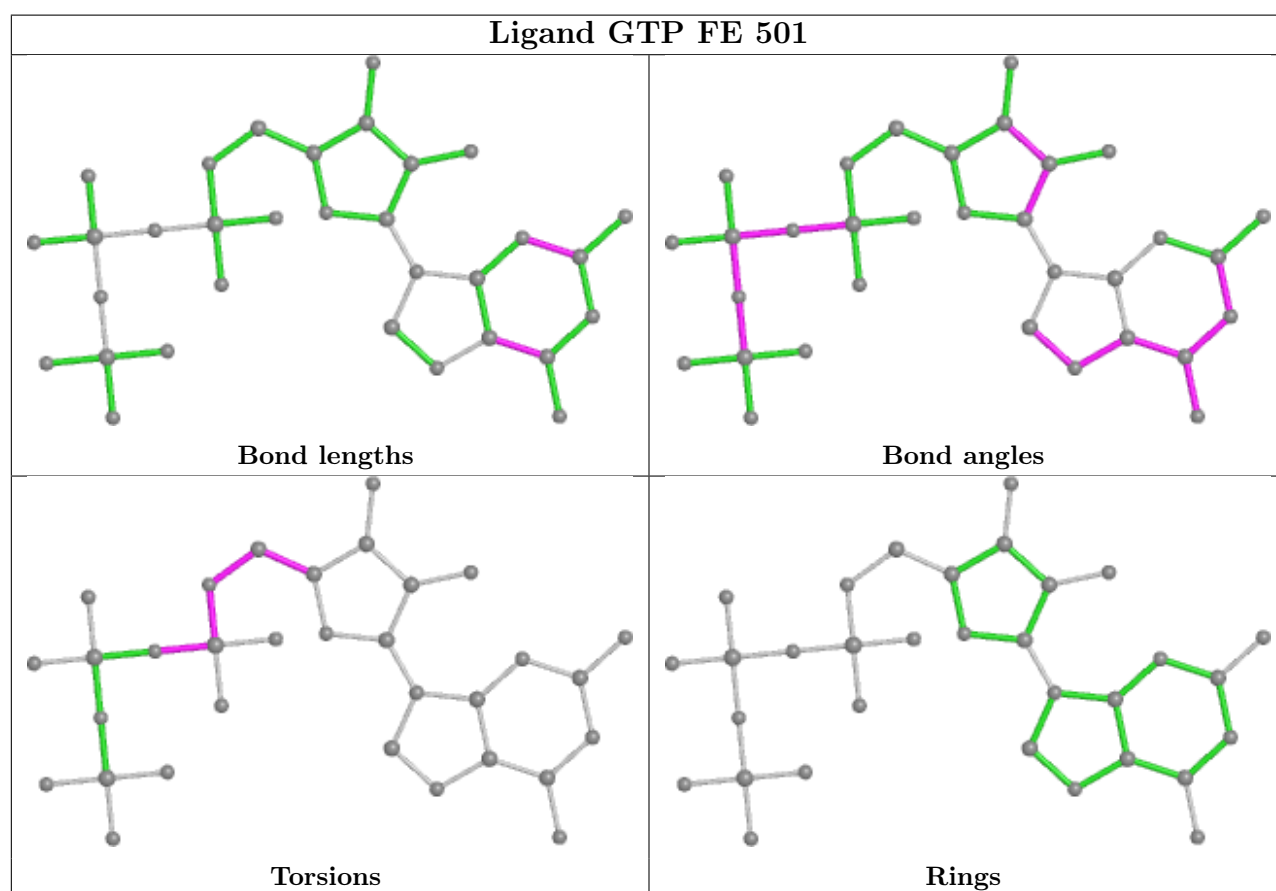
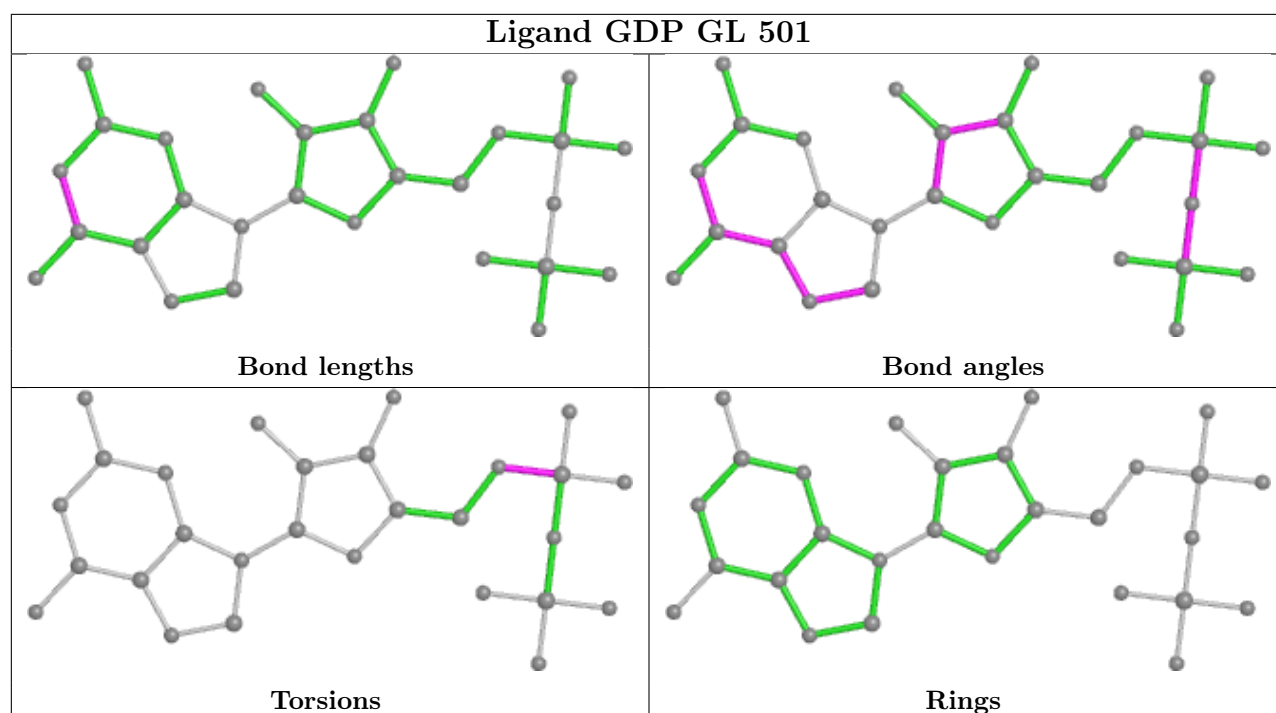




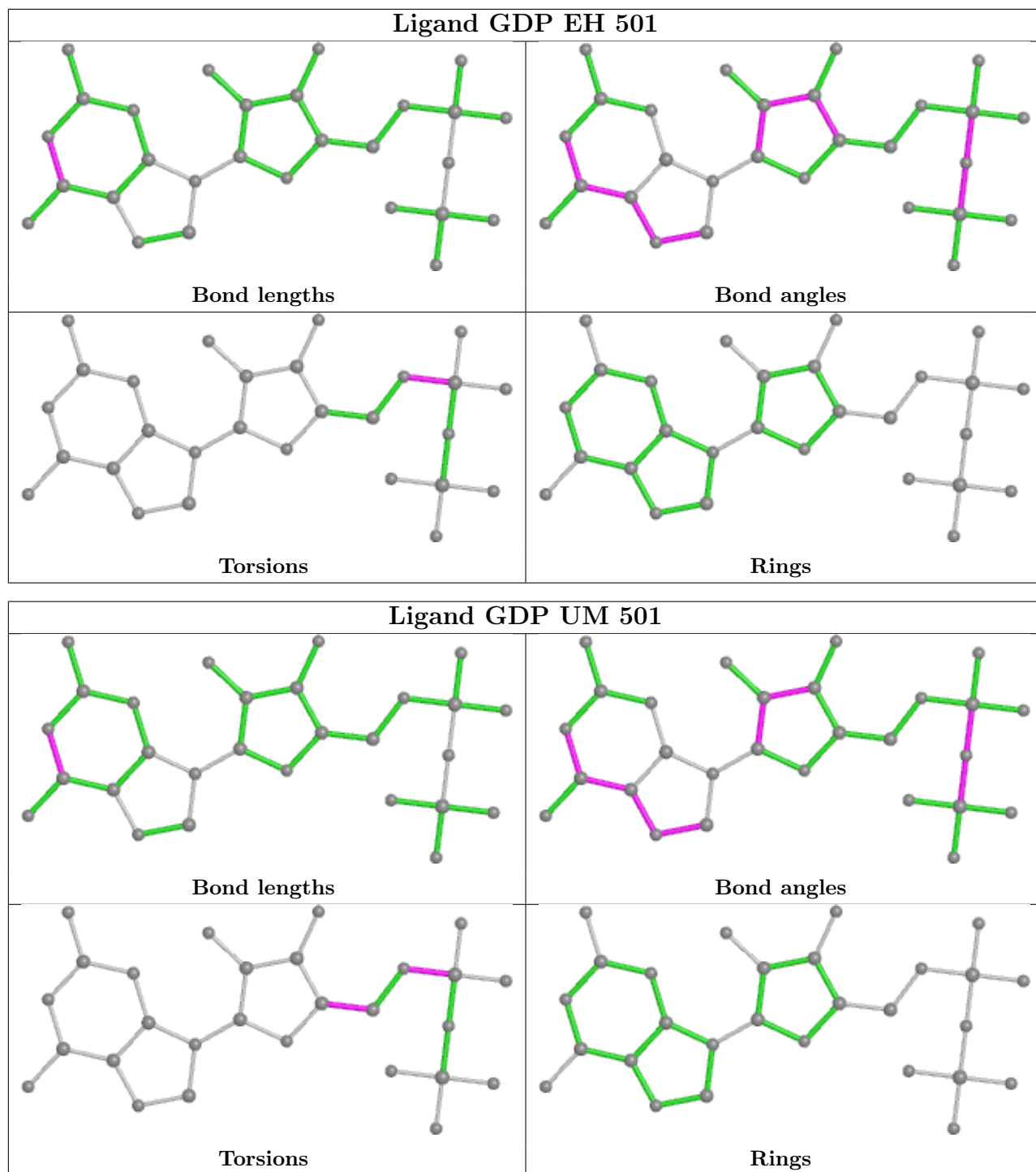


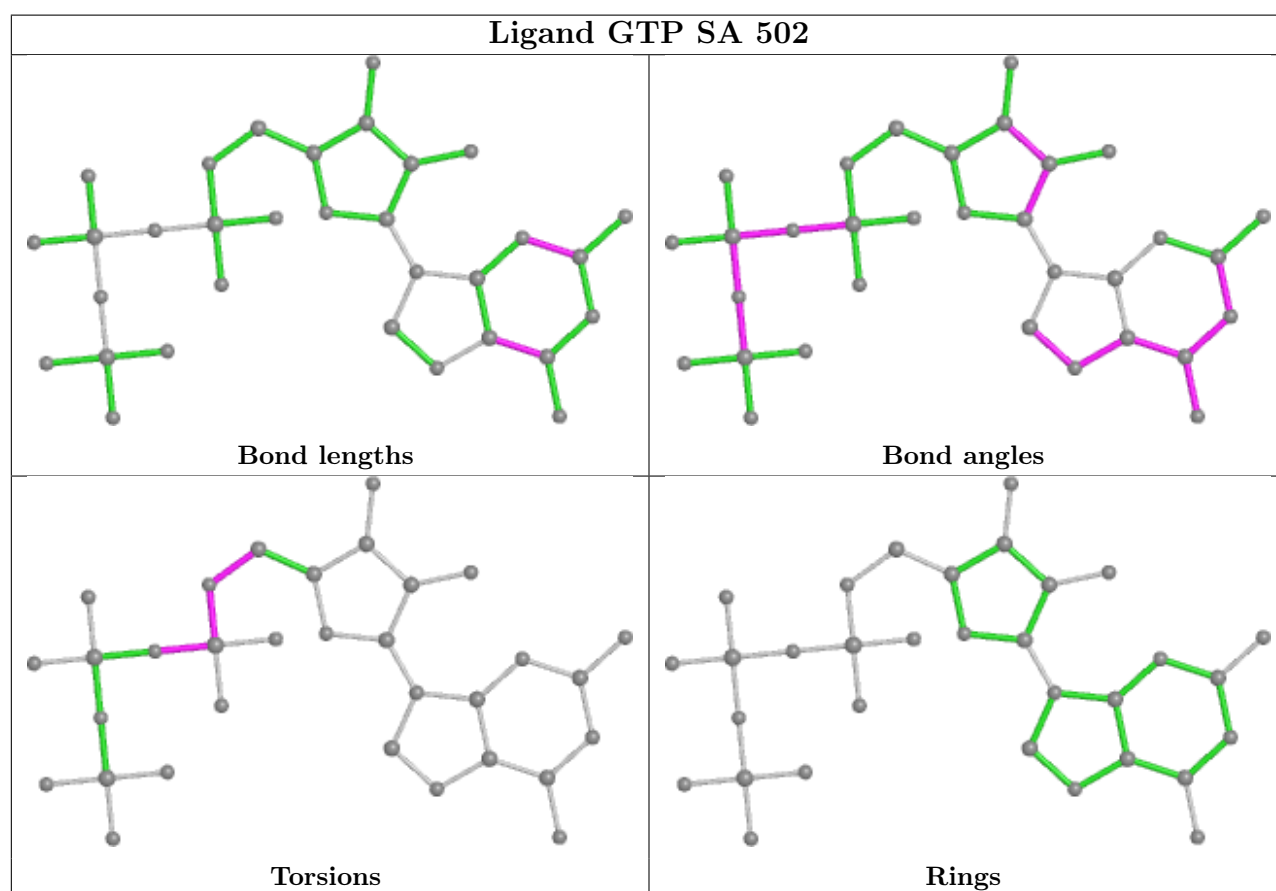
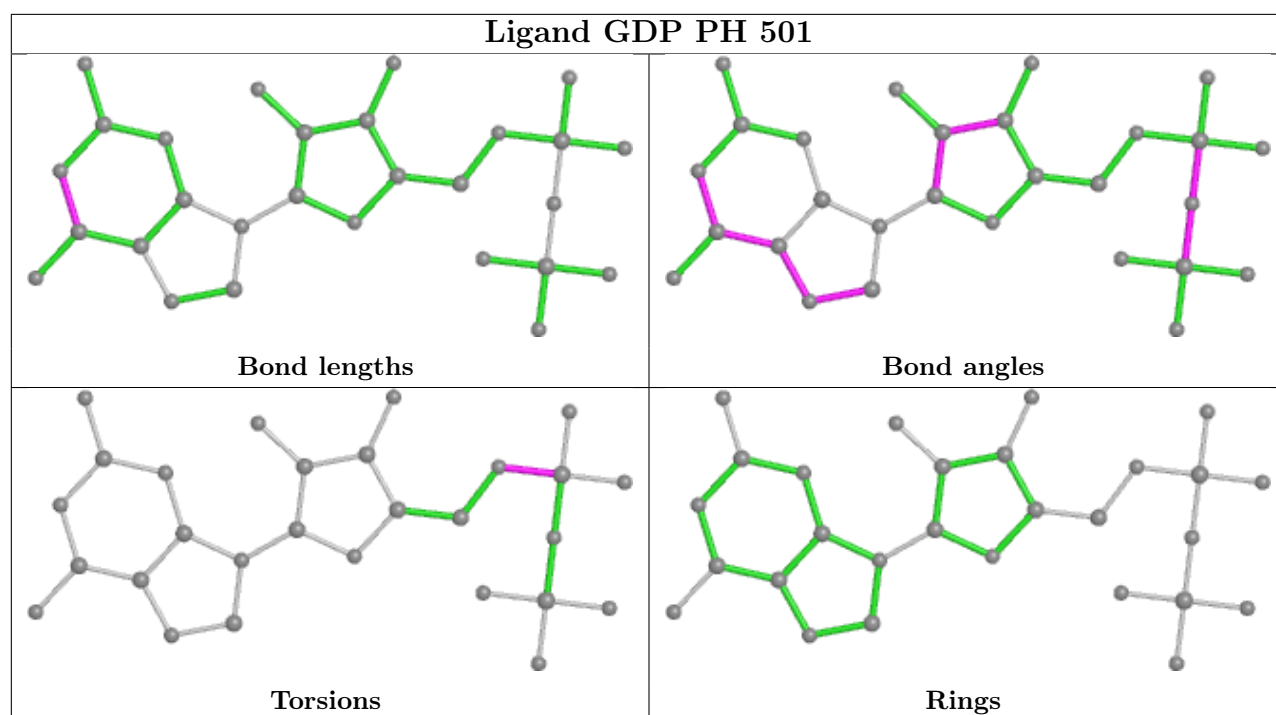


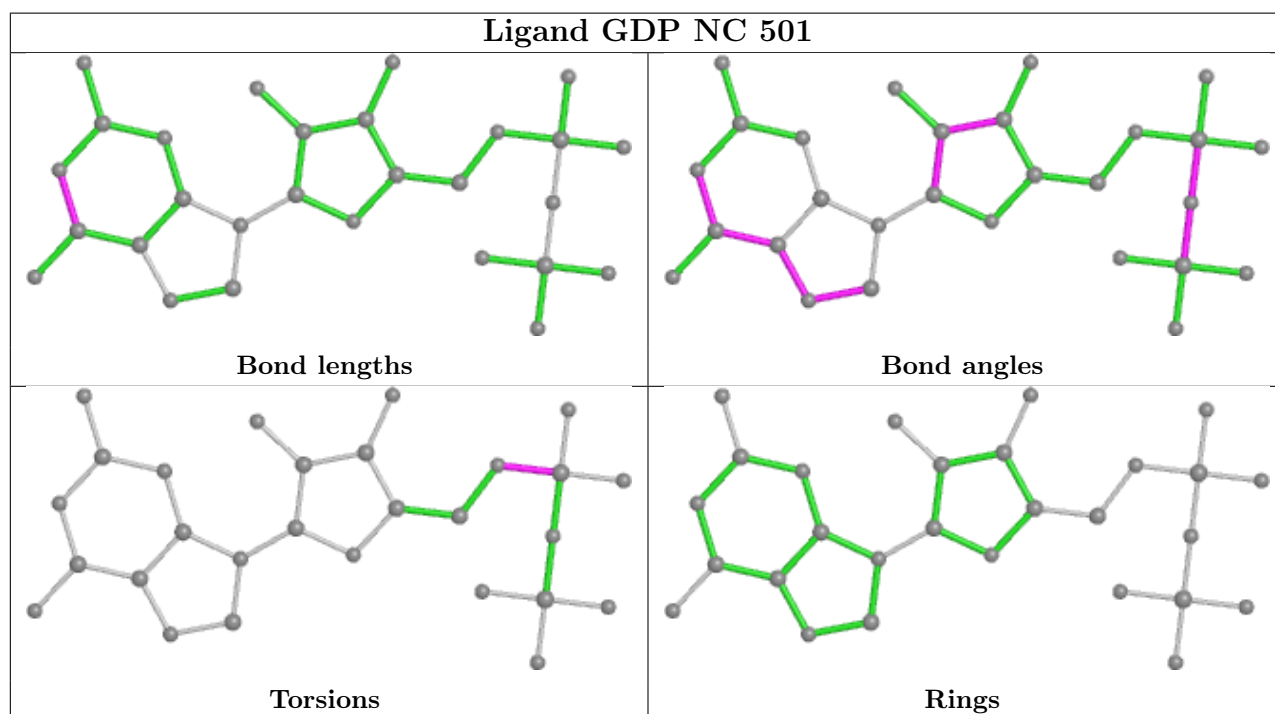
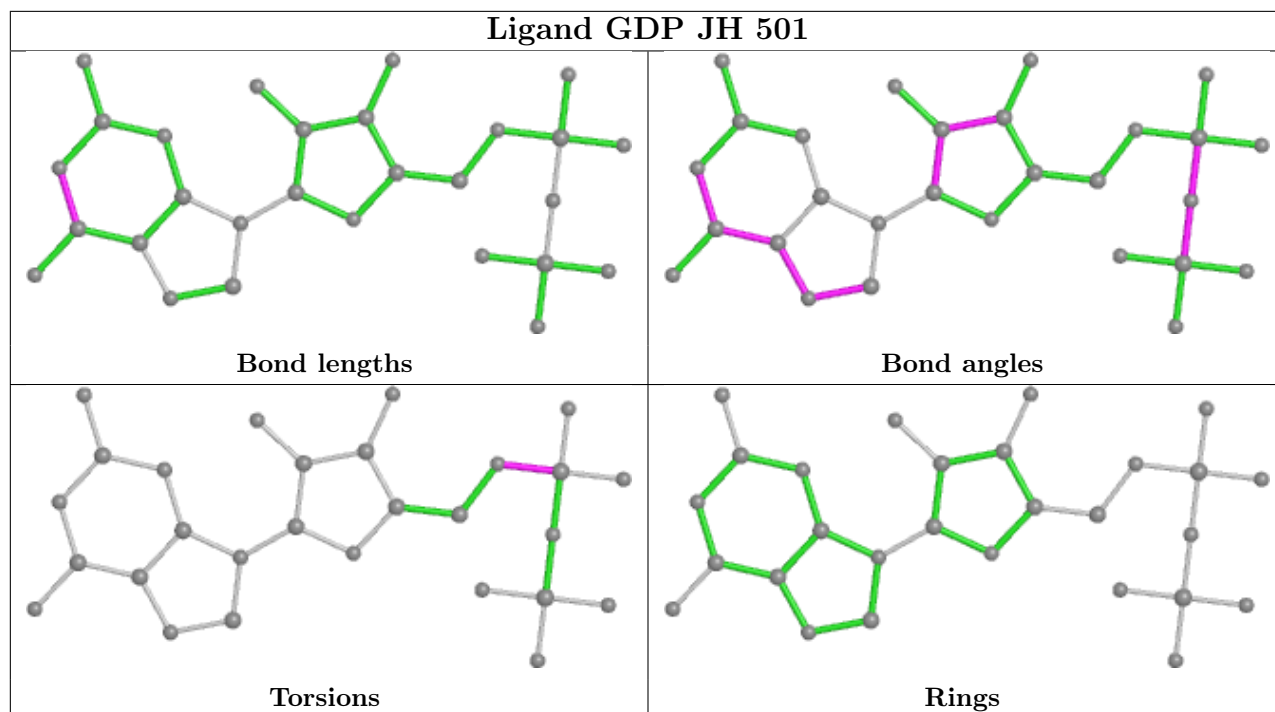


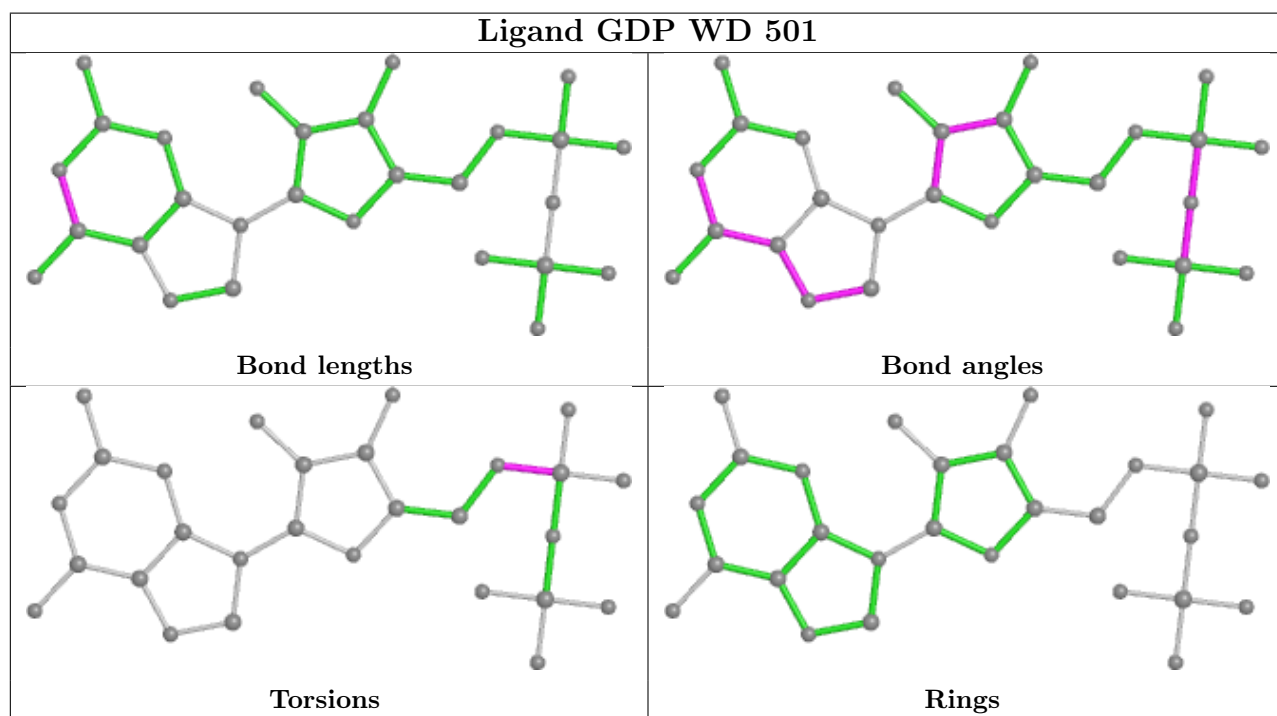
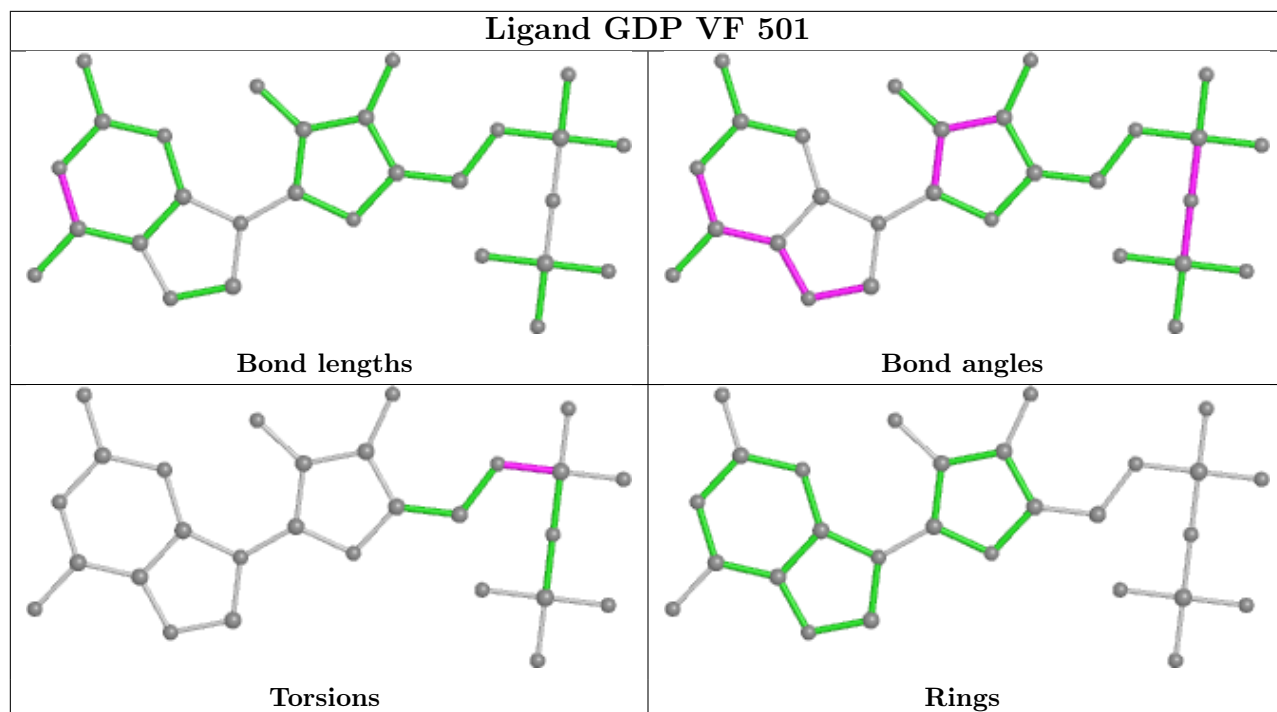


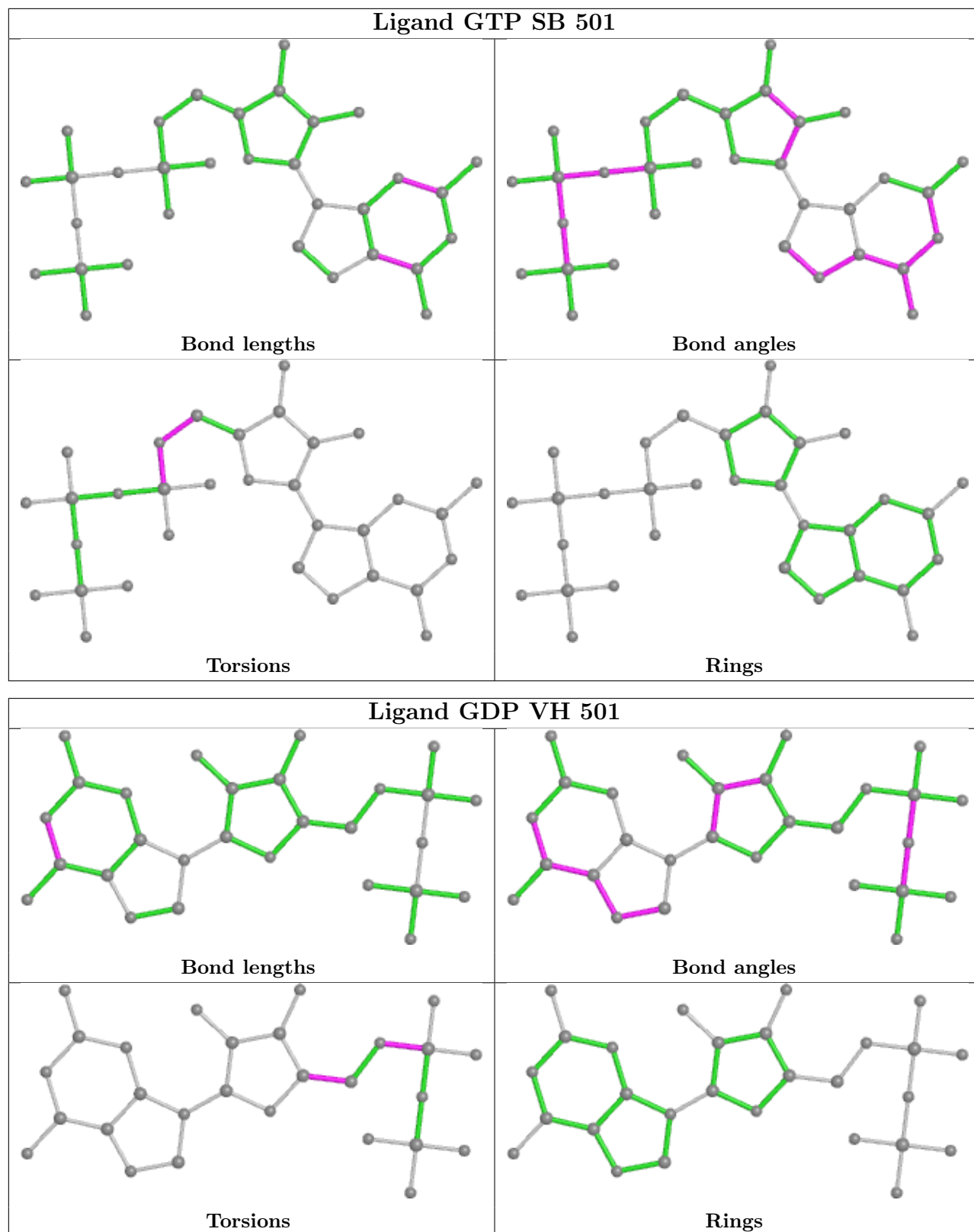


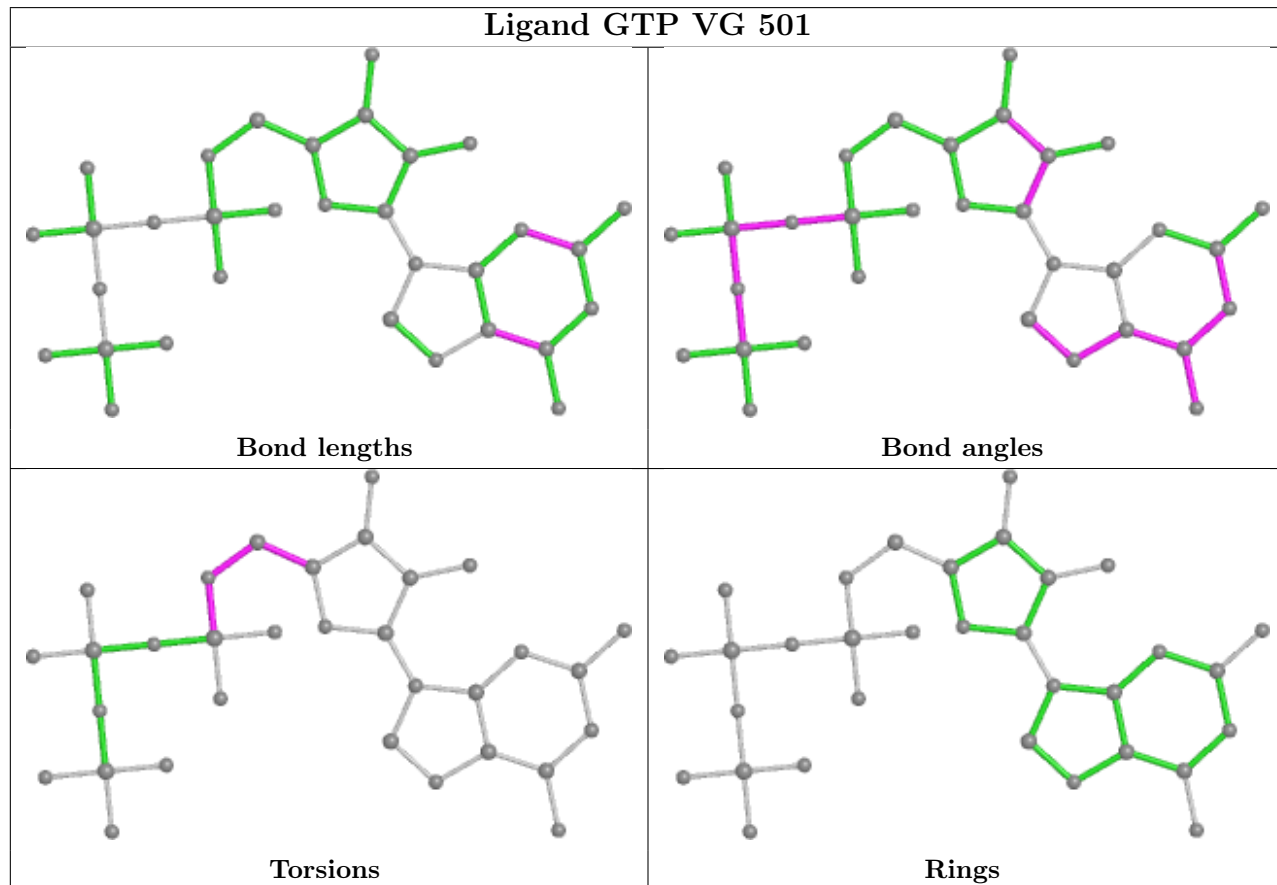
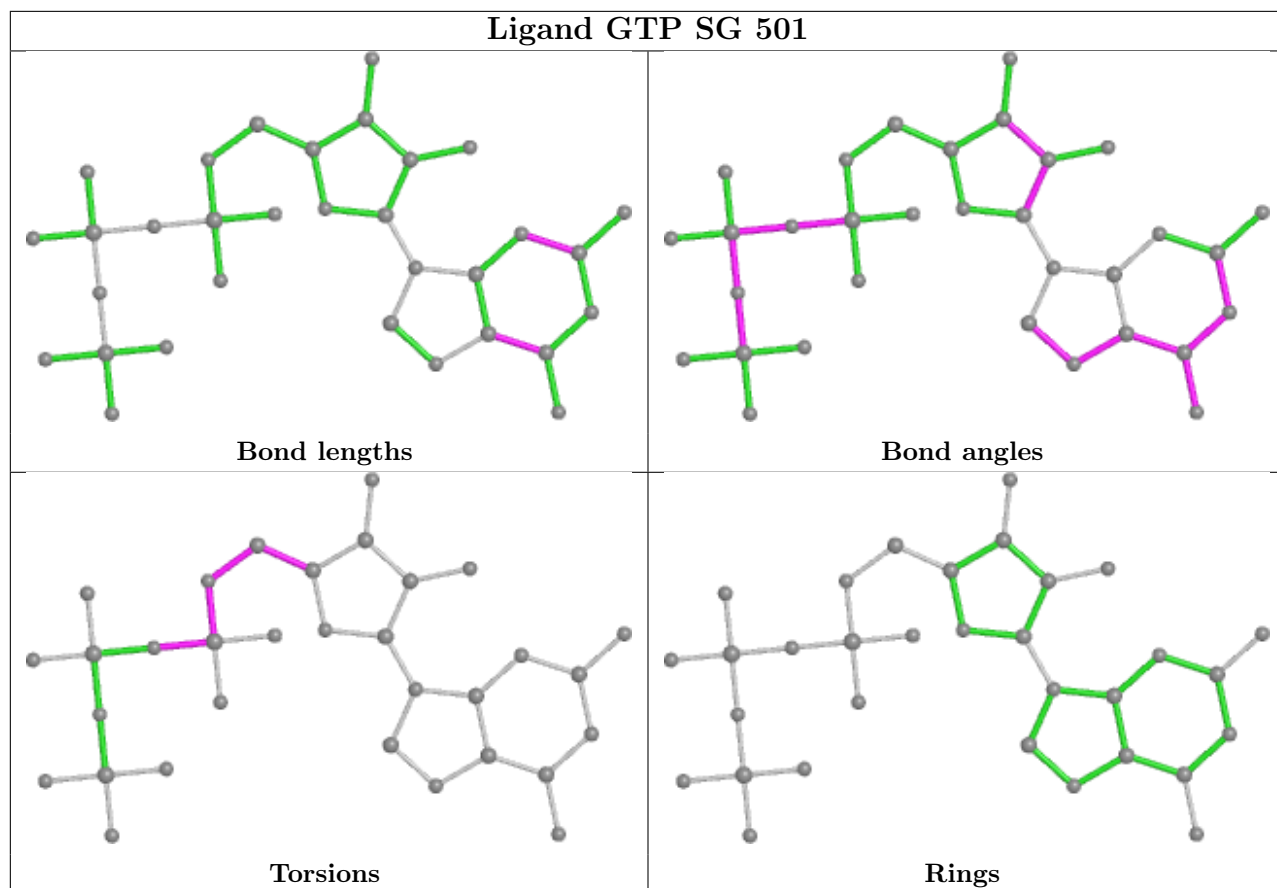


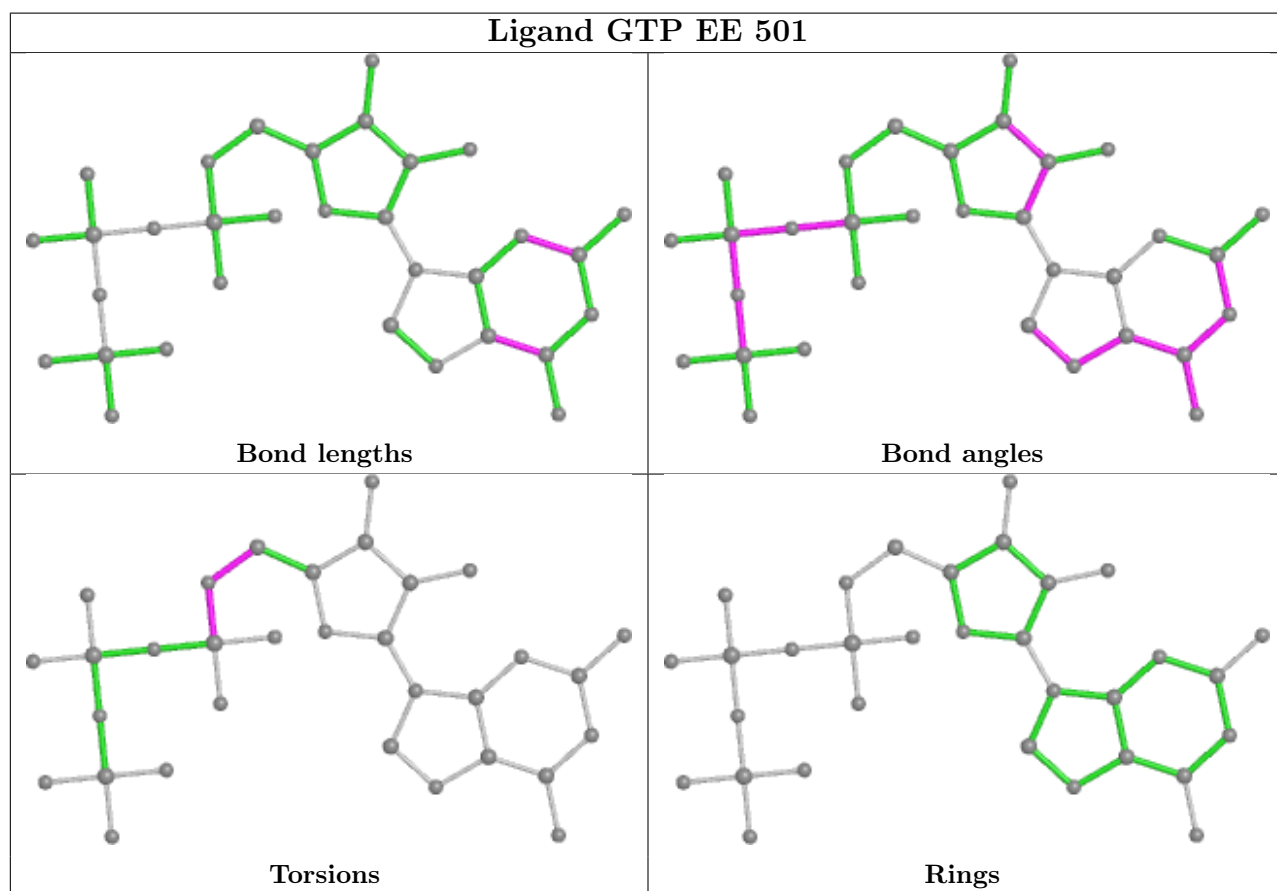
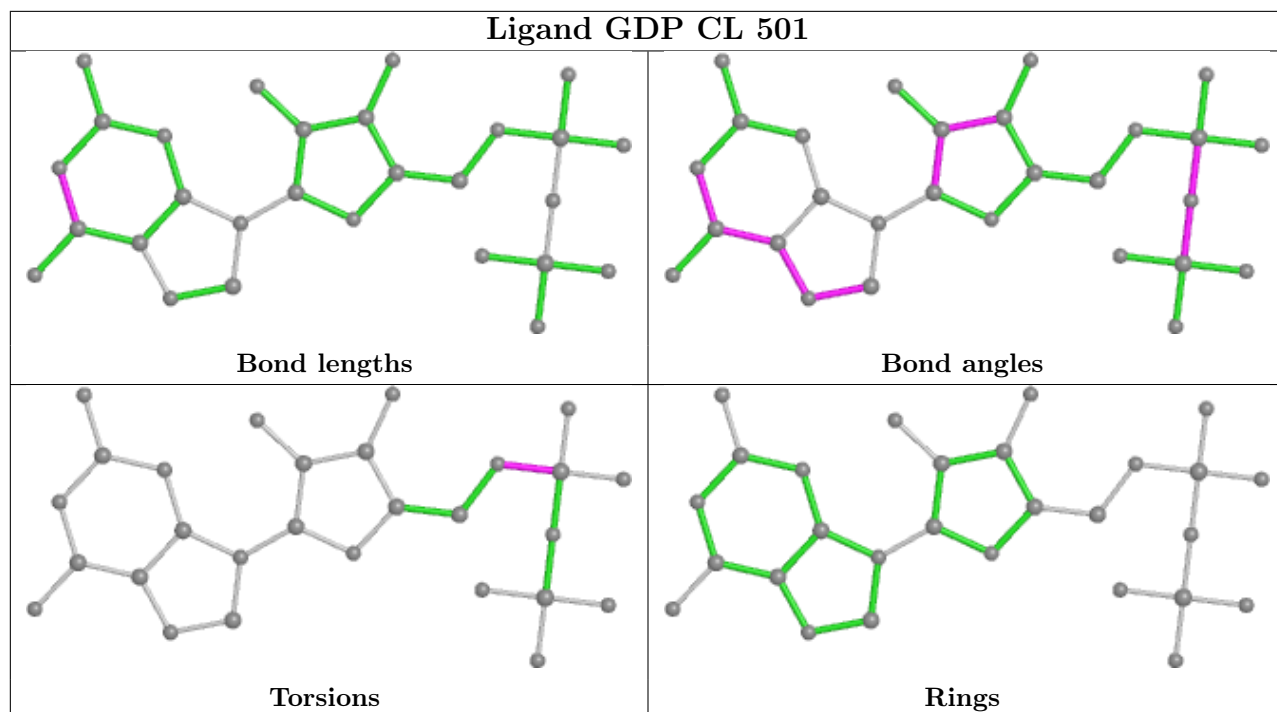


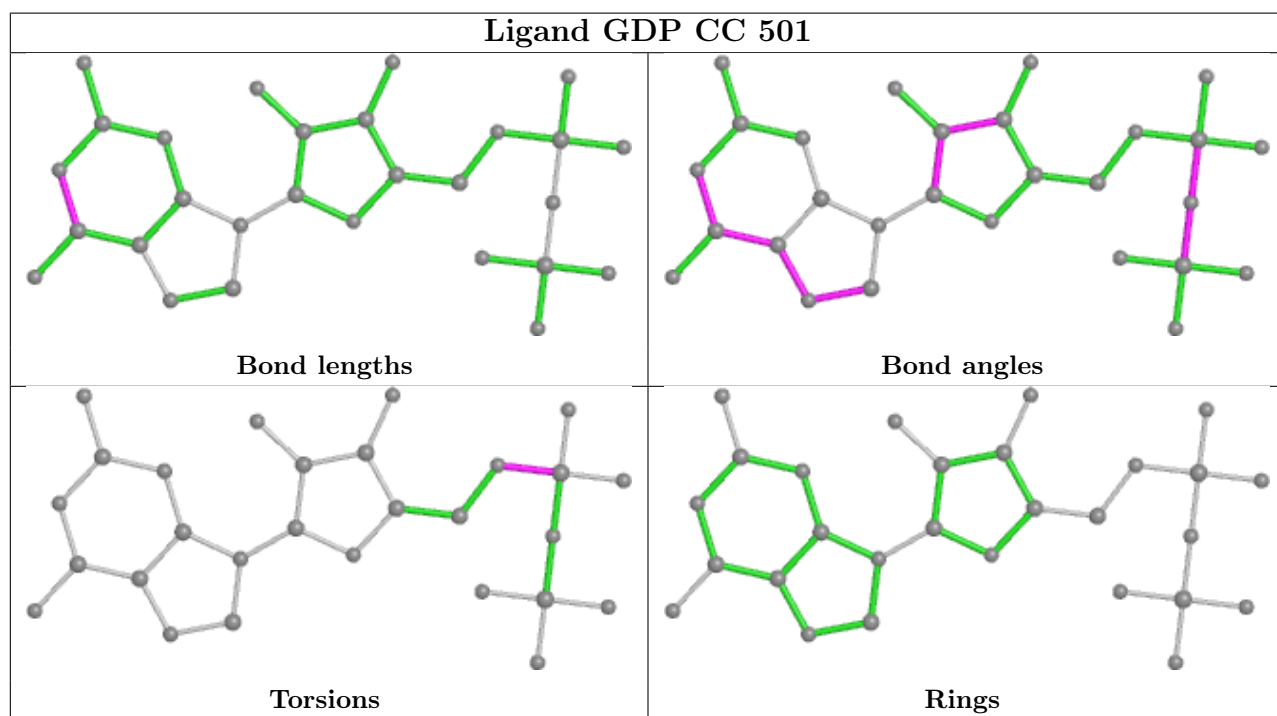
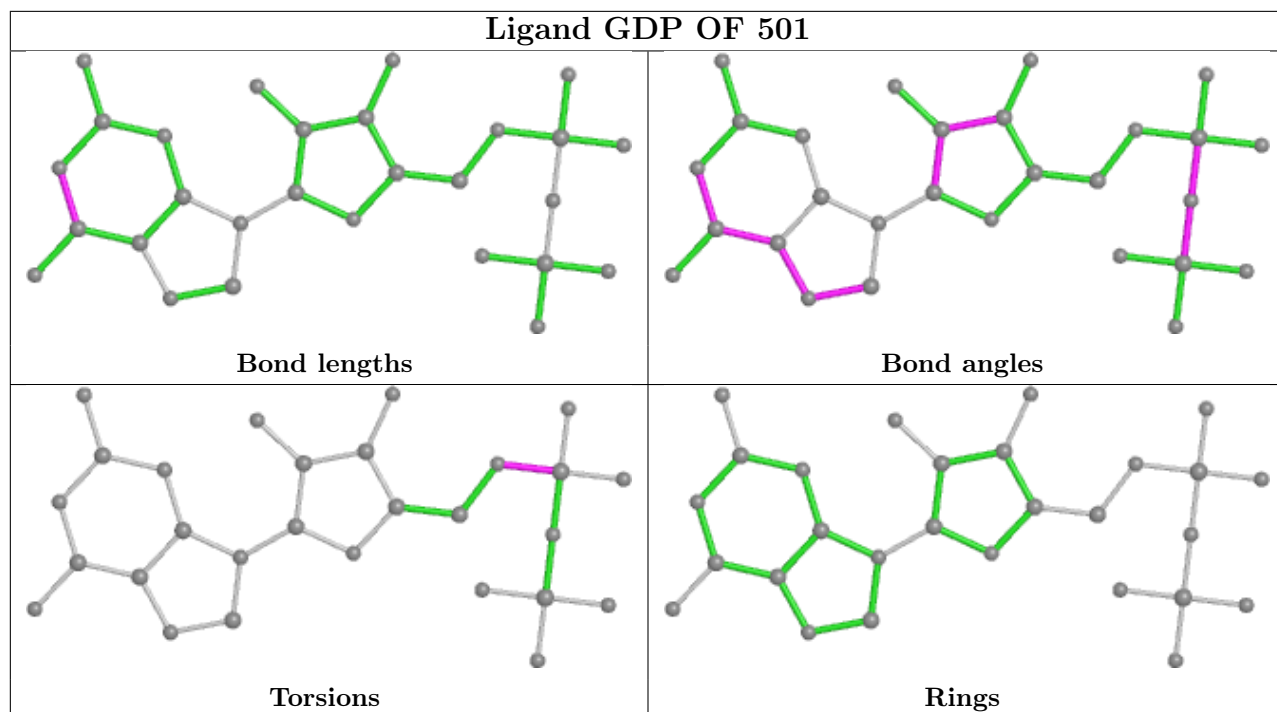




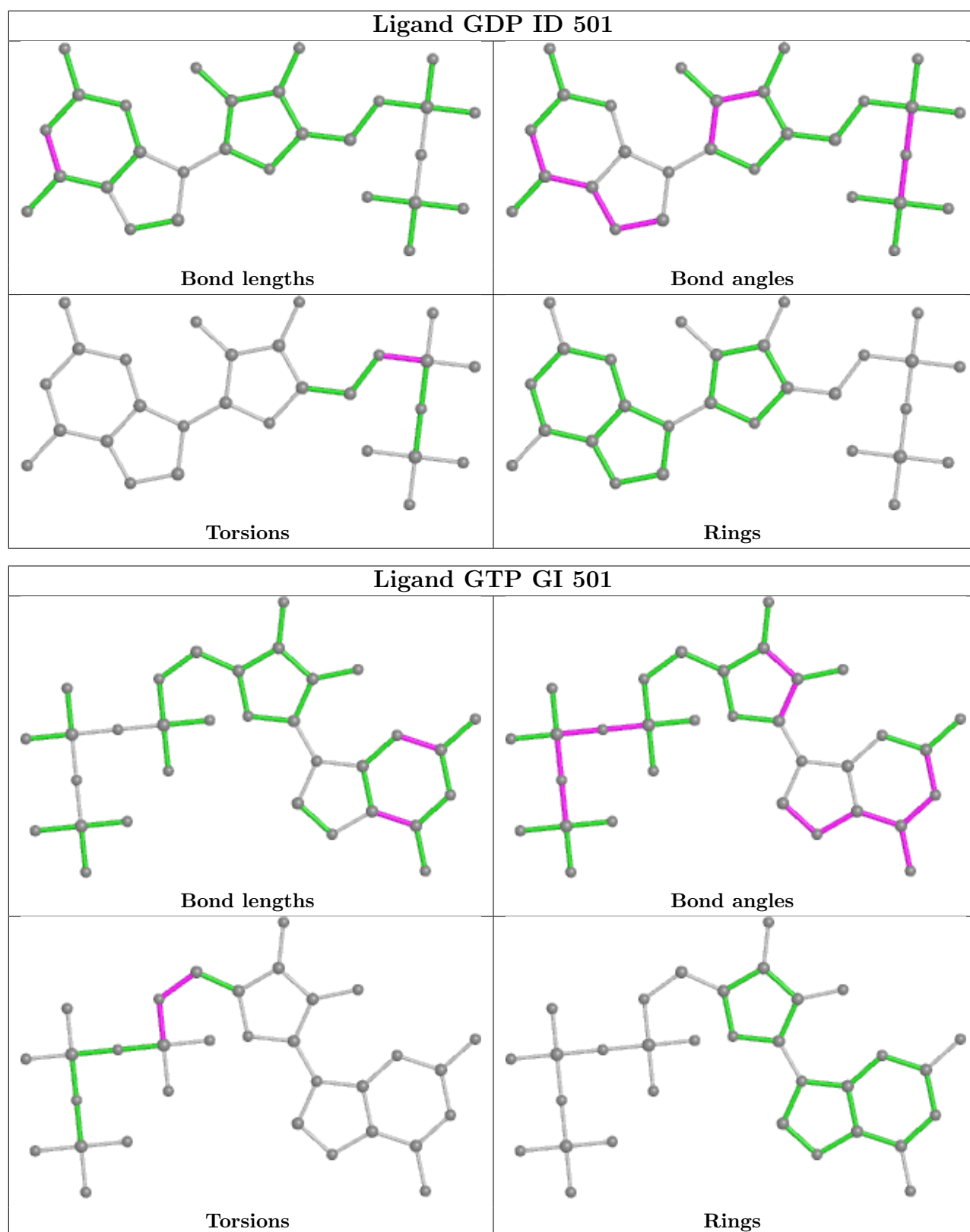












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

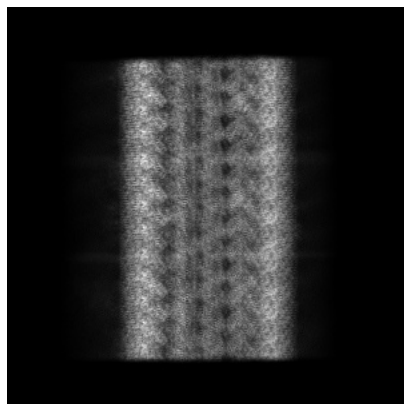
## 6 Map visualisation [i](#)

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.

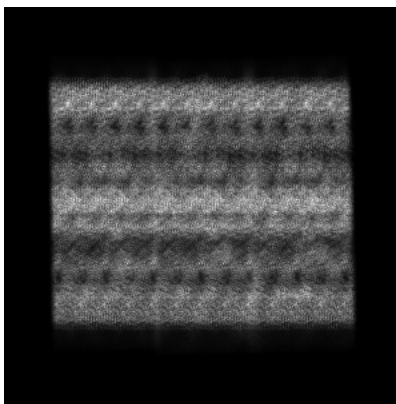
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

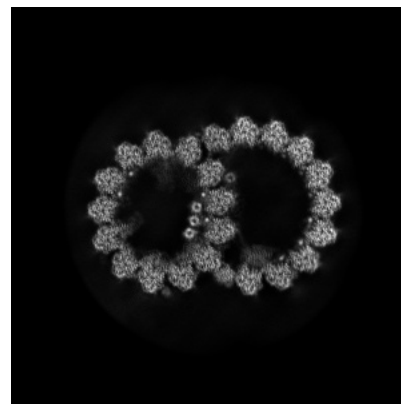
#### 6.1.1 Primary map



X

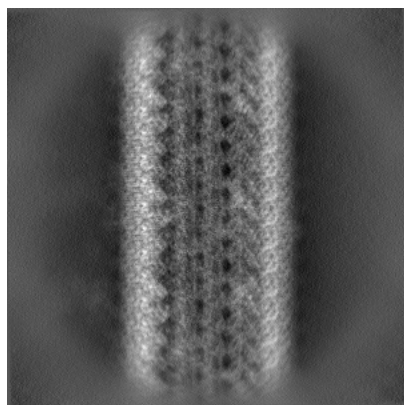


Y

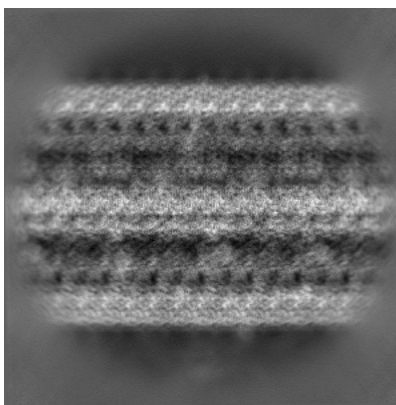


Z

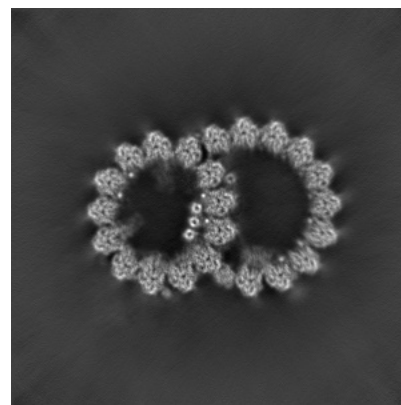
#### 6.1.2 Raw map



X



Y

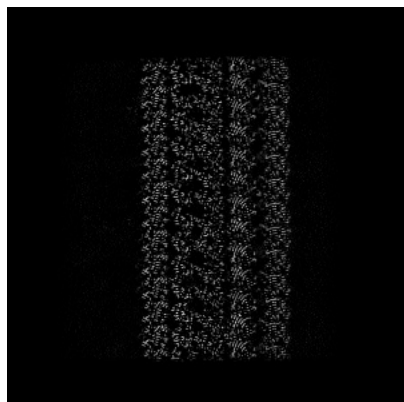


Z

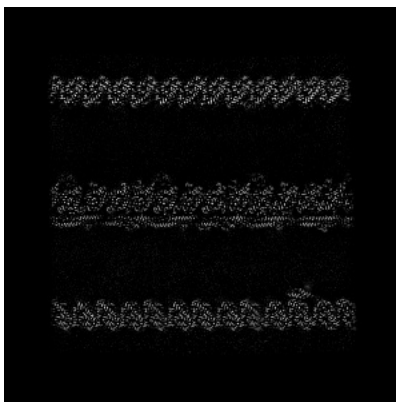
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

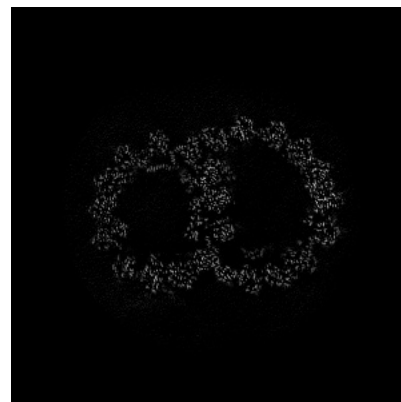
### 6.2.1 Primary map



X Index: 256

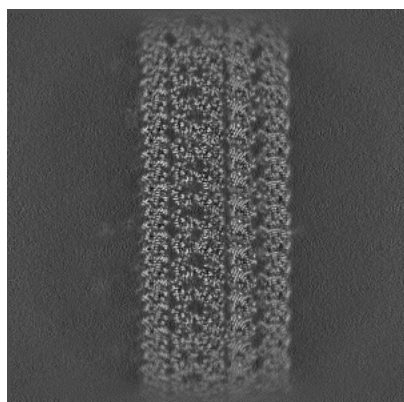


Y Index: 256

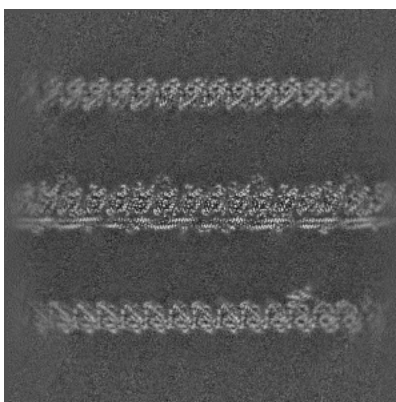


Z Index: 256

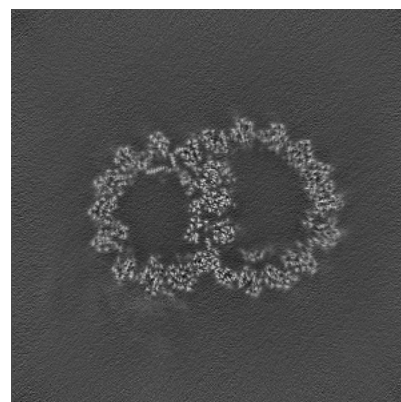
### 6.2.2 Raw map



X Index: 256



Y Index: 256

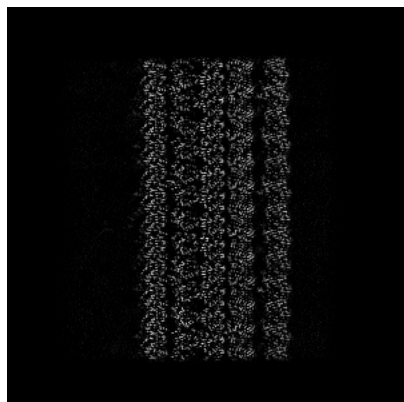


Z Index: 256

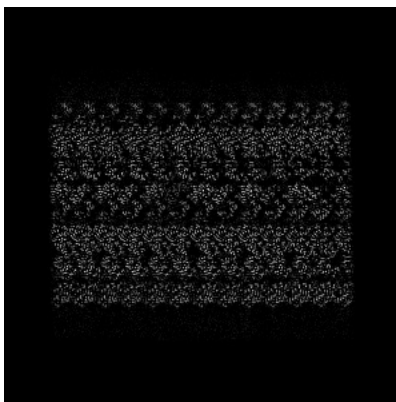
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

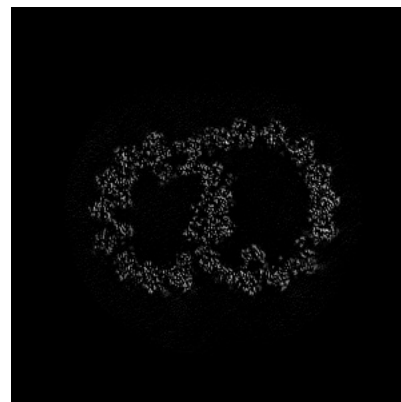
### 6.3.1 Primary map



X Index: 258

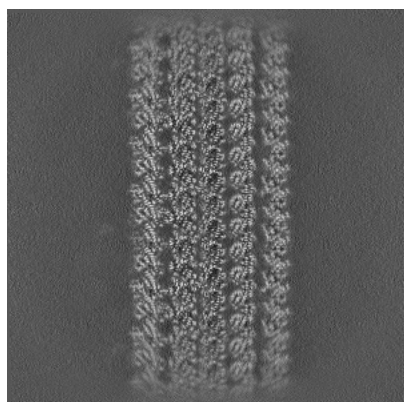


Y Index: 174

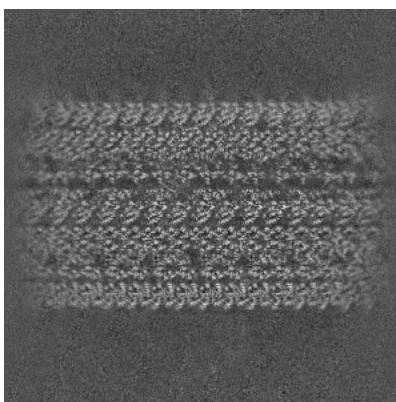


Z Index: 385

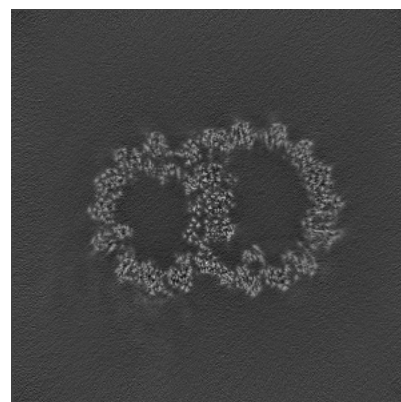
### 6.3.2 Raw map



X Index: 264



Y Index: 177

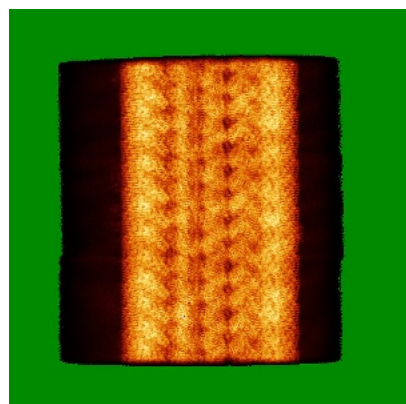


Z Index: 260

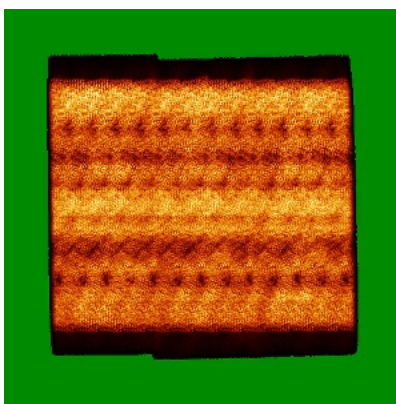
The images above show the largest variance slices of the map in three orthogonal directions.

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

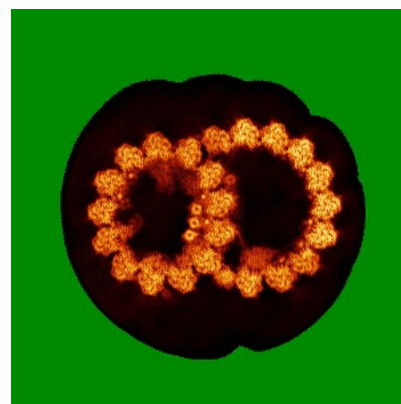
### 6.4.1 Primary map



X

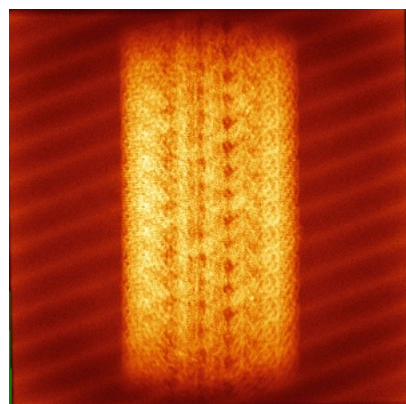


Y

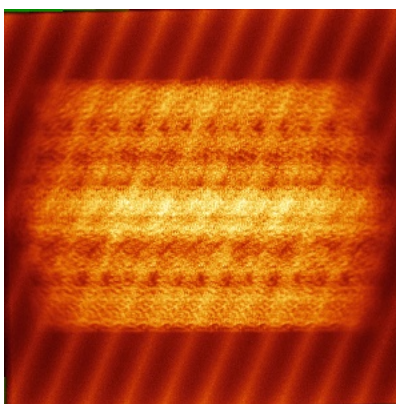


Z

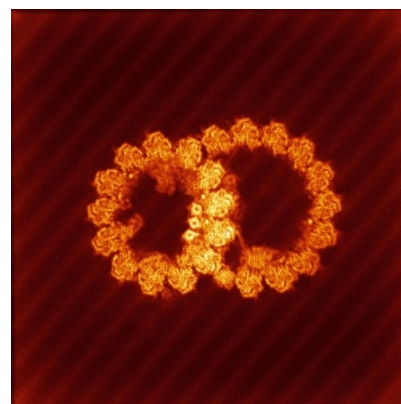
### 6.4.2 Raw map



X



Y

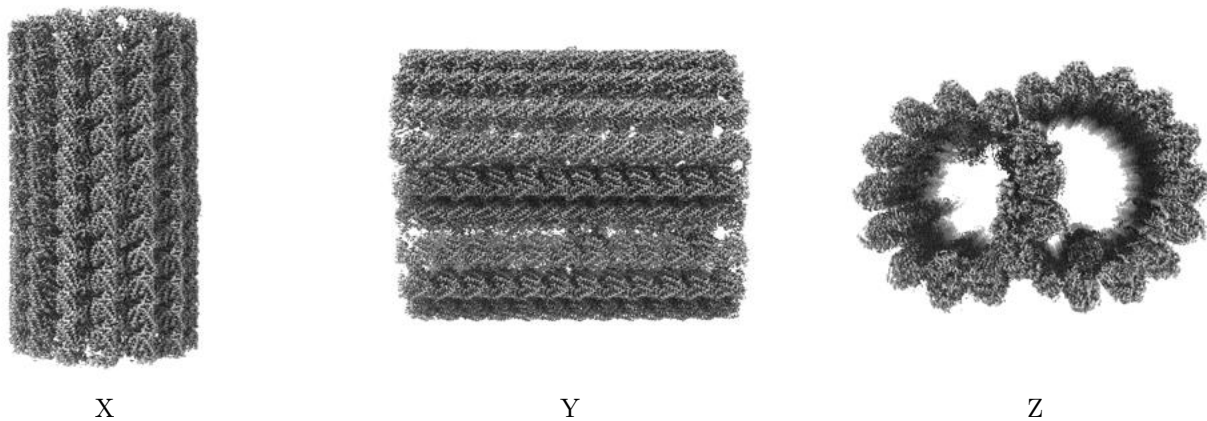


Z

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.

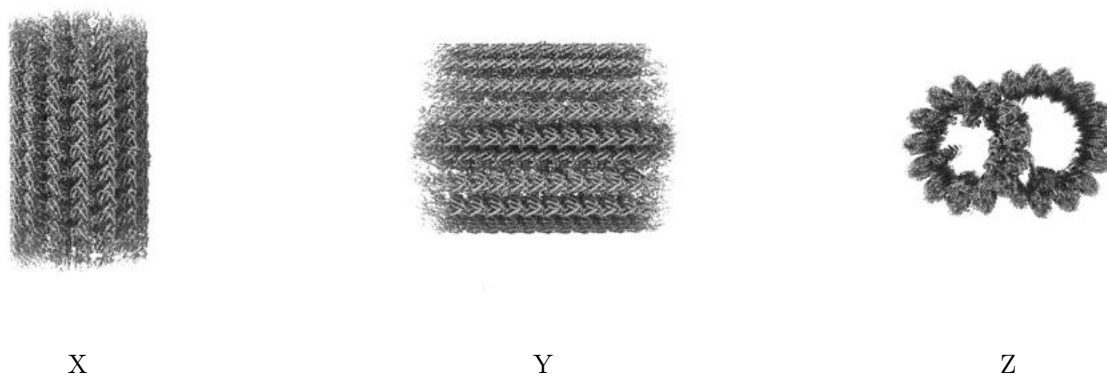
## 6.5 Orthogonal surface views [i](#)

### 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.

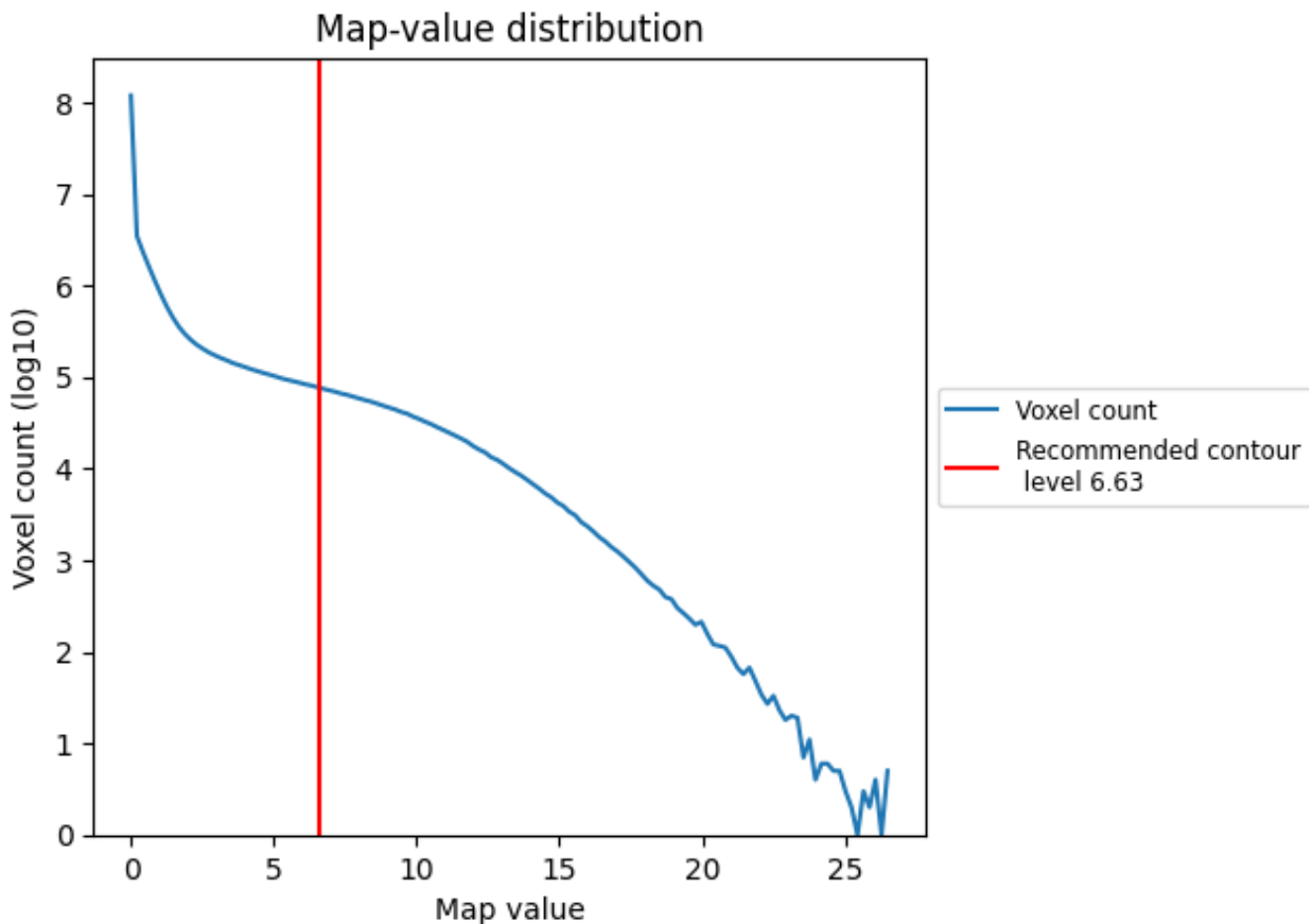
## 6.6 Mask visualisation [i](#)

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.

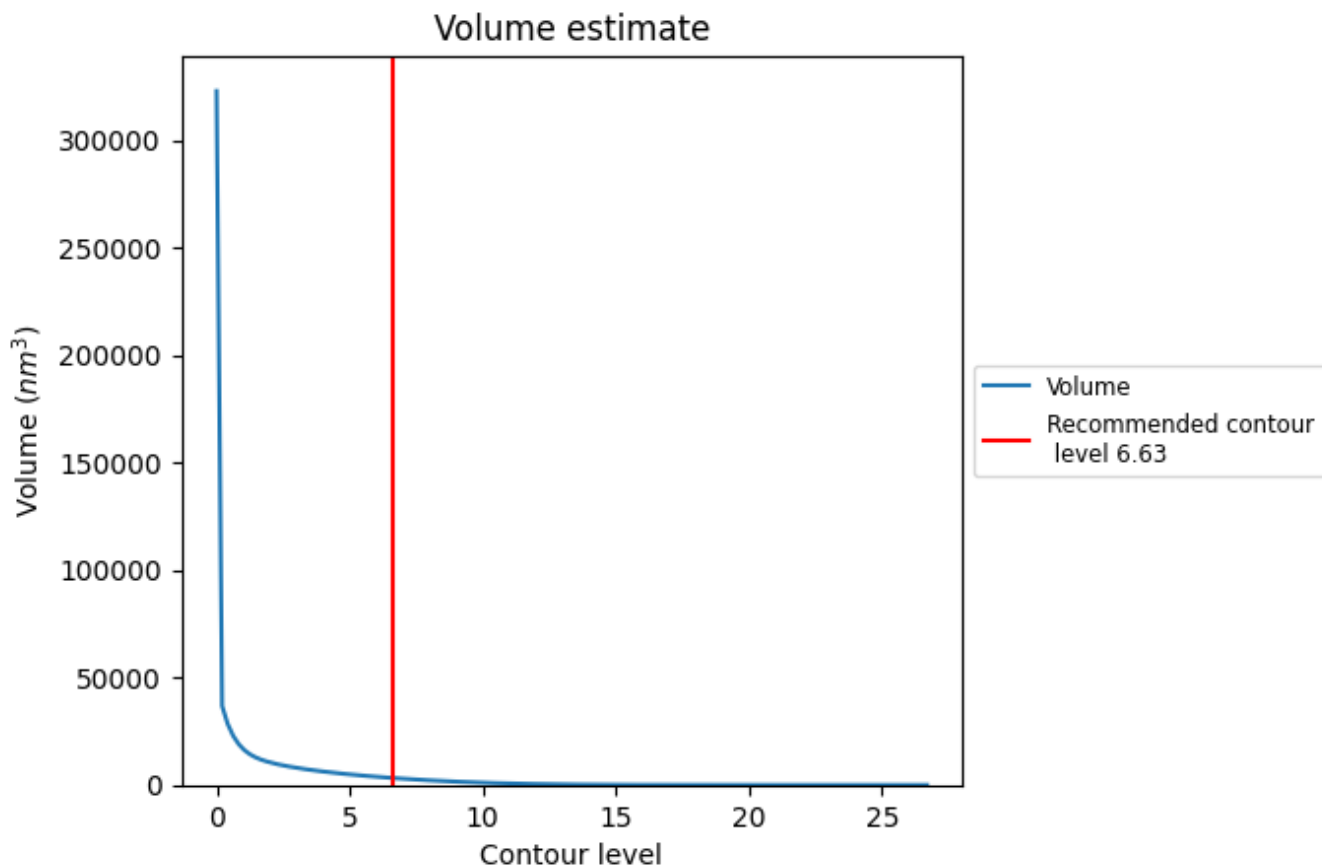
### 7.1 Map-value distribution [i](#)



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.



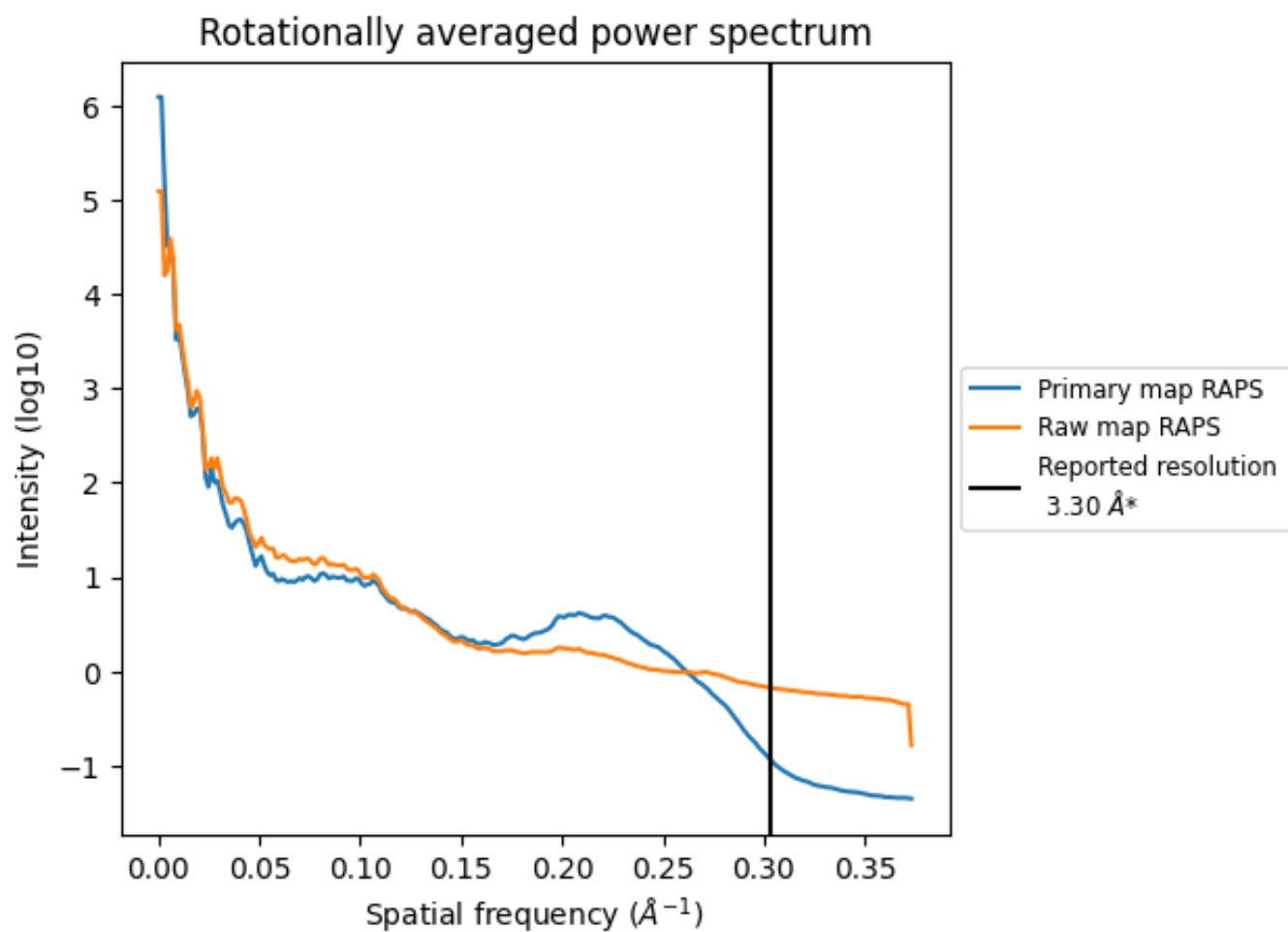
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3228  $\text{nm}^3$ ; 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](#)

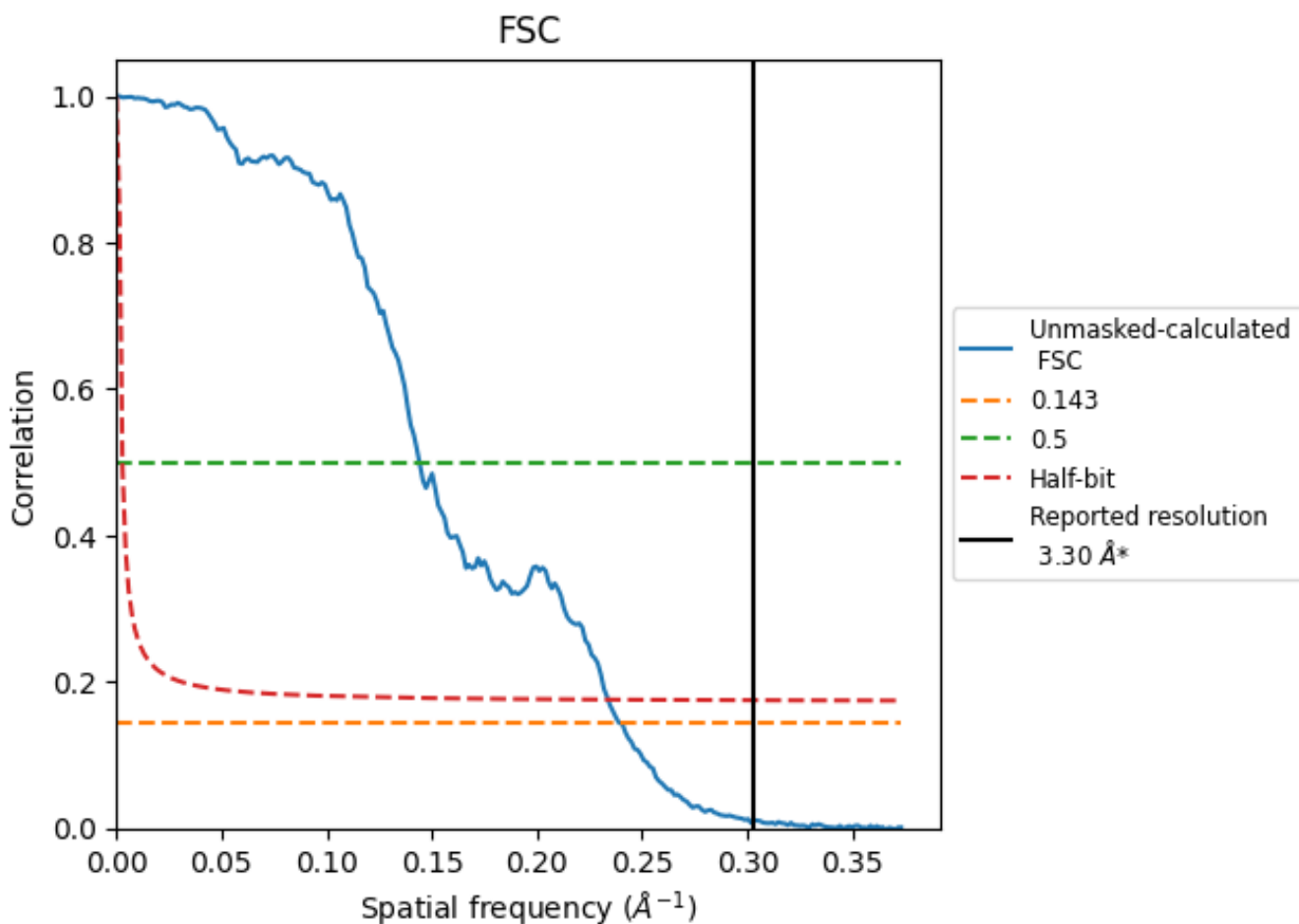


\*Reported resolution corresponds to spatial frequency of  $0.303 \text{ \AA}^{-1}$

## 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<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

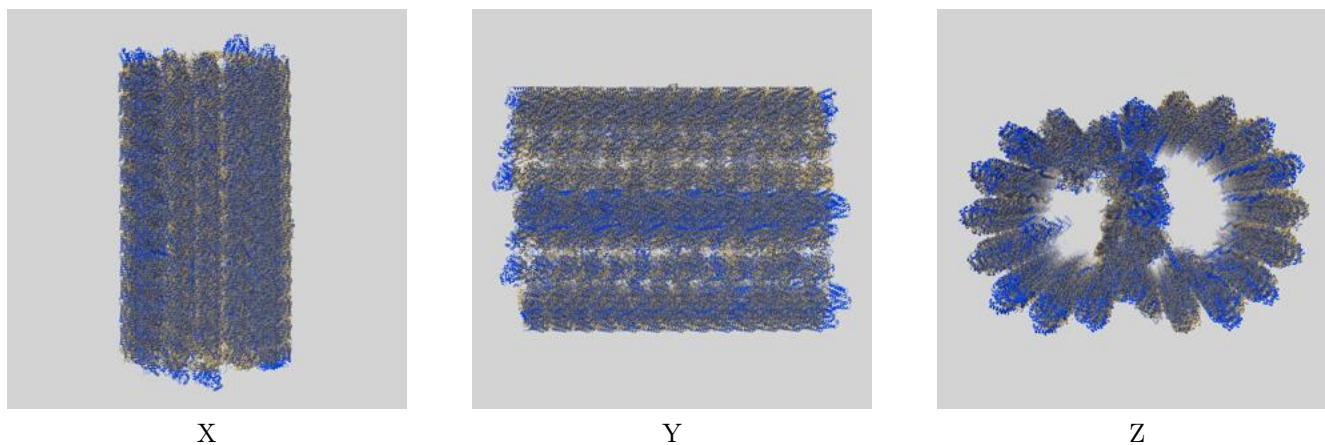
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.18	6.94	4.28

\*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](#)

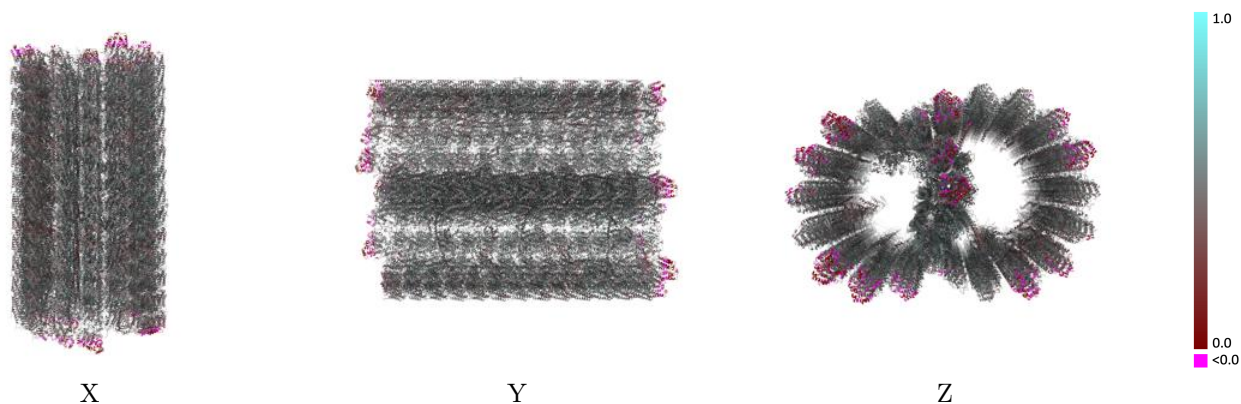
This section contains information regarding the fit between EMDB map EMD-40619 and PDB model 8SNB. Per-residue inclusion information can be found in section 3 on page 71.

### 9.1 Map-model overlay [i](#)



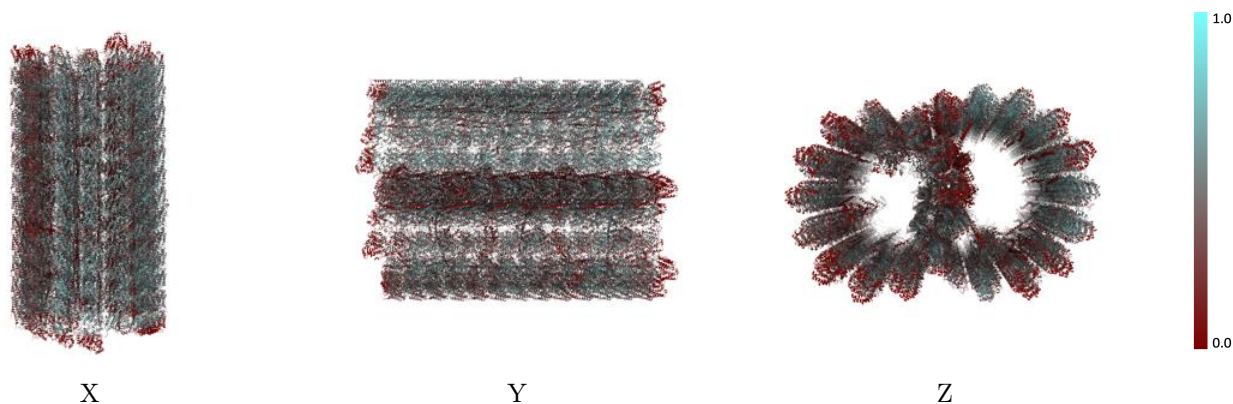
The images above show the 3D surface view of the map at the recommended contour level 6.63 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



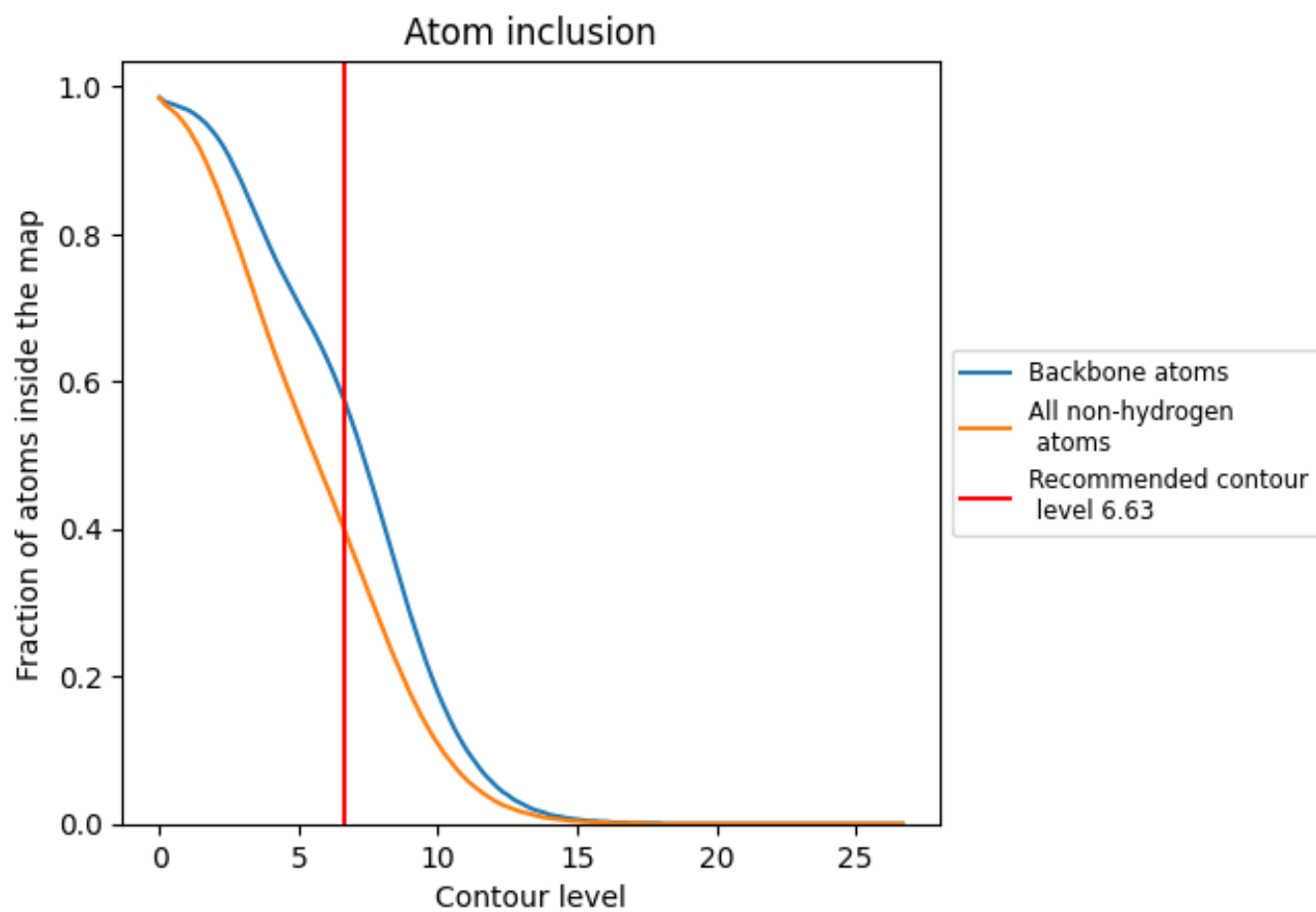
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.4790
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	0.4510
3K	0.1310	0.4050
3N	0.3440	0.4090
3O	0.3370	0.4250
3R	0.2060	0.4740
3S	0.2230	0.4720
3T	0.2020	0.4660
3W	0.1430	0.3900
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	0.2710	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	█ 0.4760
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	0.3860	0.4800
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	0.4200	0.4790
EK	0.3900	0.4810
EL	0.1180	0.2590
EM	0.3060	0.4670
FA	0.4450	0.4780
FB	0.4290	0.4770
FC	0.4600	0.4820
FD	0.3720	0.4530
FE	0.4260	0.4760
FF	0.4560	0.4760
FG	0.4200	0.4720
FH	0.3260	0.4480
FI	0.3960	0.4640
FJ	0.4490	0.4750
FK	0.4270	0.4740
FL	0.2420	0.3820
FM	0.3030	0.4210
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	█ 0.3650
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	█ 0.2350
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	0.2680
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